A NONLOCAL MODEL FOR COUPLED DAMAGE-PLASTICITY
INCORPORATING GRADIENTS OF INTERNAL STATE VARIABLES AT
MULTISCALES

A Dissertation

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By

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FOR MY GRANDPARENTS,
WHOSE LOVE HAS ALWAYS BEEN THERE TO GUIDE ME

AND THERE ARE THOSE WHO GIVE
AND KNOW NOT PAIN IN GIVING,
NOR DO THEY SEEK JOY,
NOR GIVE WITH MINDFULNESS OF VIRTUE;
THEY GIVE AS IN YONDER VALLEY
THE MYRTLE BREATHES ITS FRAGRANCE INTO SPACE.
THROUGH THE HANDS OF SUCH AS THESE GOD SPEAKS,
AND FROM BEHIND THEIR EYES HE SMILES UPON THE EARTH.

~ FROM THE PROPHET BY KALIL GIBRAN (1923) ~
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ABSTRACT

The thermodynamically consistent formulation and the subsequent numerical implementation of a gradient enhanced continuum coupled damage-plasticity model as a constitutive framework to model ill-posed localization problems is presented. By the introduction of “nonlocal,” gradient-enhanced measures in the plasticity potential function and yield criterion and in the damage potential function and damage criterion, the proposed model introduces microstructural characteristic material length scales which allows the size of localized zones to be predicted based on material constants, as opposed to local models where the loss of ellipticity causes the localized zones to be mesh dependent.

The gradient model proposed introduces non-linear functions for the hardening terms and can account for a wide range of material models. Gradients of hardening terms are found directly by operating on the respective hardening terms, and numerical methods are used to compute these gradients. The gradient enhanced measure used in this work consists of a combination of the local measure and the local measure’s Laplacian as justified by an approximation to nonlocal theory; however, through the expansion of various gradient terms in this nonlinear hardening plasticity model, gradients of both odd and even orders are introduced into the constitutive model.

The numerical implementation uses a small deformation finite element formulation and includes the displacements, the plastic multiplier, and the damage multiplier as nodal degrees of freedom, thus allowing the three fields to have different interpolation functions. The displacement field is interpolated using standard continuous elements; higher order elements (cubic Hermitian) are used for the plastic multiplier and for the damage multiplier to enforce continuity of the second order gradients. The effectiveness of the model is evaluated by studying the mesh-dependence issue in localization problems through numerical examples. Numerical results from this work are qualitatively compared with numerical simulations by other authors for different formulations.
CHAPTER 1 : INTRODUCTION

1.1 PROBLEM STATEMENT

Engineering materials contain defects that lead in some cases to specific pattern formation due to a coupling of inelastic mechanisms such as micro-crack and micro-void growth with plastic flow and fracture. Initially, loading of heterogeneous materials causes non-interacting micro-cracks and micro-voids; however, experimental observations indicate that further loading will cause failure mechanisms to occur at localized zones of plasticity and damage where interaction and coalescence of micro-cracks and micro-voids take place. When investigating problems where the material defects induce localization or where the structure and boundary conditions induce localization such as shear banding in a biaxial test (Figure 1.1) or localization of chip segmentation in high speed machining of titanium alloys, the absence of any material length scale from a conventional continuum solution causes the element size in finite element solutions to become the characteristic length. This means that traditional numerical simulations of localization problems suffer from a pathological mesh dependence. This problem arises as the shear bands develop at a bifurcation point where the governing equations go from elliptic to hyperbolic and the mathematical model becomes ill-posed.

This type of mesh-dependency is not physically based, as the numerical prediction of the observed characteristic width of the shear bands is based on the size of the finite element as opposed to a material length scale. In traditional finite element solutions, as

Figure 1.1: Mesh dependence on the numerical analysis of a biaxial test for various finite element meshes.
the finite element mesh is refined, the width of the localized deformation decreases to a vanishing width. In actuality, the width of a localized zone is dependent not on the numerical method that is used, but on material parameters. Specifically, the width is dependent on the “length scales” of the material, where examples of length scales in various inhomogeneous materials are shown in Figure 1.2.

1.2 BACKGROUND

Enhanced continuum models, including but not limited to gradient theories, seek to introduce a “length scale” into the continuum. In nonlocal models, long-range microstructural interaction is introduced where the stress response at a material point is assumed to depend on the state of its neighborhood in addition to the state of the point itself. A nonlocal measure is used for the local variable which is defined as the weighted average at the position of the local counterpart over a surrounding volume at a small

![Figure 1.2](image)

Figure 1.2: Various length scales in an inhomogeneous material: (a) void size; (b) fiber size and spacing; (c) crack and/or dislocation density; and (d) grain size.

Gradient models have been investigated as approximations to nonlocal integral models. In these gradient models, the integral form of the nonlocal internal state variable is approximated by using a truncated Taylor series expansion. Since gradient theories are justified as approximations to nonlocal theories, similar length scales are introduced into the continuum model (Voyiadjis et al., 2005; Voyiadjis & Abu Al-Rub, 2005). Bammann & Aifantis (1981, 1982) and Aifantis (1984a,b) suggested a gradient approach to deformation to describe plastic instabilities including dislocation patterning and spatial characteristics of shear bands. This initial work and subsequent articles by Aifantis and co-workers (e.g. Aifantis & Hirth, 1985; Walgraef & Aifantis, 1985; Aifantis, 1987; Zbib & Aifantis, 1988a; Walgraef & Aifantis, 1988; Vardoulakis & Aifantis, 1989; Mühlhaus & Aifantis, 1991; Voyiadjis et al., 2001a) have contributed to appreciating the potential and applicability of the gradient approach to a variety of material instability problems ranging from metal fatigue and polycrystal/soil shear banding to the failure of concrete and liquefaction. The gradient approach has also been extended to problems of size effect (Fleck & Hutchinson, 1993; Shu & Fleck, 1999; Bammann et al., 1999) when investigating such problems as micro-bending (Stolken & Evans, 1998) and micro-torsion (Fleck & Hutchinson, 1993; Fleck et al., 1994). Computational issues of the gradient theory for plasticity (e.g. de Borst et al., 1995; Mühlhaus & Aifantis, 1991; Ramaswamy & Aravas, 1998; Bammann et al., 1999; Voyiadjis & Dorgan, 2004ab, 2005), damage (e.g. Pijaudier-Cabot & Bažant, 1987; Bammann et al., 1999; Peerlings et al., 1996; Kuhl et al., 2000), and coupled damage-plasticity (e.g. Pamin & de Borst, 1999; Voyiadjis & Dorgan, 2001, 2004c, 2005; Voyiadjis et al., 2001a,b, 2004; Dorgan & Voyiadjis, 2006) have been discussed extensively in the literature.

1.3 Objectives

The use of a gradient enhanced nonlocal continuum model is investigated in this work in order to introduce a microstructural characteristic length through gradient enhancements to plasticity and damage theories. A formulation is given in which gradients are incorporated in the constitutive model by the introduction of nonlocal measures in the plasticity potential function and yield criterion and in the damage potential function and damage criterion. The gradient enhanced constitutive model used is developed from a thermodynamically consistent framework for a small strain, rate-independent material in which there is a strong coupling between gradient-enhanced plasticity and gradient-enhanced damage. The development of evolution equations for plasticity and damage are treated in a similar mathematical approach and formulation since both address defects such as dislocations for the former and cracks/voids for the
later. Depending on the material of interest (e.g. ductile damaged material, brittle damaged material, etc.), different microstructural mechanisms will be prominent in the constitutive model. As these mechanisms do not act independently, the model is developed such that the plasticity flow rule and the damage flow are dependent on both the plastic potential and the damage potential (Voyiadis & Deliktas, 2000).

By following a mathematically consistent formulation in the expansion of Laplacians of hardening variables, first order gradients as well as the Laplacians of several variables are incorporated into the model. As opposed to previous theories in the literature with linear hardening, the gradient model used here consistently expands the Laplacian evolution equations to allow different nonlinear material models. The gradients of the hardening terms are found directly by operating on the respective hardening term, and numerical methods are used to compute these gradients of the hardening terms.

The specific choice of the nonlocal measure should be based on the behavior to be captured. Typically, researchers make use of the Laplacian to help in the regularization of numerical problems involving patterning, i.e. shear bands. However, when investigating micro-bending (Stolken & Evans, 1998) and micro-torsion (Fleck & Hutchinson, 1993; Fleck et al., 1994), the first order gradient captures size effects (Bammann et al., 1999). In order to account for both of these effects, both gradients should be incorporated into the model. Though other researchers have introduced nonlocal measures as combinations of first-order gradients, second-order gradients, and higher-order gradients, this model is unique in that (a) the Laplacian based measure is directly derived from the Taylor’s series approximation of a nonlocal measure and (b) the model incorporates first-order up to fourth-order gradients including odd-ordered gradients. Thus, the proposed capability of this model is increased to account for not just shape patterning such as localization problems, but also to properly simulate size dependent behavior of the materials.

The main focus of this work is the formulation and implementation of this complex, gradient enhanced model into a finite element framework. In order to solve the boundary value problem, a multifield approach is adopted such that the plastic and damage multipliers are discretized in addition to the displacement field. Since the degrees of freedom are increased, two additional governing equations (i.e. the weak forms of the consistency conditions in damage and plasticity) are used to obtain a solution.

The governing equations involve both the first order gradient and the Laplacian of the plastic and damage multipliers; however, the governing equations only involve first order derivatives of the displacement field (i.e. strains). Thus, the discretization procedure for the plastic and damage multipliers use C\(^1\) continuous interpolation functions such as the Hermitian shape functions, and hence discretization procedure for the displacement field only use C\(^0\) continuous interpolation functions. This type of discretization is a mixed finite element solution whereby different interpolation functions are used for different discretized fields.
1.4 OUTLINE

This dissertation begins with a discussion in CHAPTER 2 on the main purpose of the present study: strain localization phenomena in metals. A discussion is given on the occurrence of shear bands as well as the defining characteristics of the width of shear bands. As the shear bands cause numerical problems in conventional continuum solutions, some methods are discussed which attempt to resolve these issues. The nonlocal justification for the gradient theory is given here, and the nonlocal approximation measure used in the gradient enhanced model is derived.

CHAPTER 3 gives the thermodynamically consistent theoretical formulations and the numerical implementation of a classical continuum plasticity model. The framework developed here will be used to derive the coupled damage-plasticity model and subsequently the gradient enhanced coupled damage-plasticity model. In deriving the constitutive model, a local yield surface is used to determine the occurrence of plasticity. Isotropic hardening and kinematic hardening are incorporated as state variables to describe the change of the yield surface. The plasticity model is unique in that the hardening conjugate forces (stress like terms) are general functions of their corresponding hardening state variables (strain like terms) and can be defined based on the desired material behavior. It is shown that, depending on the functions used, standard models from the literature can be recovered. The fully implicit backward Euler scheme is developed for this model, and the equilibrium equation is posed in a standard finite element framework to be solved in a Newton-Raphson solution procedure.

Following the framework developed for plasticity in CHAPTER 3, CHAPTER 4 presents the thermodynamically consistent theoretical formulations and the numerical implementation of a classical continuum plasticity model fully coupled with damage. The damage is introduced through a continuum damage mechanics framework and utilizes an anisotropic damage measure to quantify the reduction of the material stiffness. In deriving the constitutive model, a local yield surface is used to determine the occurrence of plasticity and a local damage surface is used to determine the occurrence of damage. As in CHAPTER 3, isotropic hardening and kinematic hardening are incorporated as state variables to describe the change of the yield surface. Additionally, a damage isotropic hardening is incorporated as a state variable to describe the change of the damage surface. As with the plasticity model, the hardening conjugate forces (stress like terms) are general functions of their corresponding hardening state variables (strain like terms) and can be defined based on the desired material behavior. The fully implicit backward Euler scheme is developed for this model, and the equilibrium equation is posed in a standard finite element form to be solved in a Newton-Raphson solution procedure.

CHAPTER 5 gives the thermodynamically consistent theoretical formulations and the numerical implementation of the gradient enhanced continuum plasticity model fully coupled with a gradient enhanced damage model. The plasticity and damage frameworks presented in CHAPTER 3 and CHAPTER 4 are followed in this chapter, and gradient enhancements of the hardening conjugate forces are incorporated into the yield surface
and into the damage surface. Gradients and Laplacians are computed based on the definitions of the material models used for the hardening conjugate forces. As the governing equations involve both the first order gradient and the Laplacian of the plastic and damage multiplier degrees of freedom, the discretization procedure for the plastic and damage multipliers requires higher order interpolation functions such as the Hermitian shape functions. Thus, a mixed finite element solution is used whereby different interpolation functions are used for the multiplier degrees of freedom and the displacement degrees of freedom. The fully implicit solution scheme is developed for this model, and the governing equations are posed in a standard finite element form to be solved in a Newton-Raphson solution procedure.

Utilizing the gradient model presented in CHAPTER 5, CHAPTER 6 discusses the implementation of the gradient theory model accounting for isotropic hardening plasticity into the commercial finite element code ABAQUS (2003). Analytical and numerical examples of localization are given to demonstrate the effectiveness of the gradient model in removing the mesh sensitivity problem.

CHAPTER 7 discusses the length scale introduced through gradient enhanced plasticity. This length scale is defined in terms of microstructure in an attempt to bridge the length scales. A discussion is given for size effect problems in which the length scale is defined in terms of dislocation densities, and a discussion is also given for localization problems in which the length scale is defined in terms of grain sizes.

CHAPTER 8 gives a summary of the work presented in this dissertation as well as some concluding remarks regarding this work.
CHAPTER 2 : LITERATURE REVIEW

2.1 INTRODUCTION

The present study is focused on strain localization phenomena in metals. When investigating such problems as shear banding in a biaxial test (Figure 1.1) and localization of chip segmentation in high speed machining of titanium alloys, the numerical solutions using classical continuum mechanics suffer from ill-posed mathematics. The shear bands that occur develop in the bifurcation regime where the governing equations go from elliptic to hyperbolic. The absence of any material length scale in conventional continuum solutions causes the element size in finite element solutions of localization problems to become the characteristic length, meaning that traditional numerical simulations of localization problems suffer from a pathological mesh dependence. The mathematical model becomes an ill-posed initial value problem and no convergence can be obtained with mesh refinement. In order to solve these types of problems, the numerical methods should incorporate an internal length scale in the formulation. Some methods discussed here to address this issue include Cosserat theory, nonlocal theory, and gradient theory.

2.2 STRAIN LOCALIZATION

A state of localized deformation is described by a state where, after a point of instability, all further deformation concentrates in a small but finite region called a shear band or necking region. This occurs despite the fact that the external loading conditions do not vary. As all of the strains localize in this region, the structure tends to unload elastically in the structure outside of this localized zone. The width, point of emergence, and angle of inclination of the shear bands can depend on material factors including the grain diameter (either soil or metal crystal); the distribution and density of fibers in a metal-matrix composite; and the angle of internal friction and density and can depend on structural factors including the geometry of the body and the loading boundary conditions. Examples of a number of predictions for the thickness of the shear band in a soil based on the material grain size are listed in Table 2.1, where \( w_{sb} \) is the shear band width and \( l_{gs} \) is the grain size (see for example Voyiadjis et al., 2005; Voyiadjis and Song, 2005).

Following the occurrence of a state of localized deformation, the state of stress will tend to decrease with a continued application of deformation. This reduction of the load carrying capacity is known as

<table>
<thead>
<tr>
<th>( w_{sb} / l_{gs} )</th>
<th>Researcher</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 – 10</td>
<td>Roscoe (1970)</td>
</tr>
<tr>
<td>10 – 15</td>
<td>Vardoulakis (1978)</td>
</tr>
<tr>
<td>18.5 – 13</td>
<td>Mühlhaus &amp; Vardoulakis (1987)</td>
</tr>
<tr>
<td>7.5 – 9.6</td>
<td>Mokni and Desrues (1998)</td>
</tr>
<tr>
<td>10.6 – 13.9</td>
<td>Alshibli and Sture (1999)</td>
</tr>
</tbody>
</table>
softening. Softening behavior typically occurs when the shape of the body and the boundary conditions induce an inhomogeneous state of deformation. An experimental investigation of the problem in Figure 2.1 was examined in Bammann et al. (1999). In this example, the non-uniform shape of the body triggers localization to occur; however, material microstructure also gives rise to an inhomogeneous state of deformation. Shear bands occurring from material inhomogeneities can occur in a number of materials such as metals, polymers, and granular materials and are typically originated due to a material heterogeneity or defect in the material, such as micro-cracks, micro-voids, or dislocations (Figure 2.2). This localization can be attributed to a coupling of inelastic mechanisms such as micro-crack and micro-void growth with plastic flow and fracture.

The defects in these engineering materials, along with any additional defects occurring during loading, cause a nonlinear behavior and a local weakness in the material. Initially, the micro-cracks and micro-voids in the heterogeneous material will not interact with loading. However, experimental observations indicate that further loading will cause failure mechanisms to occur where the micro-cracks and micro-voids interact along localized zones of plasticity and damage. These interactions lead to a degradation of the global stiffness and to a subsequent decrease of the load carrying capacity of the material. As damage in the form of micro-cracks and micro-voids and plasticity in the form of dislocations localizes over the narrow region of the continuum, the characteristic length scale governing the variations of plasticity and damage falls far below the scale of the local state variables of strain and damage used to describe the

![Figure 2.1: Tensile specimen with array of holes and localization between the holes.](image)
response of the continuum. Gradients of strain then begin to take effect when this characteristic length scale is of the same order as the material length-scale.

2.3 THEORETICAL PREDICTIONS OF LOCALIZATION

Much research work has been done on localization in various materials since the early 1900’s. A theory of strain localization was proposed by Hadamard (1903) and later developed by researchers such as Thomas (1961), Hill (1962), Mandel (1965), and Rice (1976) who analyzed the emergence and inclination of shear bands. Further work was performed on utilizing this theory to predict the existence and orientation of shear bands within various types of materials, including elasto-plastic soils and rocks. Rudnicki & Rice (1975) investigated localization in triaxial compression of pressure-sensitive materials. They showed that the accuracy of localization predictions due to the elasto-plastic Drucker-Prager model can be greatly increased by the inclusion of a nonassociative flow rule and a vertex-like yield surface. Hill & Hutchinson (1974) and Biot (1965) developed a quasi-static bifurcation analysis for an incompressible solid constrained to undergo plane strain tension, and Vardoulakis (1980) extended this bifurcation analysis to localization in sands in order to define the inclination of shear bands.

Though bifurcation theories have been widely successful in determining the point of emergence shear bands and the orientation of shear bands, they do not take into account the width of the shear band. The shear bands occur in the bifurcation regime where the governing equations go from elliptic to hyperbolic and the absence of any material length scale from a conventional continuum solution causes the element size in finite element solutions of localization problems to become the characteristic length defining the width of the shear band.

Figure 2.2: Material inhomogeneities which may trigger localization: (a) dislocation networks and (b) micro-cracks in a composite.
This type of mesh-dependency is not physically based, as the prediction of the observed characteristic width of the shear bands is based on the size of the finite element as opposed to a material length scale. In traditional finite element solutions, as the finite element mesh is refined, the width of the localized deformation decreases to a vanishing width (Figure 1.1). In actuality, the width of a localized zone is dependent not on the numerical method that is used, but on the material parameters. Specifically, the width is dependent on the “length scales” of the material. When determining the length scale of the material, the researcher must analyze the problem being investigated. Several potential length scales for different problems are shown in Figure 1.2.

Enhanced continuum models, including but not limited to gradient theories, seek to introduce “length scales” into the continuum in order to accurately compute the width of shear bands. Mühlhaus & Vardoulakis (1987) and Vardoulakis (1989) made use of the Cosserat (micropolar) theory which was first introduced by the two Cosserat brothers (Cosserat & Cosserat, 1909). A nonlocal integral equation was introduced by Kröner (1967) and Eringen & Edelen (1972) for elastic material models, and Bažant & Pijaudier-Cabot (1988) and Pijaudier-Cabot & Bažant (1987) extended this into continuum damage mechanics. Bammann & Aifantis (1981, 1982) and Aifantis (1984a,b) suggested a gradient approach to deformation to describe plastic instabilities including dislocation patterning and spatial characteristics of shear bands. Zbib & Aifantis (1988b) compared the evolution and thickness of shear bands in metals as computed using the gradient theory with experimental observations. In addition to successfully detecting the emergence and inclination of shear bands, these enhanced theories have been shown to regularize the solutions such that the mesh dependence of the shear band thickness is removed.

2.3.1 Bifurcation / Ill-posedness

Bifurcation in a continuum implies that deformations migrate from a continuous mode to both continuous and discontinuous modes such that the localization zone contains all of the plastic strains and is surrounded by the elastically loading region. The theory of bifurcation has been used in the last three decades to investigate the splitting within the material continuum to capture the strain localization phenomenon that occurs in the post-bifurcation regime.

Instability which leads to bifurcation can occur due to either the material or the structure. For the case of a material instability, the constitutive relationship is defined as stable such that a solution for the material model exists and is unique if the following condition is satisfied (Hill, 1958; Maier & Hueckel, 1979):

\[ \dot{\sigma} : \dot{\varepsilon} > 0 \quad \text{(2.1)} \]

where \( \dot{\sigma} \) is the incremental Cauchy stress tensor and \( \dot{\varepsilon} \) is the incremental strain. This condition implies that the material is non-softening such that the increment of stress is positive with a positive increment of strain. A relationship can be assumed between the
incremental stress and the incremental strain through a tangent stiffness operator, $D$, such that:

$$ \dot{\sigma} = D : \dot{\varepsilon} $$

(2.2)

This tangent operator is defined based on the material constitutive model. The point at which material stability is lost from Eq. (2.1) can then be written as follows:

$$ \dot{\varepsilon} : D : \dot{\varepsilon} = 0 $$

(2.3)

which coincides with the singularity of the symmetric part of the tangent operator:

$$ \det(D^T + D) = 0 $$

(2.4)

In order to define the point at which structural stability is lost, the structural tangent stiffness matrix $K$ is defined as follows:

$$ K = \int_B B^T DB\,dV $$

(2.5)

where the $B$ matrix relates the strains to the displacements. The structural instability condition can then be written as follows:

$$ \det(K^T + K) = 0 $$

(2.6)

For the case of a band of localization such that a jump of the deformation gradient occurs across a surface, an acoustic tensor can be defined in terms of the vector, $n$, normal to the localization surface as follows:

$$ Q = n \cdot D \cdot n $$

(2.7)

Loss of ellipticity occurs when the acoustic tensor becomes singular. For $n \neq 0$, the following condition defines the singularity point:

$$ \det(Q) = \det(n \cdot D \cdot n) = 0 $$

(2.8)

If one considers only the homogenous solution for the boundary value problem then no bifurcation will be observed and only homogenous stress and strain fields will be obtained. However, if the non-trivial solution is considered, a bifurcation mode will occur. Using the tangent modulus from the material constitutive model as defined by Eq. (2.2), the normals to the localization zone which define the direction of the shear band are determined from Eq. (2.8); however, this method does not provide the shear band width.
2.3.2 Cosserat Theory

In classical continuum mechanics, the strain tensor can be decomposed into a symmetric part which represents the stretch of the material and an antisymmetric part which represents the rotation of the material. The two Cosserat brothers (Cosserat & Cosserat, 1909) proposed a method to separate rotations from translations such that a field of curvatures is obtained in addition to and separate from the field of strains. This type of separation can be seen in granular materials where each individual grain moves and rotates. This can be further applied to metals, where the translations and rotations occur in the crystal grains.

In order to accomplish this separation (Cosserat & Cosserat, 1909; de Borst, 1991), rotational degrees of freedom ($\omega_1$, $\omega_2$, and $\omega_3$) are introduced in addition to the standard translational degrees of freedom ($u_1$, $u_2$, and $u_3$). The curvatures are then obtained as the gradient of the field of rotations. As stresses are associated with the field of strains, couple-stresses result from the field of curvatures. The constitutive relations between the curvatures and the couple-stresses can be shown to introduce an internal length into the material model. This embedded length scale helps to regularize problems of localization such that the shear band is dependent on the length scale rather than the numerical mesh.

2.3.3 Nonlocal Theory

The nonlocal integral introduces long-range microstructural interaction by assuming the variable response at a material point is dependent on the state of its neighborhood in addition to the state of the point itself. Integral equations have been investigated by a

![Figure 2.3](image-url): The nonlocal measure at a point in the homogeneous continuum, (a), is assumed to depend on the state of its neighborhood at the mesoscale, (b).
number of researchers whereby the components of the stress and strain fields are expressed by an averaging integral (e.g. Kunin, 1968; Eringen & Edelen, 1972; Bažant, 1984; Bažant, & Chang, 1984; Bažant et al., 1984; Pijaudier-Cabot & Bažant, 1987; Bažant & Pijaudier-Cabot, 1988). At a material point \( x \) (Figure 2.3), a nonlocal tensor, \( \overline{A} \), is expressed as the weighted average of its local counterpart \( A \) over a surrounding volume \( V \) at a small distance \( s \) from \( x \) such that:

\[
\overline{A} = \frac{1}{V} \int_V h(s) A(x + s) dV
\]  

(2.9)

where \( l \) is an internal characteristic length, which is a material property, and \( h(s) \) is an empirical weighting function subject to the normalizing condition \( \int_V h(s) dV = V \). The normalizing condition ensures that \( \overline{A} = A \) when \( A(x) \) is a constant. Bažant & Chang (1984) examined a number of weighting functions that have been used in the integral equation of nonlocal theories, and some typical examples of this weighting function are presented in Figure 2.4.

### 2.3.4 Strain Gradient Theories

With regard to using gradients to describe the non-local behavior of the material, a gradient dependent, nonlocal measure, \( A \), is introduced for the local variable of interest:

![Image of Figure 2.4](image)

**Figure 2.4:** 1D isotropic weighting functions used in the definition of the nonlocal measure.
\[ \overline{A} = A + cA^G \]  

(2.10)

The local measure, \( A \), and its gradients, \( A^G \), are combined to create the gradient measure through a material length scale, \( c \). This coefficient is not necessarily a constant (Voyiadjis & Abu Al-Rub, 2005), and may be defined in terms of the microstructure (e.g., dislocation density and spacing, grain size, etc.). The gradient enhanced variable \( \overline{A} \) is a nonlocal measure of the variable \( A \) in that it takes into account the state of its neighborhood in addition to the state of the point itself. Note that these variables may be either scalars or tensors. In this form, the gradient enhancement, \( A^G \), may have any combination of gradients as chosen by the researcher (e.g., \( |\nabla A| + c_a \nabla^2 A + c_b |\nabla A|^2 \)). This allows for a more general and powerful formulation, wherein the form of the nonlocal measure can be defined by the microstructure.

The specific choice of the nonlocal measure should be based on the behavior to be captured. For instance, the inclusion of the Laplacian helps in the regularization of numerical problems involving patterning, i.e. shear bands. However, when investigating micro-bending (Stolken & Evans, 1998) and micro-torsion (Fleck & Hutchinson, 1993; Fleck et al., 1994), the first order gradient captures size effects (Bammann et al., 1999). In order to account for both of these effects, both gradients should be incorporated into the model.

Rather than making a definition for the gradient enhancement term, the form of the “nonlocal” measure used in this work is justified from the discussion of approximating the nonlocal integral equation, Eq. (2.9), by using a truncated Taylor’s expansion for an isotropic distribution. In order to develop the gradient dependent approximation of this averaging equation, the local tensor \( A \) can be first approximated by a Taylor series expansion at \( s = 0 \) such that (e.g. Mühlhaus & Aifantis, 1991):

\[
A(x + s) \approx A + \nabla A \cdot s + \frac{1}{2!} \nabla^{(2)} A \cdot s \otimes s + \cdots \tag{2.11}
\]

where \( \nabla^{(i)} \) denotes the \( i \)-th order gradient operator evaluated at the macroscale. For a general three-dimensional case, the surrounding volume can be assumed to be a sphere with a radius equal to the material characteristic length such that \( V = \frac{4}{3} \pi l^3 \). The integration is thus performed using the spherical coordinate system with the coordinates \( r \ (0 \leq r \leq l) \), \( \theta \ (0 \leq \theta \leq 2\pi) \), and \( \varphi \ (0 \leq \varphi \leq \pi) \). The relations between the Cartesian and the spherical coordinate systems are given as follows:

\[
\hat{x}_1 = r \sin \phi \cos \theta \tag{2.12}
\]

\[
\hat{x}_2 = r \sin \phi \sin \theta \tag{2.13}
\]

\[
\hat{x}_3 = r \cos \phi \tag{2.14}
\]
In the spherical coordinate system, the vector $\mathbf{s}$ is actually the vector in the direction of the outward unit normal to the sphere, $\mathbf{n}$, with a magnitude of the spherical coordinate $r$, where the outward normal is a unit vector defined in spherical coordinates as follows:

$$\mathbf{n} = \begin{bmatrix} \sin \phi \cos \theta \\ \sin \phi \sin \theta \\ \cos \phi \end{bmatrix}$$  \hspace{1cm} (2.15)

Setting the weighting function in Eq. (2.9) to the identity tensor and using the transformation relations between the Cartesian and the spherical coordinate systems, the integral equation can be written in terms of the spherical coordinates as follows:

$$\overline{\mathbf{A}} = \frac{1}{V} \int_0^{2\pi} \int_0^\pi \left[ \mathbf{A} + r \nabla \mathbf{A} \cdot \mathbf{n} + \frac{r^2}{2!} \nabla^{(2)} \mathbf{A} \cdot \mathbf{n} \otimes \mathbf{n} + \cdots \right] r^2 \sin \phi \, dr \, d\phi \, d\theta$$  \hspace{1cm} (2.16)

which can be expanded as:

$$\overline{\mathbf{A}} = \mathbf{A} + \frac{I^4}{4V} \nabla \mathbf{A} \cdot \int_0^{2\pi} \int_0^\pi \left[ \sin \phi \mathbf{n} \right] d\phi \, d\theta$$

$$+ \frac{1}{2!} \frac{I^5}{5V} \nabla^{(2)} \mathbf{A} \cdot \int_0^{2\pi} \int_0^\pi \left[ \sin \phi \mathbf{n} \otimes \mathbf{n} \right] d\phi \, d\theta + \cdots$$  \hspace{1cm} (2.17)

From the definition of the unit normal as given by Eq. (2.15), it can be shown that

$$\int_0^{2\pi} \int_0^\pi \left[ \sin \phi \mathbf{n} \right] d\phi \, d\theta = 0, \quad \int_0^{2\pi} \int_0^\pi \left[ \sin \phi \mathbf{n} \otimes \mathbf{n} \right] d\phi \, d\theta = 0, \quad \text{and so forth such that all of the terms involving odd gradients are zero. It can also be shown that}$$

$$\int_0^{2\pi} \int_0^\pi \left[ \sin \phi \mathbf{n} \otimes \mathbf{n} \right] d\phi \, d\theta = \frac{4}{3} \pi \mathbf{I}.$$  \hspace{1cm} \text{Furthermore, truncating the Taylor series after the second order gradient term, the following expression is used for the nonlocal tensor:}

$$\overline{\mathbf{A}} = \mathbf{A} + \frac{4\pi I^5}{2! \cdot 15V} \nabla^2 \mathbf{A}$$  \hspace{1cm} (2.18)

where $\nabla^2$ is the Laplacian operator and is defined as the trace of the second gradient. After substitution of the volume over which the local variable is averaged, the nonlocal approximation which is used in this work is found to have the following form (Mühlhaus & Aifantis, 1991):

$$\overline{\mathbf{A}} = \mathbf{A} + c \nabla^2 \mathbf{A}$$  \hspace{1cm} (2.19)

In this equation, the coefficient $c$ is defined to be proportional to an internal characteristic length squared. If one assumes a more general tensorial character for $\mathbf{h}(\mathbf{s})$ not necessarily confined to the expression in terms of an identity tensor, then one obtains
a different weighting of the individual coefficients. This will give a weighting function
with a tensorial nature \(c\) containing several different integration constants \(c_{ij}\). This type of
tensorial length scale is required for anisotropic material behavior as presented by
Voyiadjis & Song (2005). Additionally, with a more general weighting function, the terms
involving \(i\)-th order gradients with \(i\) being odd must be included in the nonlocal measure.

Though this form of the gradient enhanced measure includes only the local measure
and its Laplacian, first order gradients will also be brought into the formulation using
consistent thermodynamics. Thus, the gradient measure retains the justification of being
an approximation to the nonlocal integral equation, and both first order gradients and the
Laplacian are brought into the model in order to account both for localization and for size
effect problems.

\[ \nabla^2 A > 0 \]

\[ \nabla^2 A < 0 \]

\[ x \]

\[ x \]

\[ \nabla^2 A \]

Figure 2.5: Spreading of the shear band through the use of a gradient enhanced measure.
Figure 2.5 presents the behavior of the nonlocal approximation given by Eq. (2.19) when applied to a localized band of the measure, $A$. At the edges of this band, the change in the slope is positive, and so the Laplacian is negative. When used in the combination given by the gradient measure, this increases the width of the shear band allowing the band to spread to the surrounding elements. In numerical simulations of localization, this serves to remove the mesh dependency such that the shear band width extends beyond a single row of elements. At the center of the band, the change in the slope is negative, and so the negative Laplacian reduces the magnitude of the local measure in the gradient measure, thus acting as a localization limiter.

### 2.4 Conclusions

In this chapter, strain localization phenomena was discussed and criteria for material and structural instability were given. In order to account for the mesh dependence of numerical simulations of localization problems, some numerical methods which incorporate an internal length scale into the continuum framework were discussed. Included in these enhanced continuum models was the gradient theory. In the discussion of the gradient theory, the gradient measure to be used in the development of the gradient model was derived. However, before developing the gradient model, the next chapter begins with the thermodynamically consistent theoretical formulations and the numerical implementation of a classical continuum plasticity model. The framework developed here will then be used to derive the coupled damage-plasticity model and subsequently the gradient enhanced coupled damage-plasticity model.
CHAPTER 3 : LOCAL PLASTICITY MODEL

3.1 INTRODUCTION

A simple plot of the stress-strain behavior for a plastically loaded material is presented in Figure 3.1. Linear elasticity is the simplest material model and is one of the most commonly used for designing engineering structures. Elastic loadings are typically small and are such that, when the material is loaded elastically from point \( n_0 \) to point \( n_1 \), the state will return to its original state at point \( n_0 \) after removal of the external loading conditions. Though elasticity is satisfactory for most engineering materials early on in deformation, larger plastic deformations which exceed a critical threshold (the yield stress, \( \sigma_{yp} \)) will cause a state of deformation which will not return to its original state when the external loading conditions are removed; however, as the material will first have undergone an elastic deformation, the state will partially return to the original state along the elastic curve defined by point \( n_2 \) and point \( n_3 \). The part of the strain that is able to be recovered is denoted as the elastic strain (\( \varepsilon^e \)), and the irreversible part of the deformation is denoted as the plastic strains (\( \varepsilon^p \)).

Plastic deformation of ductile materials can be explained in terms of the theory of dislocations as independently introduced in 1934 by Orowan, Taylor, and Polanyi. Although movement of dislocations occurs with all loading, this movement is insignificant until the yield point occurs. At this point, loading causes dislocations to be generated, moved, and stored. The ease with which dislocations are able to move determines the hardness of the material. With an increase in the dislocation density, there

![Figure 3.1: Stress – strain curve for a plastically loaded material.](image-url)
begins to be more dislocation-dislocation interactions such that movement becomes more difficult and the stress required to produce additional plastic deformation increases, i.e. the material hardens. For a perfectly plastic material where the dislocations move infinitely, the plastic loading would occur along a path defined by points \( n_1 \) to \( n_4 \); however, in real situations, hardening of the material causes the yield stress of the material to increase along the path defined by points \( n_1 \) and \( n_2 \). As the dislocation movements are permanent, the hardening is stored in the material such that, after elastic unloading from point \( n_2 \) to point \( n_3 \), the stress-strain curve does not begin to yield at point \( n_4 \) but continues to the hardened yield stress at point \( n_2 \) where plastic loading continues past point \( n_2 \) to \( n_5 \).

Plasticity material models are used to describe this behavior by defining the critical stress (the yield stress) through a yield criterion. Various plasticity models have been used throughout the literature to define the yield surface as well as the change in size, shape, and position of the yield surface. In this work, a von Mises type yield criterion is used with both isotropic hardening (for example see Hill, 1950; Chaboche, 1989; etc.) corresponding to the change in the size of the yield surface and kinematic hardening (for example see Prager, 1956; Frederick & Armstrong, 1966, etc.) corresponding to the change in the location of the yield surface.

The constitutive model is derived using consistent thermodynamics in the same fashion as a classical rate-independent continuum J2 plasticity model (e.g. Doghri, 1993; Simo & Hughes, 1998; Belytschko, 2000). Based on the first law of thermodynamics, the Helmholtz free energy is introduced to describe the current state of energy in the material (Malvern, 1969; Coussy, 1995), and is a function of the strain and the internal state variables under consideration.

### 3.2 Continuum Mechanics and Thermodynamics

In order to derive the model equations, the thermodynamics of irreversible processes is followed by introducing a local state consisting of state variables (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000). A thermodynamic potential is used which allows the state laws to be defined based on the state variables. The evolution of the thermodynamic conjugate forces are then obtained by assuming the physical existence of the dissipation potential at the macroscale and through the use of the theory of functions of several variables with a Lagrange multiplier.

#### 3.2.1 State Variables

The local plasticity model is defined through the use of the method of material local state identification. In this method, a model is developed such that the thermodynamic state at a given point in space and time is completely determined by a given set of state variables at that point in space and time. As this set of state variables does not include
gradients for the local theory, the state at the given point is independent of the behavior surrounding the point; however, in CHAPTER 5, gradients will be introduced as state variables and the method of material nonlocal state identification will be followed to derive the thermodynamic equations.

The set of state variables defined here is due to only plasticity related phenomena, as the plasticity model will be coupled with a damage model in CHAPTER 4. The plasticity state variables are separated into a set of observable state variables and a set of internal state variables. The observable variables are those that can be measured and which appear regardless of the material phenomena such as elasticity and plasticity. The observable state variables used here are the temperature denoted by the scalar $T$ and the total strain denoted by the second-order tensor $\varepsilon$. For pure elasticity, this set of observable state variables entirely defines the point; however, for elasto-plasticity, the material has a history dependency which requires an additional set of internal state variables.

For a uniaxial loading case, the strain at a given stress has two parts: a recoverable elastic strain, $\varepsilon^e$, and an irreversible plastic strain, $\varepsilon^p$ (Figure 3.1). The reversible part is related to the stress through the usual linear elastic equations. Plasticity theory is concerned with characterizing the irreversible part which remains when external loads are removed. Similarly, for a general 3D state, the strain decomposition is assumed to be written additively as follows:

$$\varepsilon = \varepsilon^e + \varepsilon^p$$

where $\varepsilon^e$ is the reversible thermo-elastic component of the strain and $\varepsilon^p$ is the irreversible plastic component of the strain.

Additional internal state variables are required to define the plasticity hardening. These hardening internal state variables are unitless, strain like quantities and are accumulated into a set, $V^p$, of macroscopic measures of irreversible phenomena:

$$V^p = [r, \alpha]$$

where the internal state variables considered here are the plasticity related variables representing the fluxes of the isotropic and kinematic hardening behaviors denoted by the scalar $r$ and the second-order tensor $\alpha$, respectively. The isotropic hardening (Hill, 1950) corresponds to the change in the size of the yield surface and the kinematic hardening (Prager, 1956) corresponds to the change in the location of the yield surface.

### 3.2.2 Equations of State

In order to determine state laws which relate the internal state variable fluxes to their conjugate thermodynamic forces, a thermodynamic potential defined as the Helmholtz
free energy is introduced which is a state function of a thermodynamic system (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000). This thermodynamic potential is used to describe the current state of energy in the material, and is a function of the observable state variables and the internal state variables under consideration:

\[ \psi = \psi(\epsilon, T, \epsilon^p, \epsilon^e, V^p) \]  

(3.3)

However, in modeling the material using elasto-plasticity, it will be seen that the total strains and the plastic strains appear only in the form of the following decomposition from the constraint Eq. (3.1):

\[ \epsilon - \epsilon^p = \epsilon^e \]  

(3.4)

Thus, the set of variables that the free energy is dependent on can be written as:

\[ \psi = \psi(\epsilon - \epsilon^p, T, V^p) \]  

(3.5)

or equivalently as:

\[ \psi = \psi(\epsilon^e, T, V^p) \]  

(3.6)

The second law of thermodynamics imposes restrictions on the constitutive relations. From the second law of thermodynamics, the Clausius-Duhem inequality can be written as follows:

\[ \sigma : \dot{\epsilon} - \rho (\dot{\psi} + s \dot{T}) - q \frac{\nabla T}{T} \geq 0 \]  

(3.7)

where \( \sigma \) is the second order Cauchy stress tensor, \( \rho \) is the mass density, \( q \) is the heat flux vector, \( s \) is the entropy per unit mass representing the amount of disorder or randomness in a system, \( \nabla T \) is the temperature gradient, and \( \dot{\psi} \) is the time derivative of \( \psi \), such that:

\[ \dot{\psi} = \frac{\partial \psi}{\partial \epsilon^e} : \epsilon^e + \frac{\partial \psi}{\partial T} \dot{T} + \frac{\partial \psi}{\partial V^p} : \dot{V}^p \]  

(3.8)

The dot in the third term indicates that this term is summed over the components of the set, \( V^p \), of macroscopic measures of irreversible phenomena such that:

\[ \frac{\partial \psi}{\partial V^p} : \dot{V}^p = \frac{\partial \psi}{\partial r} \dot{r} + \frac{\partial \psi}{\partial \alpha} : \alpha \]  

(3.9)
Using Eq. (3.8) along with the strain decomposition given by Eq. (3.1), the Clausius-Duhem inequality can be expanded in the following form:

\[
\sigma : \dot{\varepsilon}^p + \left( \sigma - \rho \frac{\partial \psi}{\partial \varepsilon^e} \right) : \dot{\varepsilon}^e - \rho \left( \frac{\partial \psi}{\partial T} + s \right) \dot{T} - \rho \frac{\partial \psi}{\partial V^p} \cdot \dot{V}^p - q \cdot \frac{\nabla T}{T} \geq 0
\]  

(3.10)

In order to obtain thermodynamic laws, independent processes are assumed that satisfy this inequality. The first independent process is a case of elastic loading \((\varepsilon^p = 0; \dot{V}^p = 0)\) occurring at a constant, uniform temperature \((\dot{T} = 0; \nabla T = 0)\). Thus, for the Clausius-Duhem inequality to hold at any given elastic strain increment, the following must be true:

\[
\sigma - \rho \frac{\partial \psi}{\partial \varepsilon^e} = 0
\]  

(3.11)

The next independent process is that of uniform thermal load \((\nabla T = 0)\) in addition to the elastic loading \((\varepsilon^p = 0; \dot{V}^p = 0)\). Assuming Eq. (3.11) holds, the Clausius-Duhem inequality holds at any given temperature increment only if the following equation is true:

\[
\sigma_j = C^e : (\varepsilon_j - \varepsilon^p_j) = \sigma_0 + C^e : (\Delta \varepsilon_j - \Delta \varepsilon^p_j)
\]  

(3.12)

From these last two equations, the thermo-elastic state laws are defined:

\[
\sigma = \rho \frac{\partial \psi}{\partial \varepsilon^e}
\]  

(3.13)

\[
s = -\frac{\partial \psi}{\partial T}
\]  

(3.14)

Thus, the stress, \(\sigma\), and the enthalpy, \(s\), are defined as the conjugate forces corresponding to the state variables \(\varepsilon^e\) and \(T\), respectively. Similarly, a set of conjugate forces, \(A^p\), is defined which correspond to the hardening internal state variables:

\[
A^p = [R, X]
\]  

(3.15)

where the scalar \(R\) measures the expansion or contraction of the yield surface in the stress space while maintaining its shape and having a fixed center and the second-order tensor \(X\) measures the movement and distortion of the yield surface. Whereas the internal state variables are unitless, strain like quantities, the thermodynamic conjugate forces are a set of stress like quantities that are related to the state variables as the stress is related to the
strain. These conjugate forces are defined in the Clausius-Duhem inequality by the following set of state laws:

\[ A^p = \rho \frac{\partial \psi}{\partial N^p} \quad (3.16) \]

### 3.2.3 Conjugate Forces

Since the internal state variables are selected independently of one another, one can express the analytical form of the Helmholtz free energy in terms of its internal state variables as:

\[ \rho \psi = \frac{1}{2} \epsilon^e \cdot : C^e \cdot \epsilon^e + W^p \left( V^p \right) - \rho Ts \quad (3.17) \]

where the fourth-order tensor \( C^e \) is the elastic tangent modulus, the scalar \( \rho \) is the material density, and the superscripted “\( e \)” and “\( p \)” imply terms associated with elasticity and plasticity, respectively. For this form of the Helmholtz free energy and from the state law Eq. (3.13), the stress applied to stretch or compress a body is defined to be proportional to the elastic strain thus produced in the form of a Hookean relationship as follows:

\[ \sigma = C^e \cdot : \epsilon^e \quad (3.18) \]

For isotropic elasticity, the elastic stiffness tensor is expressible as:

\[ C^e = \kappa^e \mathbf{I} + 2 \mu^e \mathbf{D}^I = \lambda^e \mathbf{I} + 2 \mu^e \mathbf{I} \quad (3.19) \]

where \( \mathbf{I} \) and \( \mathbf{D}^I \) are the second-order identity tensor and the fourth-order deviatoric identity tensors, respectively, as defined in the APPENDIX A. From the definition of the dyadic product, the first term in this definition of the elastic stiffness tensor has components \( \kappa^e (\mathbf{1} \otimes \mathbf{1})_{ijkl} = \kappa^e \delta_{ij} \delta_{kl} \). The two independent material constants \( \lambda^e \) and \( \mu^e \) are the Lamé constants. The coefficient \( \mu^e \) is also known as the shear modulus. These constants can be expressed in terms of the bulk modulus, \( \kappa^e \); Young’s modulus, \( E \); and Poisson’s ratio, \( \nu \), as follows:

\[ \mu^e = \frac{E}{2(1 + \nu)} \quad (3.20) \]

\[ \lambda^e = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \quad (3.21) \]

\[ \kappa^e = \lambda^e + \frac{2}{3} \mu^e = \frac{E}{3(1 - 2\nu)} \quad (3.22) \]
Utilizing this isotropic elastic modulus, the Hookean relationship can alternately be written as follows:

$$\sigma = \lambda \varepsilon \left(1 : \varepsilon^e\right) + 2\mu \varepsilon^e$$  \hspace{1cm} (3.23)

The term $W^p \left( V^p \right)$ accounts for energy introduced into the system by the hardening terms. In general, the hardening term for the energy may be introduced as fully coupled for the isotropic and kinematic hardening. However, in this work it is assumed that the energy introduced by the hardening terms is uncoupled so that the energy term is a sum of two terms:

$$W^p \left( V^p \right) = W^r \left( r \right) + W^a \left( \alpha \right)$$  \hspace{1cm} (3.24)

The energy term relating to the plasticity isotropic hardening – conjugate force relationship can be, but is not exclusively, in the form of a power or exponential relationship (Doghri, 1993). Similarly, power and exponential relationships can be defined for the kinematic hardening energy terms (Voyiadis & Dorgan, 2004b, 2005). Thus, the energy terms can be selected from one of the following:

**Power Laws**

$$W^r \left( r \right) = \frac{H}{m_i} r^{m_i+1}$$  \hspace{1cm} (3.25)

$$W^a \left( \alpha \right) = \frac{H_a}{m_{\alpha}^{\alpha+1}} \left\| \alpha \right\|^{m_{\alpha}+1}$$  \hspace{1cm} (3.26)

**Exponential Laws**

$$W^r \left( r \right) = R_i \left( r + \frac{1}{\gamma_i} e^{-\gamma_i r} - \frac{1}{\gamma_i} \right)$$  \hspace{1cm} (3.27)

$$W^a \left( \alpha \right) = X_{\alpha} \left( \left\| \alpha \right\| + \frac{1}{\gamma_{\alpha}} e^{-\gamma_{\alpha} \left\| \alpha \right\|} - \frac{1}{\gamma_{\alpha}} \right)$$  \hspace{1cm} (3.28)

In these relationships, $H_i$, $m_i$, $R_i$, $X_{\alpha}$ are positive material and geometrical dependent parameters, where $i = r, \alpha$. For example, for the case of a composite, the geometrical properties may include size, shape, and spacing of the fibers. Utilizing the energy terms into the Helmholtz free energy, the state laws, Eq. (3.16), result in definitions for the hardening - thermodynamic conjugate forces as power and exponential relations of the corresponding state variables:

**Power Laws**

$$R = H_i r^{m_i}$$  \hspace{1cm} (3.29)

$$X = H_{\alpha} \left\| \alpha \right\|^{m_{\alpha}+1}$$  \hspace{1cm} (3.30)
Exponential Laws

\[
R = R_c \left(1 - e^{-\gamma r}\right)
\]

\[
X = X_c \frac{\alpha}{\| \alpha \|} \left(1 - e^{-\gamma \| \alpha \|} \right)
\]

Note that these laws are subject to the constraint that \( X = 0 \) when \( \| \alpha \| = 0 \).

The internal state variable - thermodynamic conjugate force relationships are defined based on the material being investigated, and different relationships can be selected for the isotropic hardening law and for the kinematic hardening law. For example, the isotropic hardening relationship can be selected as linear with an exponential law for the kinematic hardening. Though two typical models, the power and exponential laws, are used here to introduce the isotropic and kinematic hardening relations, more complex models can be incorporated in the same manner; however, the analysis of the material model is beyond the scope of this work. This work is focused on the development of a formulation based on a general functional form of the thermodynamic conjugate forces. This allows the constitutive model to be developed without making an assumption as to the behavior of the material model such that the conjugate forces are written as a general function of their corresponding internal state variable:

\[
R = R(r) \quad (3.33)
\]

\[
X = X(\alpha) \quad (3.34)
\]

For an example of how these relationships can be defined, consider the isotropic hardening conjugate force for plasticity, \( R \). This conjugate force, which is a stress quantity, measures the expansion or contraction of the yield surface in the stress space while maintaining its shape and having a fixed center. Thus, the radius of the yield surface, i.e. the current yield stress, is computed as the sum of the initial yield stress, \( \sigma_{ys} \), and the isotropic hardening conjugate force. Some possible softening curves for the relationship between the current yield stress and the isotropic hardening are plotted in Figure 3.2.

3.2.4 Dissipation Potential and Flow Rules

The evolution of the thermodynamic conjugate forces can be obtained through the evolution relations of the internal state variables, which are obtained by assuming the physical existence of the dissipation potential at the macroscale. The energy dissipation processes are set in conjunction to the Clausius-Duhem inequality with the thermodynamic state laws substituted and are thus given as the product of the thermodynamic conjugate forces with the respective flux variables as follows:
\[ \Pi^p = \sigma : \dot{\varepsilon}^p - \rho A^p \cdot \dot{\nabla}^p - q \cdot \frac{\nabla T}{T} \geq 0 \]  

(3.35)

The theory of functions of several variables is used with the Lagrange multiplier \( \lambda^p \) to construct the objective function \( \Omega \) in the following form:

\[ \Omega = \Pi^p - F \lambda^p \]  

(3.36)

where \( F \) is the plastic potential and will be defined later. In order to obtain the plastic strain rate, the following condition is used to extremize the objective function:

\[ \frac{\partial \Omega}{\partial \sigma} = 0 \]  

(3.37)

From this condition for the case when \( F \geq 0 \), the corresponding evolution equation for the plastic strain is given as follows:

\[ \dot{\varepsilon}^p = \frac{\partial F}{\partial \sigma} \lambda^p \]  

(3.38)

In order to derive the evolution equations for the hardening state variables, the following condition is used to extremize the objective function:

\[ \frac{\partial \Omega}{\partial A^p} = 0 \]  

(3.39)

Figure 3.2: Softening curves: possible relations between the isotropic hardening, \( r \), and the corresponding conjugate force, \( R \)
From this condition for the case when $F \geq 0$, the corresponding set of evolution equations for the hardening state variables is given as follows:

$$\dot{V}^p = -\frac{\partial F}{\partial A^p} \dot{\lambda}^p$$  \hspace{1cm} (3.40)

The following loading-unloading conditions known as the Kuhn-Tucker conditions (Kuhn & Tucker, 1951) must be enforced:

$$\dot{\lambda}^p \geq 0; \quad f \leq 0; \quad \dot{\lambda}^p f = 0$$  \hspace{1cm} (3.41)

The first relationship states that the plastic flow rate is always non-negative, while the second condition shows that the stress state is always within the yield surface or on the yield surface. The last condition can be met for two different loading cases. If the stress is in a state of elastic loading/unloading, then $\dot{\lambda}^p = 0$ and the condition is met. If, however, there is plastic loading ($\dot{\lambda}^p > 0$), then the last condition forces the stress state to remain on the yield surface ($f = 0$). In order for this condition to be enforced with loading, there can be no evolution of the yield surface ($\dot{f} = 0$). This last implication is the consistency condition for plasticity, and it will be used to obtain the evolution of the plastic multiplier.

### 3.2.5 Yield Condition

Associative plasticity can be used here to derive the evolution equations for the constitutive model such that the plastic potential, $F$, is set equal to the yield criterion, $f$:

$$F = f = \|\xi\| - \sqrt{\frac{2}{3}} \left[ \sigma^{ij} + R \right] \leq 0$$  \hspace{1cm} (3.42)

where $\|\xi\|$ is the norm of the relative stress tensor, $\xi$, and is defined in terms of the deviatoric stress, $s$, and the backstress, $X$, as follows:

$$\xi = s - X$$  \hspace{1cm} (3.43)

The deviatoric stress, $s$, is defined in APPENDIX A and is rewritten here as:

$$s = \sigma - \frac{1}{3} \nu (\sigma) 1$$  \hspace{1cm} (3.44)

Based on the assumption of an elastic stiffness tensor from isotropic elasticity given by Eq. (3.19), the Hookean relationship given by Eq. (3.18) may alternatively be written as follows:
\[ \sigma = \kappa \text{tr} \left( \varepsilon^e \right) 1 + 2 \mu \varepsilon^e \]  
\[ \text{(3.45)} \]

where \( \varepsilon^e \) is the deviatoric part of the strain tensor. Thus, the deviatoric part of the stress tensor is written as:

\[ s = 2 \mu \varepsilon^e \]  
\[ \text{(3.46)} \]

and the deviatoric relative stress is written as:

\[ \xi = 2 \mu \varepsilon^e - X \]  
\[ \text{(3.47)} \]

With the plastic potential defined by Eq. (3.42), the normals to the plastic potential required in Eqs. (3.38) and (3.40) are derived to have the following forms:

\[ \frac{\partial F}{\partial \sigma} = \frac{\partial f}{\partial \sigma} = \frac{\xi}{\| \xi \|} = f_\sigma \]  
\[ \text{(3.48)} \]

\[ \frac{\partial F}{\partial R} = \frac{\partial f}{\partial R} = -\sqrt{\frac{1}{3}} = f_R \]  
\[ \text{(3.49)} \]

\[ \frac{\partial F}{\partial X} = \frac{\partial f}{\partial X} = f_X = -f_\sigma \]  
\[ \text{(3.50)} \]

Thus, the complete set of constitutive equations for the local plasticity model have been derived and are summarized as follows:

**Yield Criterion**

\[ F = f = \| \xi \| - \sqrt{\frac{1}{3}} \left[ \sigma_{\text{yy}} + R \right] \leq 0 \]  
\[ \text{(3.51)} \]

**State Laws**

\[ \sigma = C^e : (\varepsilon - \varepsilon^p) \]  
\[ \text{(3.52)} \]

\[ R = R(r) \]  
\[ \text{(3.53)} \]

\[ X = X(\alpha) \]  
\[ \text{(3.54)} \]

**State Variable Evolution Equations**

\[ \dot{\varepsilon}^p = f_\sigma \dot{\lambda}^p \]  
\[ \text{(3.55)} \]

\[ \dot{r} = -f_R \dot{\lambda}^p = \ddot{\varepsilon}^p_{\text{eq}} \]  
\[ \text{(3.56)} \]

\[ \dot{\alpha} = -f_X \dot{\lambda}^p = f_\sigma \dot{\lambda}^p = \ddot{\varepsilon}^p \]  
\[ \text{(3.57)} \]

**Kuhn-Tucker Conditions**

\[ \dot{\lambda}^p \geq 0 ; \quad r \leq 0 ; \quad \dot{\lambda}^p f = 0 \]  
\[ \text{(3.58)} \]
In these equations, $\dot{\varepsilon}_{\text{eq}}^p$ is defined as the evolution of the equivalent plastic strain and takes the following form:

$$\dot{\varepsilon}_{\text{eq}}^p = \sqrt{\frac{2}{3}} \dot{\varepsilon}^p : \dot{\varepsilon}^p = \sqrt{\frac{2}{3}} \dot{\lambda}^p$$

(3.59)

### 3.2.6 Plasticity Consistency Condition

At a plastic state where $f = 0$, the consistency condition $\dot{f} = 0$ results from the loading-unloading conditions of Eq. (3.41). Thus, as the yield criterion is a function of the effective Cauchy stress, the backstress, and the isotropic hardening, the consistency condition can be expanded in terms of the conjugate forces:

$$\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial r} \dot{r} + \frac{\partial f}{\partial X} \dot{X} \equiv 0$$

(3.60)

As the conjugate forces have been defined as general functions of the state flux variables as defined in Eqs. (3.53) and (3.54), the consistency condition can be rewritten in terms of the flux variables as follows:

$$\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial r} \dot{r} + \frac{\partial f}{\partial X} \dot{X} : \dot{\alpha} \equiv 0$$

(3.61)

After substitution of the normals to the yield surface as defined in Eqs. (3.48) to (3.50) and the evolution equations for the internal state variables as defined in Eqs. (3.55) to (3.57), the plastic multiplier can be solved from this consistency condition in terms of the incremental stress as follows:

$$\dot{\lambda}^p = \frac{1}{H} \sigma_{\alpha} : \dot{\sigma}$$

(3.62)

where $H$ is defined here as:

$$H = f_r \frac{\partial R(r)}{\partial r} + f_{\alpha} \frac{\partial X(\alpha)}{\partial \alpha} : f_{\alpha}$$

(3.63)

Alternately, the incremental stress found by differentiating the Hookean law, Eq. (3.52), is first substituted into the consistency condition, Eq. (3.61), and the evolution of the plastic strain, Eq. (3.55), is substituted into the resulting equation, the plastic multiplier can be solved for in terms of the incremental strain as follows:

$$\dot{\lambda}^p = \frac{1}{h} f_{\alpha} : C^\alpha : \dot{\varepsilon}$$

(3.64)
where \( h \) is defined here as:

\[
h = H + f_\sigma : C^e : f_\sigma
\]  

(3.65)

As the normal to the yield surface \( f_\sigma \) is a deviatoric tensor as defined by Eq. (3.48), the following relationships can be derived from the assumption of isotropic elasticity given by Eq. (3.19):

\[
C^e : f_\sigma = 2\mu f_\sigma
\]  

(3.66)

\[
f_\sigma : C^e : f_\sigma = 2\mu^e
\]  

(3.67)

such that the plastic multiplier and the hardening coefficient, \( h \), can be rewritten as follows:

\[
\lambda^p = \frac{1}{H} f_\sigma : \dot{\sigma} = \frac{2\mu^e}{h} f_\sigma : \dot{\varepsilon}
\]  

(3.68)

\[
h = H + 2\mu^e
\]  

(3.69)

Now again using the rate form of the Hookean relationship given by Eq. (3.52) and pre-multiplying by \( f_\sigma \), the following relation is obtained:

\[
f_\sigma : \dot{\sigma} = f_\sigma : C^e : \dot{\varepsilon} - f_\sigma : C^e : f_\sigma \lambda^p
\]  

(3.70)

Using Eq. (3.64), the above equation is expressed as:

\[
f_\sigma : \dot{\sigma} = h\lambda^p - f_\sigma : C^e : f_\sigma \lambda^p
\]  

(3.71)

or:

\[
\frac{f_\sigma : \dot{\sigma}}{\lambda^p} = \frac{\dot{\varepsilon}^p : \dot{\sigma}}{(\dot{\lambda}^p)^2} = h - f_\sigma : C^e : f_\sigma = H
\]  

(3.72)

As seen from this equation, since the terms \( \dot{\varepsilon}^p \) and \((\dot{\lambda}^p)^2\) are always positive, this hardening modulus is positive when hardening occurs (i.e. positive increments of stress), and it is negative when softening occurs (i.e. negative increments of stress).

### 3.2.7 Elasto-Plastic Tangent Modulus

In order to define the constitutive equation, the rate form of the Hookean stress must be derived by differentiating the stress-strain relation of Eq. (3.52):
\[ \dot{\sigma} = C^e : (\dot{\varepsilon} - \dot{\varepsilon}^p) \]  

(3.73)

Using the evolution of the plastic strain and of the plastic multiplier defined by Eqs. (3.55) and (3.64), the constitutive law can now be defined by the following expression:

\[ \dot{\sigma} = D^{ep} : \dot{\varepsilon} \]  

(3.74)

where the elastic-plastic continuum tangent modulus, \( D^{ep} \), is expressed as:

\[
D^{ep} = \begin{cases} 
C^e & \text{if } \dot{\lambda}^p = 0 \\
C^e - \frac{1}{h} C^e : f_{\sigma} \otimes f_{\sigma} : C^e & \text{if } \dot{\lambda}^p > 0 
\end{cases}
\]  

(3.75)

Alternatively, if the plastic multiplier defined in terms of the incremental stress, Eqs. (3.62), is used, then the inverse of the elastic-plastic continuum tangent modulus takes the following form:

\[
D^{-ep} = \begin{cases} 
C^{-e} & \text{if } \dot{\lambda}^p = 0 \\
C^{-e} + \frac{1}{H} f_{\sigma} \otimes f_{\sigma} & \text{if } \dot{\lambda}^p > 0 
\end{cases}
\]  

(3.76)

It should be noted that, in order to avoid spurious loading-unloading at yield due to the abrupt transition from elasticity to plasticity (Belytschko et al., 2000), a consistent tangent modulus will be derived in a subsequent section.

### 3.2.8 Uniaxially Loaded Bar

In order to better understand the equations, the model developed in this chapter is reduced here to a one-dimensional, uniaxially loaded bar. For this loading case, as there are no shear stresses or shear strains, the Cauchy stress tensor is written in symmetric vector form in terms of axial components and reduced to be in terms of a single axial component:

\[
\{\sigma\} = \begin{bmatrix} \sigma_{11} \\ 0 \\ 0 \end{bmatrix}
\]  

(3.77)

Utilizing this uniaxial stress tensor in Eq. (3.23), and writing the elastic coefficients in terms of the Poisson’s ratio and the Young’s modulus, the following relations between the uniaxial stress and strain components are obtained:
\[
\begin{bmatrix}
\sigma_{11} \\
0 \\
0
\end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix}
1-\nu & \nu & \nu \\
\nu & 1-\nu & \nu \\
\nu & \nu & 1-\nu
\end{bmatrix} \begin{bmatrix}
\varepsilon_{11}^e \\
\varepsilon_{22}^e \\
\varepsilon_{33}^e
\end{bmatrix}
\]

(3.78)

Alternatively, the inverse of this relation gives the components of the elastic strain as follows:

\[
\begin{bmatrix}
\varepsilon_{11}^e \\
\varepsilon_{22}^e \\
\varepsilon_{33}^e
\end{bmatrix} = \frac{1}{E} \begin{bmatrix}
1 & -\nu & -\nu \\
-\nu & 1 & -\nu \\
-\nu & -\nu & 1
\end{bmatrix} \begin{bmatrix}
\sigma_{11} \\
0 \\
0
\end{bmatrix} = \begin{bmatrix}
-\nu \varepsilon_{11}^e \\
-\nu \varepsilon_{11}^e \\
-\nu \varepsilon_{11}^e
\end{bmatrix}
\]

(3.79)

As the Poisson’s ratio is 0.5 for incompressible plasticity, the plastic strain tensor can also be reduced using this relationship as follows:

\[
\begin{bmatrix}
\varepsilon_{11}^p \\
\varepsilon_{22}^p \\
\varepsilon_{33}^p
\end{bmatrix} = \begin{bmatrix}
\varepsilon_{11}^p \\
-\frac{1}{2} \varepsilon_{11}^p \\
-\frac{1}{2} \varepsilon_{11}^p
\end{bmatrix}
\]

(3.80)

which, from Eq. (3.57), allows the backstress flux tensor to be reduced as follows:

\[
\begin{bmatrix}
\alpha_{11} \\
\alpha_{22} \\
\alpha_{33}
\end{bmatrix} = \begin{bmatrix}
\alpha_{11} \\
-\frac{1}{2} \alpha_{11} \\
-\frac{1}{2} \alpha_{11}
\end{bmatrix}
\]

(3.81)

The relationships between the backstress and its corresponding conjugate force given by Eqs. (3.30) and (3.32) were defined such that, from Eq. (3.81), the following relation holds:

\[
\begin{bmatrix}
X_{11} \\
X_{22} \\
X_{33}
\end{bmatrix} = \begin{bmatrix}
X_{11} \\
-\frac{1}{2} X_{11} \\
-\frac{1}{2} X_{11}
\end{bmatrix}
\]

(3.82)

The total strain can be written from the additive combination of the elastic strain and the plastic strain as follows:

\[
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33}
\end{bmatrix} = \begin{bmatrix}
\varepsilon_{11}^e + \varepsilon_{11}^p \\
-\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p \\
-\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p
\end{bmatrix}
\]

(3.83)
Utilizing the definition of a deviatoric tensor, the relative stress tensor given by Eq. (3.43) can be written in the following form:

\[
\begin{bmatrix}
\xi_{11} \\
\xi_{22} \\
\xi_{33}
\end{bmatrix} = \left( \frac{2}{3} \sigma_{11} - X_{11} \right) \begin{bmatrix}
1 \\
-\frac{1}{2} \\
-\frac{1}{2}
\end{bmatrix}
\]  
(3.84)

From the definition of the norm, the yield condition given by Eq. (3.51) can now be written for the uniaxial loading case as follows:

\[
f = \sqrt{\frac{2}{3} \left[ \sigma_{11} - \frac{3}{2} X_{11} \right] - \left( \sigma_{sp} + R \right)} \leq 0
\]  
(3.85)

If plasticity occurs with loading, i.e. if \( \dot{\lambda}^p > 0 \), then the normals to the yield surface which will be required to compute the inverse elasto-plastic modulus can be written as follows:

\[
\{f_{,\sigma}\} = \frac{\{\xi\}}{\|\xi\|} = \sqrt{\frac{2}{3}} \begin{bmatrix}
1 \\
-\frac{1}{2} \\
-\frac{1}{2}
\end{bmatrix}
\]  
(3.86)

\[
f_{,r} = -\sqrt{\frac{2}{3}}
\]  
(3.87)

\[
\{f_{,X}\} = -\frac{3}{2} \{f_{,\sigma}\}
\]  
(3.88)

The relation between the increment of the uniaxial stress and the increment of uniaxial strain can be found from the inverse of the constitutive relation, Eq. (3.74):

\[
D_{1111}^{\text{sp}} \dot{\sigma}_{11} = \dot{\epsilon}_{11}
\]  
(3.89)

where the inverse elasto-plastic modulus can be defined for the uniaxial case as follows:

\[
\left[ D^{\text{sp}} \right] = \frac{1}{E} \begin{bmatrix}
1 & -\nu & -\nu \\
-\nu & 1 & -\nu \\
-\nu & -\nu & 1
\end{bmatrix} + \frac{2}{3H} \begin{bmatrix}
1 & -\frac{1}{2} & -\frac{1}{2} \\
-\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
-\frac{1}{2} & \frac{1}{4} & \frac{1}{4}
\end{bmatrix}
\]  
(3.90)

The hardening modulus, \( H \), used in this inverse modulus is defined from Eq. (3.63):

\[
H = \frac{2}{3} \frac{\partial R(r)}{\partial r} + \frac{2}{4} \frac{\partial X_{11}}{\partial \alpha_{11}}
\]  
(3.91)
where the following definition of the derivative of the kinematic hardening conjugate force with respect to the backstress was also used:

\[
\frac{\partial X(\alpha)}{\partial \alpha} = \frac{\partial X_{11}}{\partial \alpha_{11}} \begin{bmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & 1 \\ -\frac{1}{2} & 1 & 1 \end{bmatrix}
\]  

(3.92)

Thus, a relation can be obtained between the total incremental strain and the uniaxial stress:

\[
\bar{\sigma}_{11} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{E + \frac{2}{3H}} \end{bmatrix} \dot{\epsilon}_{11}
\]  

(3.93)

Note that this last relation holds when plasticity occurs, i.e. when \( f \geq 0 \). Otherwise, Eq. (3.93) becomes an elastic strain relation where \( \bar{\sigma}_{11} = E \dot{\epsilon}_{11} \).

### 3.3 Conjugate Force Definitions

Now that the constitutive model has been derived, the definitions of the conjugate forces are revisited here in order to demonstrate the applicability of the material models used. In order to understand how these relationships can be defined, various models for defining the isotropic hardening conjugate force and the kinematic hardening conjugate force will be considered, and it will be shown the hardening models take the form of standard models from the literature.

#### 3.3.1 Linear Isotropic Hardening Model

The simplest case in plasticity hardening is to assume a linear hardening model such that the isotropic hardening conjugate force is a linear function of the equivalent plastic strain:

\[
\dot{R} = a \dot{\varepsilon}_{eq}^p
\]  

(3.94)

where the coefficient \( a \) is a constant derived from a simple monotonic uniaxial curve. In order to obtain this linear model using the model presented in this chapter, a linear state law is utilized for the isotropic hardening as defined by setting \( m_r = 1 \) in Eq. (3.29). By taking the time derivative of this equation, and utilizing the evolution equation, Eq. (3.56), the evolution equation of the isotropic hardening conjugate force is obtained in the desired form:
\[
\dot{R} = H_r \dot{\varepsilon}_p^H
\]  
(3.95)

where the previously defined coefficient, \( a \), is defined to be equal to the linear coefficient, \( H_r \).

The derivative of the linear state law with respect to the isotropic hardening state variable to be used in Eq. (3.63) is defined as follows:

\[
\frac{\partial R}{\partial r} = H_r
\]  
(3.96)

Using an incremental scheme for the evolution of the isotropic hardening, Eq. (3.56) and the uniaxial constitutive relationship given by Eq. (3.93), the resulting stress-strain behavior for this type of material can be plotted. As an example, consider a material with a Young’s modulus \( E = 11920 \text{N/mm}^2 \), a Poisson’s ratio \( \nu = 0.49 \), and no kinematic hardening. In Figure 3.3, the stress-strain curve is plotted for both an isotropic hardening material and an isotropic softening material:

![Stress-strain curve](image)

**Figure 3.3**: Stress-strain curve for a material behaving according to the linear state law for isotropic hardening and softening.
Hardening
\[
(\sigma_{yp}, H_R) = \left( 100 \text{N/mm}^2, 600 \text{N/mm}^2 \right)
\] (3.97)

Softening
\[
(\sigma_{yp}, H_R) = \left( 100 \text{N/mm}^2, -600 \text{N/mm}^2 \right)
\] (3.98)

3.3.2 Chaboche Isotropic Hardening Model

Chaboche (1989) introduced a nonlinear relationship between the isotropic hardening and the equivalent plastic strain such that:

\[
\dot{R} = a (b - R) \dot{\varepsilon}_p^p
\] (3.99)

In order to obtain this Chaboche model using the model presented in this chapter, the exponential state law is utilized for the isotropic hardening as defined by Eq. (3.31). Differentiating this equation gives the following evolution of the isotropic hardening conjugate force:

![Stress-strain curve for a material behaving according to the exponential state law corresponding to the Chaboche isotropic hardening model.](image)

**Figure 3.4:** Stress-strain curve for a material behaving according to the exponential state law corresponding to the Chaboche isotropic hardening model.
\[
\dot{R} = R_e \gamma_r e^{-\gamma r_r} \dot{r}_{eq} 
\]

(3.100)

Use of the original state law, Eq. (3.31), and the evolution equation, Eq. (3.56), results in the desired form depicted by Eq. (3.99):

\[
\dot{R} = \gamma_r (R_e - R) \dot{\varepsilon}_{eq}^p 
\]

(3.101)

Thus, the Chaboche model has been derived where the previously defined coefficient, \(a\), is defined to be equal to \(\gamma_r\) and the coefficient \(b\) is defined to be equal to \(R_e\). These coefficients can be determined from a plot of \(R\) versus \(r\) such that the coefficient \(R_e\) is the saturation stress at large values of \(r\) and the combination of coefficients \(R_e \gamma_r\) is the initial slope of the curve near \(\varepsilon_{eq}^p = 0\).

The derivative of the linear state law with respect to the isotropic hardening state variable to be used in Eq. (3.63) is defined as follows:

\[
\frac{\partial R}{\partial r} = R_e \gamma_r e^{-\gamma r_r} 
\]

(3.102)

Using an incremental scheme for the evolution of the isotropic hardening, Eq. (3.56) and the uniaxial constitutive relationship given by Eq. (3.93), the resulting stress-strain behavior for this type of material can be plotted. As an example, consider a material with a Young’s modulus \(E = 11920 \text{ N/mm}^2\), a Poisson’s ratio \(\nu = 0.49\), and no kinematic hardening. In Figure 3.4, the stress-strain curve is plotted for both an isotropic hardening material and an isotropic softening material with the following parameters:

**Hardening**

\[
(\sigma_{yp}, R_e, \gamma_r) = (100 \text{ N/mm}^2, 100 \text{ N/mm}^2, 10.0) 
\]

(3.103)

**Softening**

\[
(\sigma_{yp}, R_e, \gamma_r) = (100 \text{ N/mm}^2, -100 \text{ N/mm}^2, 10.0) 
\]

(3.104)

3.3.3 Prager Kinematic Hardening Model

The Prager model (1956) was introduced to describe the motion of the yield surface such that the yield surface translates linearly with the plastic strain. Thus, the evolution of the back-stress can be defined by the following relationship:

\[
\dot{X} = a \dot{\varepsilon}_p 
\]

(3.105)
where the coefficient $a$ is a constant derived from a simple monotonic uniaxial curve. In order to obtain this Prager model using the model presented in this chapter, a linear state law is utilized for the kinematic hardening as defined by setting $m_a = 1$ in Eq. (3.30). By taking the time derivative of this equation, and utilizing the evolution equation, Eq. (3.57), the evolution equation of the kinematic hardening conjugate force is obtained in the desired form:

$$\dot{X} = H_a \dot{\varepsilon}$$

(3.106)

where the previously defined coefficient, $a$, is defined to be equal to the presented model’s linear coefficient, $H_a$.

The derivative of the linear state law with respect to the isotropic hardening state variable to be used in Eq. (3.63) is defined as follows:

$$\frac{\partial X}{\partial a} = H_a$$

(3.107)

Using an incremental scheme for the evolution of the isotropic hardening, Eq. (3.56)

---

**Figure 3.5**: Stress-strain curve for a material behaving according to the linear state law corresponding to the Prager kinematic hardening model.
and the uniaxial constitutive relationship given by Eq. (3.93), the resulting stress-strain behavior for this type of material can be plotted. As an example, consider a material with a Young’s modulus $E = 11920 \, N/\text{mm}^2$, a Poisson’s ratio $\nu = 0.49$, and no isotropic hardening. In Figure 3.5, the stress-strain curve is plotted for both a kinematic hardening material and a kinematic softening material with the following parameters:

$$\left(\sigma_{yp}, H_\alpha\right) = \left(100 \, N/\text{mm}^2, 600 \, N/\text{mm}^2\right)$$  (3.108)

$$\left(\sigma_{yp}, H_\alpha\right) = \left(100 \, N/\text{mm}^2, -600 \, N/\text{mm}^2\right)$$  (3.109)

### 3.3.4 Armstrong - Frederick Kinematic Hardening Model

The Armstrong & Frederick model (1956) was introduced to describe the motion of the yield surface, to simulate the multiaxial Bauschinger effect, and to introduce non-linear hardening. Its kinematic hardening rule was predicted by the following expression:

$$\dot{X} = a \dot{\varepsilon}^{\text{eq}} - b \dot{\varepsilon}^{\text{eq}} X$$  (3.110)

where the constants $a$ and $b$ are determined from uniaxial tests. In order to obtain this Armstrong-Frederick model using the model presented in this chapter, either a power or an exponential state law is utilized for the kinematic hardening as defined by Eqs. (3.30) and (3.32), respectively. By taking the time derivative of these equations, the following evolution equations are obtained:

**Power:**

$$\dot{X} = H_\alpha \left[ \|\alpha\|^\mu_\alpha - \dot{\varepsilon}^{\text{eq}} - H_\alpha \left(1 - m_\alpha\right) \|\alpha\|^\mu_\alpha \left(\alpha : \dot{\alpha}\right) \right]$$  (3.111)

**Exponential:**

$$\dot{X} = X \left[ \frac{\dot{\alpha}}{\|\alpha\|} - \frac{\alpha}{\|\alpha\|^2} \left(\alpha : \dot{\alpha}\right) \right] \left(1 - e^{-\gamma \varepsilon}\right) + \left(\gamma_\alpha \frac{\alpha}{\|\alpha\|} \left(e^{-\gamma \varepsilon}\right) \left(\alpha : \dot{\alpha}\right)ight)$$  (3.112)

subject to the constraint that $\dot{X} = 0$ when $\|\alpha\| = 0$.

Use of the original state laws, Eqs. (3.30) and (3.32), and the evolution equation, Eq. (3.57), results in the desired forms for the evolution of the kinematic hardening:
Power:
\[
\dot{\mathbf{X}} = \left[ H_\alpha \|\mathbf{a}\|^{\nu_\alpha - 1} \right] \dot{\mathbf{e}}^p - \left( 1 - m_\alpha \right) \left( \frac{\mathbf{a}}{\|\mathbf{a}\|} : \frac{\dot{\mathbf{e}}_\text{eq}^p}{\dot{\mathbf{e}}^p} \right) \mathbf{X}^p \mathbf{X}
\] (3.113)

Exponential:
\[
\dot{\mathbf{X}} = X_\alpha \left( 1 - e^{-\gamma_\alpha \|\mathbf{a}\|} \right) \dot{\mathbf{e}}^p - \left( 1 - e^{-\gamma_\alpha \|\mathbf{a}\|} \left( 1 + \|\mathbf{a}\| \gamma_\alpha \right) \right) \left( \frac{\mathbf{a}}{\|\mathbf{a}\|} : \frac{\dot{\mathbf{e}}_\text{eq}^p}{\dot{\mathbf{e}}^p} \right) \mathbf{X}^p \mathbf{X}
\] (3.114)

Thus, a modified form of the Armstrong-Frederick given by Eq. (3.110) has been derived. In this form, the coefficients are no longer constant. The coefficient \( a \) is now a function of the norm of the kinematic hardening flux variable, \( \|\mathbf{a}\| \), such that:

Power:
\[
a = H_\alpha \|\mathbf{a}\|^{\nu_\alpha - 1} \] (3.115)

Exponential:
\[
a = X_\alpha \left( 1 - e^{-\gamma_\alpha \|\mathbf{a}\|} \right) \] (3.116)

and the coefficient, \( b \), is now a function of the kinematic hardening flux variable, \( \mathbf{a} \); its norm, \( \|\mathbf{a}\| \); and the evolutions of the plastic strain, \( \dot{\mathbf{e}}^p \), and accumulated plastic strain, \( \dot{\mathbf{e}}_\text{eq}^p \), such that:

Power:
\[
b = \left( 1 - m_\alpha \right) \left( \frac{\mathbf{a}}{\|\mathbf{a}\|} : \frac{\dot{\mathbf{e}}_\text{eq}^p}{\dot{\mathbf{e}}^p} \right) \] (3.117)

Exponential:
\[
b = \left( 1 - e^{-\gamma_\alpha \|\mathbf{a}\|} \left( 1 + \|\mathbf{a}\| \gamma_\alpha \right) \right) \left( \frac{\mathbf{a}}{\|\mathbf{a}\|} : \frac{\dot{\mathbf{e}}_\text{eq}^p}{\dot{\mathbf{e}}^p} \right) \] (3.118)

The derivatives of the exponential and power state laws with respect to the kinematic hardening state variable to be used in Eq. (3.63) are defined as follows:

Power:
\[
\frac{\partial \mathbf{X}}{\partial \mathbf{a}} = H_\alpha \|\mathbf{a}\|^{\nu_\alpha - 1} \mathbf{1} \mathbf{1} + H_\alpha \left( m_\alpha - 1 \right) \|\mathbf{a}\|^{\nu_\alpha - 1} \mathbf{a} \mathbf{a}
\] (3.119)
Exponential:
\[
\frac{\partial X}{\partial \alpha} = X_\alpha \left\{ \frac{1}{\|\alpha\|} \left( \frac{1}{\|\alpha\|} \right) \left( 1 - e^{-\gamma_\alpha \|\alpha\|} \right) + X_\alpha \gamma_\alpha \left( \frac{1}{\|\alpha\|} \right) \left( e^{-\gamma_\alpha \|\alpha\|} \right) \right\} (3.120)
\]

subject to the constraint that $\dot{X} = 0$ when $\|\alpha\| = 0$.

Of further interest is the case of a uniaxial tension/compression loading as discussed in Section 3.2.8. For the reduced form of the backstress flux tensor given in Eq. (3.81), the following relationships can be used:

\[
\|\alpha\| = \sqrt{\alpha_{11}^2 + \alpha_{22}^2 + \alpha_{33}^2} = \sqrt{\frac{3}{2}} \alpha_{11} \quad (3.121)
\]
\[
\alpha : \dot{\alpha} = \alpha_{11} \dot{\alpha}_{11} + \alpha_{22} \dot{\alpha}_{22} + \alpha_{33} \dot{\alpha}_{33} = \frac{3}{2} \alpha_{11} \dot{\alpha}_{11} \quad (3.122)
\]

These relations allow the evolution equations for the kinematic hardening in a 1D state to be written in terms of the uniaxial components as follows:

**Power:**
\[
\dot{X}_{11} = H_{\alpha}^{m_0} m_\alpha \left( \sqrt{\frac{3}{2}} X_{11} \right)^{m_\alpha - 1} \dot{\varepsilon}_{eq} \quad (3.123)
\]

**Exponential:**
\[
\dot{X}_{11} = \gamma_\alpha \left( X_\alpha - \sqrt{\frac{3}{2}} X_{11} \right) \dot{\varepsilon}_{eq} \quad (3.124)
\]

It is important to note that Eq. (3.124), the nonlinear kinematic hardening evolution rule for a 1D state, is identical to the 1D form of the Armstrong-Frederick equation.

The uniaxial forms of the derivatives of the exponential and power state laws with respect to the kinematic hardening state variable to be used in Eq. (3.63) are defined as follows:

**Power:**
\[
\frac{\partial X_{11}}{\partial \alpha_{11}} = m_\alpha H_{\alpha} \left( \sqrt{\frac{3}{2}} \alpha_{11} \right)^{m_\alpha - 1} \quad (3.125)
\]

**Exponential:**
\[
\frac{\partial X_{11}}{\partial \alpha_{11}} = X_\alpha \gamma_\alpha e^{-\gamma_\alpha \sqrt{\frac{3}{2}} \alpha_{11}} \quad (3.126)
\]
Using an incremental scheme for the evolution of the isotropic hardening, Eq. (3.56) and the uniaxial constitutive relationship given by Eq. (3.93), the resulting stress-strain behavior for this type of material can be plotted. As an example, consider a material with a Young’s modulus \( E = 11920 \, N/mm^2 \), a Poisson’s ratio \( \nu = 0.49 \), and no isotropic hardening. In Figure 3.6, the stress-strain curve is plotted for both a kinematic hardening material and an kinematic softening material with the following parameters:

\[
\text{Hardening} \quad \left( \sigma_{yp}, X, \gamma_a \right) = \left( 100 \, N/mm^2, 100 \, N/mm^2, 10.0 \right)
\]  

(3.127)

\[
\text{Softening} \quad \left( \sigma_{yp}, X, \gamma_a \right) = \left( -100 \, N/mm^2, 100 \, N/mm^2, 10.0 \right)
\]  

(3.128)

### 3.4 Rate Boundary Value Problem

In the analysis of a 3D small deformation plasticity rate boundary value problem, the body has a plastic region, \( V_p \), and an elastic region outside of this zone. \( V \) denotes the

![Figure 3.6: Stress-strain curve for a material behaving according to the exponential state law corresponding to the Armstrong-Frederick kinematic hardening model.](image-url)
total domain. The rate boundary value problem in the strong form is described by the following governing equations:

**Equilibrium equation:**
\[ \nabla \cdot \sigma + b = 0 \]  \hspace{1cm} (3.129)

**Applied tractions boundary condition**
\[ n \cdot \sigma + t = 0 \text{ on } \Gamma_t \]  \hspace{1cm} (3.130)

**Applied displacements boundary condition**
\[ u = \bar{u} \text{ on } \Gamma_u \]  \hspace{1cm} (3.131)

where \( \Gamma_t \) is the boundary over which tractions, \( \hat{t} \), are applied, \( \Gamma_u \) is the boundary over which displacements, \( \bar{u} \), are applied, and \( b \) are body forces. In this local model using finite elements, only the equilibrium equation is required in order to obtain a unique solution of the boundary value problem. The weak form of the equilibrium equation can be written by multiplying Eq. (3.129) by a virtual displacement rate vector, \( \delta \bar{u} \), and integrating. The equilibrium equation is integrated over the entire body:

\[ \int_V \delta \bar{u} \cdot (\nabla \cdot \sigma + b) dV = 0 \]  \hspace{1cm} (3.132)

Integrating by parts the weak form of the equilibrium equation gives the following:

\[ \int_V \delta \dot{\varepsilon} : C^e : (\dot{\varepsilon} - f^e \dot{\lambda}^p) dV - \int_V \delta \bar{u} \cdot b dV - \int_{\Gamma_t} \delta \bar{u} \cdot \hat{t} d\Gamma = 0 \]  \hspace{1cm} (3.133)

**3.5 INTEGRATION ALGORITHM**

In the solution procedure, a linearized form of the governing equation given by Eq. (3.133) is solved within an incremental iterative Newton-Raphson solution procedure for the increment of strain over the time increment \( \Delta t_j \) such that:

\[ \varepsilon_j = \varepsilon_0 + \Delta t_j \dot{\varepsilon} = \varepsilon_0 + \Delta \varepsilon_j \]  \hspace{1cm} (3.134)

where the subscripted \( j \)'s and 0 indicate that the variable is computed at iteration \( j \) and at the previously converged state, respectively; and the symbol \( \Delta \) denotes a total increment from the previously converged state to the iteration, \( j \). The increment of the plastic multiplier, \( \Delta \lambda_j^p \), is then computed, and the state of the material is updated such that:
\[ \theta_j^p = \sigma_j^0 + \Delta \theta_j^p \]  
\[ r_j = r_j^0 + \Delta r_j \]  
\[ a_j = a_j^0 + \Delta a_j \]  
\[ \sigma_j = C^e : (\epsilon_j - \epsilon_j^0) = \sigma_j^0 + C^e : (\Delta \epsilon_j - \Delta \epsilon_j^p) \]  

Early computational work would update the state using the plastic multiplier from Eq. (3.62), \( \lambda_0^p \), such that the increment of the plastic multiplier over the time increment \( \Delta t_j \) would be computed as:

\[ \Delta \lambda_j^p = \hat{\lambda}_0^p \Delta t_j = \frac{\Delta t_j}{h_0} f_{s_0} : C^e : \Delta \epsilon \]  

where \( h_0 \) is written as:

\[ h_0 = f_{\sigma_0} : C^e : f_{\sigma_0} + f_{r_0}^2 \frac{\partial R (r_0)}{\partial r} + f_{\sigma_0} \frac{\partial X (\sigma_0)}{\partial \sigma} : f_{\sigma_0} \]  

and the unit normal, \( f_{s_0} \), is computed based on the state at the beginning of the time step. Based on this increment, the state would be updated for a plastic state using a simple forward Euler integration scheme where the increments in Eqs. (3.135) to (3.137) are defined as follows:

\[ \Delta \epsilon_j^p = f_{\sigma_0} \Delta \lambda_j^p \]  
\[ \Delta r_j = -f_{r_0} \Delta \lambda_j^p \]  
\[ \Delta a_j = f_{\sigma_0} \Delta \lambda_j^p \]  

In this scheme, it is not enforced that the yield condition at the end of the time step (time \( j \)) is zero such that the solution will tend to drift from the yield surface producing inaccurate solutions. In order to obtain more accurate solutions, integration schemes must be used which enforce that \( f_j = 0 \) at the end of the time step:

\[ F_j = f_j = \| \xi_j \| - \sqrt{\frac{2}{3}} \left[ \sigma_{ij} + R_j \right] = 0 \]  

where the relative stress and the deviatoric stress tensors are defined as:

\[ \xi_j = s_j - X_j \]  
\[ s_j = \left( I - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right) : \sigma_j = 2 \mu^e \epsilon_j^e \]  

and the conjugate forces are defined as functions of the state variables such that:
\[ R_j = R \left( r_j \right) \quad \text{(3.147)} \]
\[ X_j = X \left( a_j \right) \quad \text{(3.148)} \]

In order to address this type of problem, a return mapping algorithm is used. This algorithm has an initial elastic-predictor step, followed by a plastic-corrector step. In the elastic-predictor step, the incremental strains are assumed to be elastic such that an initial trial stress can be computed as:

\[ \sigma_{\text{trial}}^j = \sigma_0 + C^e : \Delta \epsilon_j \quad \text{(3.149)} \]

The trial state \( \left( \sigma_{\text{trial}}^j, \epsilon_0^p, r_0, a_0 \right) \) is then used to decide whether an elastic point enters the plastic regime or whether a plastic point elastically unloads through a trial yield criterion. For the case when \( f_{\text{trial}} \leq 0 \), the integration point is assumed to be elastic and the current state \( \left( \sigma_j, \epsilon_j^p, r_j, a_j \right) \) is set to the trial state \( \left( \sigma_{\text{trial}}^j, \epsilon_0^p, r_0, a_0 \right) \). Alternatively, when \( f_{\text{trial}} > 0 \), the current state resulting from this trial state lies outside of the yield surface. Plasticity has occurred and the state has to be returned to the yield surface. Using the definition of the Cauchy stress from Eq. (3.138) along with the definition of the trial stress, Eq. (3.149), the Cauchy stress is corrected as follows:

\[ \sigma_j = \sigma_{\text{trial}}^j - C^e : \Delta \epsilon_j^p \quad \text{(3.150)} \]

Thus, the correction to the stress during the plastic-corrector phase is defined as:

\[ \Delta \sigma_j = -C^e : \Delta \epsilon_j^p \quad \text{(3.151)} \]

While the trial stress is computed based upon the increment of the total strain, this plastic corrector is computed based upon the increment of the plastic multiplier which is computed based on the integration scheme used. In this scheme, the increment of the plastic multiplier is initially set to zero \( \left( \Delta \lambda_j^p(0) = 0 \right) \). At each iteration, \( k \), the plastic multiplier is then incremented by \( d \lambda_j^p(k) \) such that:

\[ \Delta \lambda_j^p(k+1) = \Delta \lambda_j^p(k) + d \lambda_j^p(k) \quad \text{(3.152)} \]

This increment is computed by using a linearized form of the nonlinear equation, \( f \left( \Delta \lambda_j^p \right) \), such that:
This iterative procedure is followed until the state computed from the plastic multiplier converges. This occurs when the stress has returned to the yield surface.

### 3.5.1 Fully Implicit Backward Euler Scheme

An implicit backward Euler scheme as presented in Belytschko et al. (2000) is used for the integration of the constitutive model. This type of integration scheme is implicit (computed at time \( j \)) in the plasticity multiplier, the plastic strain, the hardening variables, and the plastic flow direction. The integration scheme is defined by Eqs. (3.134) to (3.138) and Eq. (3.144), where the increments of the state variables are written as follows:

\[
\Delta e^p_j = f_\sigma \Delta \lambda^p_j \tag{3.154}
\]

\[
\Delta r_j = -f_{,R_j} \Delta \lambda^p_j \tag{3.155}
\]

\[
\Delta a_j = f_\sigma \Delta \lambda^p_j \tag{3.156}
\]

It can be seen that the problem defined by this model can be entirely defined by solving for two unknowns, \( \Delta \sigma_j \) and \( \Delta \lambda^p_j \), through the use of the following two nonlinear equations defined from Eqs. (3.154) and (3.144):

\[
a_j = -\varepsilon_j^p + \varepsilon_j^o + f_\sigma \Delta \lambda^p_j = 0 \tag{3.157}
\]

\[
f_j = \left\| \xi_j \right\| - \sqrt{\frac{2}{3}} \left[ \sigma_{yp} + R_j \right] = 0 \tag{3.158}
\]

Making use of Eq. (3.151), these two equations can be linearized as in Eq. (3.153) such that, for each iteration \( k \), the following equations hold:

\[
a_j^{(k)} + C^{-e} : d\sigma_j^{(k)} + df_{,\sigma_j}^{(k)} \Delta \lambda_j^{p(k)} + f_{,\lambda_j}^{(k)} d \lambda_j^{p(k)} = 0 \tag{3.159}
\]

\[
f_j^{(k)} + f_{,\sigma_j}^{(k)} : d\sigma_j^{(k)} + f_{,\lambda_j}^{(k)} d \lambda_j^{p(k)} = 0 \tag{3.160}
\]

where the normals to the yield surface are defined as:

\[
f_{,\sigma_j}^{(k)} = \left( \frac{\partial f}{\partial \sigma_{,j}} \right)^{(k)} = \frac{\xi_j^{(k)}}{\left\| \xi_j^{(k)} \right\|} \tag{3.161}
\]

\[
f_{,\lambda_j^{p}}^{(k)} = \left( \frac{\partial f}{\partial \lambda_j^{p(k)}} \right)^{(k)} = -f_{,R_j}^{(k)} \frac{\partial R_j^{(k)}}{\partial \rho} - f_{,\sigma_j}^{(k)} \frac{\partial X_j^{(k)}}{\partial a_j} : f_{,\sigma_j}^{(k)} \tag{3.162}
\]
The increment of the stress normal can be expanded in terms of the increments of the unknowns such that:

\[
df_{\sigma_j}^{(k)} = \left( \frac{\partial f_{\sigma}}{\partial \sigma} \right)_j : d\sigma_j^{(k)} + \left( \frac{\partial f_{\sigma}}{\partial \Delta \lambda^p} \right)_j d\lambda_j^{(k)}
\]  

\text{(3.163)}

where:

\[
\left( \frac{\partial f_{\sigma}}{\partial \sigma} \right)_j = \left( \frac{\partial f_{\sigma}}{\partial \xi} \right)_j = \frac{I - f_{\sigma_j}^{(k)} \otimes f_{\sigma_j}^{(k)}}{\sigma_j} = f_{\sigma_j, \sigma_j}^{(k)}
\]

\text{(3.164)}

\[
\left( \frac{\partial f_{\sigma}}{\partial \Delta \lambda^p} \right)_j = -f_{\sigma_j, \sigma_j}^{(k)} : \frac{\partial \mathbf{X} (a_j^{(k)})}{\partial \sigma} : f_{\sigma_j}^{(k)} = f_{\sigma_j, \Delta \lambda^p_j}^{(k)}
\]

\text{(3.165)}

After substituting Eq. (3.163) into Eq. (3.159), the increment of the stress can be solved for as follows:

\[
d\sigma_j^{(k)} = -\mathbf{A}_j^{(k)} : \mathbf{a}_j^{(k)} - \mathbf{A}_j^{(k)} : \mathbf{A}_j^{(k)} d\lambda_j^{(k)}
\]

\text{(3.166)}

where:

\[
\mathbf{A}_j^{(k)} = \left[ \mathbf{C}^{-1} + f_{\sigma_j, \sigma_j}^{(k)} \Delta \lambda_j^{(k)} \right]^{-1}
\]

\text{(3.167)}

\[
\mathbf{A}_j^{(k)} = f_{\sigma_j}^{(k)} + f_{\sigma_j, \Delta \lambda_j}^{(k)} \Delta \lambda_j^{(k)}
\]

\text{(3.168)}

This increment of stress can now be substituted into the linearized yield condition, Eq. (3.160). The resulting equation is then solved for \( d\lambda_j^{(k)} \) such that:

\[
d\lambda_j^{(k)} = \frac{f_j^{(k)} - f_{\sigma_j}^{(k)} : \mathbf{A}_j^{(k)} : \mathbf{a}_j^{(k)}}{f_{\sigma_j}^{(k)} : \mathbf{A}_j^{(k)} : f_j^{(k)} + f_{\sigma_j, \Delta \lambda_j}^{(k)} \Delta \lambda_j^{(k)}} - f_{\Delta \lambda_j}^{(k)}
\]

\text{(3.169)}

Thus, the increments of the unknown stress and the unknown plastic multiplier have been derived at iteration \( k \). Using these increments from Eqs. (3.166) and (3.169), the unknowns are updated as follows:

\[
\Delta \lambda_j^{(k+1)} = \Delta \lambda_j^{(k)} + d\lambda_j^{(k)}
\]

\text{(3.170)}

\[
\sigma_j^{(k+1)} = \sigma_j^{(k)} + d\sigma_j^{(k)}
\]

\text{(3.171)}
and the state variables are updated as follows:

\[
\begin{align*}
\epsilon^{p(k+1)}_j &= \epsilon^{p(k)}_j - C^{-e} : d\sigma^{(k)}_j \\
r^{(k+1)}_j &= r^{(k)}_j + f_{\delta_j}^{p(k)} d\lambda^{p(k)}_j \\
\alpha^{(k+1)}_j &= \alpha^{(k)}_j - C^{-e} : d\sigma^{(k)}_j
\end{align*}
\] (3.172)

The Newton iteration procedure is repeated until convergence is obtained by checking \( a_j \) and \( f_j \) from Eqs. (3.157) and (3.158). An algorithm for this solution procedure is given in Table 3.1.

### 3.5.2 Consistent Tangent Operator

The trial stress can be used to predict if an integration point has entered the plastic regime, and the internal state variables can then be updated using the integration scheme. In order to obtain proper quadratic convergence, the choice of a tangent operator must be consistent with the integration scheme. The consistent tangent operator is defined as follows (e.g. Simo & Taylor, 1985):

\[
D^{\text{alg}}_j = \left( \frac{d\sigma}{d\epsilon} \right)_j
\] (3.175)

Following the procedure given in Belytschko et al. (2000), the following set of equations are used which corresponds to the integration scheme of the previous section:

\[
\begin{align*}
d\sigma_j &= C^e : (d\epsilon_j - d\epsilon^p_j) \\
d\epsilon^p_j &= df_{\sigma_j} \Delta \lambda^p_j + f_{\sigma_j} d\lambda^p_j \\
df_j &= f_{\sigma_j} : d\sigma_j + f_{\delta_j} d\lambda^p_j = 0
\end{align*}
\] (3.176) (3.177) (3.178)

where the normals to the yield surface and the increment of the stress normal are defined by evaluating Eqs. (3.161) to (3.163) at time step \( j \). After substituting the increment of the plastic strain, Eq. (3.177), and the increment of the stress normal, Eq. (3.163) at time step \( j \), into Eq. (3.176), the increment of the stress is solved for such that:

\[
d\sigma_j = A_j : d\epsilon_j - A_j : \left( f_{\sigma_j} + f_{\delta_j} \Delta \lambda^p_j \right) d\lambda^p_j
\] (3.179)

where:

\[
A_j = \left[ C^{-e} + f_{\sigma_j} \Delta \lambda^p_j \right]^{-1}
\] (3.180)
Table 3.1: Fully Implicit Backward Euler Return Algorithm

1. Initialize and compute trial elastic state for iteration $k = 0$

\[
\Delta \lambda_j^{(0)} = 0 \\
\sigma_j^{(0)} = \sigma_j^{\text{trial}} = \sigma_j^0 + C^e : \Delta \varepsilon_j \\
\varepsilon_j^{(0)} = \varepsilon_j^0; \quad r_j^{(k)} = r_j^0; \quad a_j^{(k)} = a_j^0
\]

2. Check convergence for iteration $k$

\[
f_j^{(k)} = \|\varepsilon_j^{(k)}\| - \sqrt{\frac{1}{2} \left[ \sigma_{dp} + R_j^{(k)} \right]} \\
a_j^{(k)} = -\varepsilon_j^{(k)} + \varepsilon_j^0 + f_{\sigma_j}^{(k)} \Delta \lambda_j^{(k)}
\]

IF $f_j^{(k)} < TOL_1$ AND $\|a_j^{(k)}\| < TOL_2$, THEN:

\[
\sigma_j = \sigma_j^{(k)} \\
\varepsilon_j = \varepsilon_j^{(k)}; \quad r_j = r_j^{(k)}; \quad a_j = a_j^{(k)}
\]

EXIT

END IF

3. Compute increments of unknowns

\[
d \lambda_j^{(k)} = \frac{f_j^{(k)} - f_{\sigma_j}^{(k)} : A_j^{(k)} : a_j^{(k)}}{f_{\sigma_j}^{(k)} : A_j^{(k)} : \left( f_{\sigma_j}^{(k)} + f_{\sigma_j, \Delta \lambda_j}^{(k)} \Delta \lambda_j^{(k)} \right) - f_{\sigma_j}^{(k)}} \\
d \sigma_j^{(k)} = -A_j^{(k)} : a_j^{(k)} - A_j^{(k)} : \left( n_{\sigma_j}^{(k)} + f_{\sigma_j, \Delta \lambda_j}^{(k)} \Delta \lambda_j^{(k)} \right) d \lambda_j^{(k)}
\]

4. Update state

\[
\Delta \lambda_j^{(k+1)} = \Delta \lambda_j^{(k)} + d \lambda_j^{(k)} \\
\sigma_j^{(k+1)} = \sigma_j^{(k)} + d \sigma_j^{(k)} \\
\varepsilon_j^{(k+1)} = \varepsilon_j^{(k)} - C^{-e} : d \sigma_j^{(k)} \\
r_j^{(k+1)} = r_j^{(k)} + f_{R_j}^{(k)} d \lambda_j^{(k)} \\
a_j^{(k+1)} = a_j^{(k)} - C^{-e} : d \sigma_j^{(k)} \\
k \leftarrow k + 1, \text{ GO TO 2}
\]
This increment of stress can now be substituted into the incremental consistency condition, Eq. (3.178). The resulting equation is then solved for $d\lambda^e_j$ such that:

$$d\lambda^e_j = \frac{f_{\sigma_j} : A_j : de_j}{f_{\sigma_j} : A_j : \left(f_{\sigma_j} + f_{\sigma_j,\Delta\lambda^e_j} \Delta\lambda^e_j\right) - f_{,\Delta\lambda^e_j}}$$

(3.181)

Substituting the above relation in Eq. (3.179) gives the algorithmic relation between the increment of the stress and the elastic strain as follows:

$$d\sigma_j = D^a_{,j} : de_j$$

(3.182)

where $D^a_{,j}$ is the algorithmic elastic stiffness operator and is defined as follows:

$$D^a_{,j} = A_j - \left( A_j : \left(f_{\sigma_j} + f_{\sigma_j,\Delta\lambda^e_j} \Delta\lambda^e_j\right) \otimes f_{\sigma_j} : A_j \right) \left(f_{\sigma_j} : A_j : \left(f_{\sigma_j} + f_{\sigma_j,\Delta\lambda^e_j} \Delta\lambda^e_j\right) - f_{,\Delta\lambda^e_j}\right)^{-1}$$

(3.183)

In the next section, an algebraic form of the governing equation is formulated using the integration scheme which can be solved within an incremental iterative Newton-Raphson solution.

### 3.6 Finite Element Formulation

In order to solve a boundary value problem, the finite element approach is adopted in this work such that the displacement field is discretized. The algorithm requires a weak satisfaction of the equilibrium condition such that:

$$\int_V \delta u : \left(\nabla \cdot \sigma_j + b_j\right) dV = 0$$

(3.184)

Using integration by parts for the weak form of the equilibrium equation, and substituting the algorithmic relation Eq. (3.182), the governing equation is written as follows:

$$\int_V \delta \varepsilon : D^a_{,j} : de_j dV = \int_v \delta \varepsilon : b_j dV + \int_{\Gamma_e} \delta \varepsilon : \hat{t}_j d\Gamma - \int_V \delta \varepsilon : \sigma_j dV$$

(3.185)

Note that this equation is enforced over the entire body, including both the plastic domain and the elastic domain. In the right hand side of the governing equations, the stress at iteration $j$ must be known. As seen from the integration scheme, for each integration point
in a plastic state, the backward Euler elastic predictor-plastic corrector algorithm is used to compute the stress. The governing equation can be linearized consistently and solved within an incremental iterative Newton-Raphson solution procedure.

The displacement is discretized using a set of displacement nodal degrees of freedom contained in the vector \( \{a_j\} \). As the governing equation only involves first order derivatives of the displacement field (i.e. strains), the discretization procedure for the displacement field only requires \( C^0 \) continuous interpolation functions. The interpolating relation is defined as follows:

\[
\mathbf{u}_j = [N] \{a_j\}
\]  

(3.186)

where \([N]\) contains the set of element interpolating shape functions. By taking appropriate derivatives of Eq. (3.186), the strains are obtained through the following strain-displacement relation:

\[
\varepsilon_j = [B] \{a_j\}
\]  

(3.187)

The derivation of the shape functions, \([N]\), and the strain-displacement matrix, \([B]\), will be shown for one-dimensional and two-dimensional elements in Sections 3.6.1 and 3.6.2. To avoid volumetric locking in plane strain problems, the \( \overline{B} \) as introduced by Hughes (1980) is used.

Using the discretization relations given by Eqs. (3.186) and (3.187), the weak form of the equilibrium equation defined by Eq. (3.185) is now written as follows:

\[
\left\{ \delta a \right\}^T \left[ [B]^T [D^\text{alg}] [B] \right] \{da\} d\mathbf{V}
\]

\[
= \left\{ \delta a \right\}^T \left[ \int_{\mathbf{V}} [N]^T \left\{ b_j \right\} d\mathbf{V} + \int_{\Gamma_i} [N]^T \left\{ \tilde{t}_j \right\} d\Gamma - \int_{\mathbf{V}} [B]^T \left\{ \sigma_j \right\} d\mathbf{V} \right]
\]  

(3.188)

As this governing equation must be admissible for any variation in \( \{\delta a\} \), this equation can be written as a set of algebraic equations:

\[
[K_{aa}] \{da\} = \{f_a\} + [f_a] + [f_b]
\]  

(3.189)

where the sub-matrices are defined as follows:
Diagonal matrices

\[
[K_{aa}] = \int_{V} [B]^T [D^{\text{ele}}] [B] dV
\]  

(3.190)

External force vector and body force vector

\[
[f_e] = \int_{\Gamma} [N]^T \{ \bar{r}_j \} d\Gamma
\]  

(3.191)

\[
[f_b] = \int_{V} [N]^T \{ b_j \} dV
\]  

(3.192)

Vector of nodal forces (equivalent to internal stresses)

\[
[f_{u}] = -\int_{V} [B]^T \{ \sigma_j \} dV
\]  

(3.193)

Thus, the weak form of the governing equation has been written in terms of a stiffness matrix, a vector of degrees of freedom, and a vector of residuals in the standard form used by finite elements. These matrices and vectors can be computed for the elements which discretize a body and accumulated into global matrices and vectors for the entire body. A finite element procedure is then followed to solve the equations. The problem defined by this set of equations is nonlinear as the stiffness and the load residuals are a function of the body deformation. The degrees of freedom thus cannot automatically be solved from the system of equations. An iterative procedure is thus required to obtain the degrees of freedom such that the left-hand side of the governing equations is in equilibrium with the load vector residuals of the right-hand side. A typical procedure, which is not discussed here but is readily available from the commercial finite element program ABAQUS using the user subroutine UEL, is the Newton-Raphson method; however, other methods such as the modified Newton-Raphson may be used.

### 3.6.1 One-Dimensional Bar Elements

One-dimensional bar elements are defined here for interpolation through a standard procedure for the development of isoparametric finite elements (Taig, 1961; Irons, 1966). In this discussion, shape functions are derived for both a two-node linear interpolating element (Figure 3.7.1, a) and a three-node quadratic interpolating element (Figure 3.7.1, b). In labeling these elements, the first letter ‘C’ indicates a standard continuum stress/displacement element, the second pair ‘1D’ indicates a one-dimensional bar element, and the final number indicates the number of nodes used to discretize the displacements.

The degrees of freedom for these elements are defined by a single axial displacement, \( u_i \), at each node, \( i \). Thus, the elements can be represented by a vector containing the global coordinates for the element and by a vector containing the element degrees of freedom as follows:
Figure 3.7.1: Elements presented in the global coordinate system: (a) two-node linear bar element; (b) three-node quadratic bar element; (c) four-node bi-linear quadrilateral; and (d) eight-node bi-quadratic quadrilateral.

Figure 3.7.2: Elements presented in the natural coordinate system.
The elements considered here are derived using isoparametric formulations such that the same shape functions are used to interpolate the coordinates of the nodes and the displacements:

\[
x = [N] \{c\}
\]
\[
u = [N] \{a\}
\]

where the matrices of shape functions are defined as follows:

**Linear Element**

\[
\{c\} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}
\]
\[
\{a\} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}
\]

**Quadratic Element**

\[
\{c\} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}
\]
\[
\{a\} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}
\]

The interpolation relations of the displacement in Eq. (3.197) utilizing the degrees of freedom defined in Eq. (3.195) are presented in Figure 3.8. In order to derive the shape functions, a natural coordinate system is used as shown in Figure 3.7.2 (a) such that the reference nodal coordinates for nodes 1 and 2 are located at \(\xi = -1\) and \(\xi = +1\), respectively. Though the third node of the quadratic element is not required to be located at mid-length in the global coordinate system, it is located at mid-length \((\xi = 0)\) in the reference coordinate system. Thus, the reference nodal coordinates can be contained in the following vectors:

- Linear Element
  \[
  [N] = \begin{bmatrix} N_1 \\ N_2 \end{bmatrix}
  \]

- Quadratic Element
  \[
  [N] = \begin{bmatrix} N_1 \\ N_2 \\ N_3 \end{bmatrix}
  \]

![Figure 3.8](image.png)

**Figure 3.8**: Plots of the (a) linear and (b) quadratic interpolations of displacements, \(u\), denoting nodal degrees of freedom.
Utilizing this coordinate system, a polynomial is assumed for the discretization of the displacement field such that:

\[ u = \{ \tilde{X} \}^T \{ \tilde{d} \} \]  

(3.200)

where the vector \( \{ \tilde{X} \} \) defines the order of the interpolation and the vector \( \{ \tilde{d} \} \) contains coefficients acting as generalized degrees of freedom for this polynomial. For the two-node element, this polynomial is linear such that these vectors take the following forms:

**Linear Element**

\[ \{ \tilde{X} \} = \{ 1 \ \tilde{\xi} \}^T \]

\[ \{ \tilde{d} \} = \{ \tilde{d}_1 \ \tilde{d}_2 \}^T \]

(3.201)

**Quadratic Element**

\[ \{ \tilde{X} \} = \{ 1 \ \tilde{\xi} \ \tilde{\xi}^2 \}^T \]

\[ \{ \tilde{d} \} = \{ \tilde{d}_1 \ \tilde{d}_2 \ \tilde{d}_3 \}^T \]

(3.202)

In order to write the generalized degrees of freedom in terms of the nodal degrees of freedom, \( \{ a \} \), the following expression is used:

\[ \{ a \} = [ \tilde{A} ] \{ \tilde{d} \} \]  

(3.203)

where each row of this relation is found by evaluating Eq. (3.200) for the corresponding degree of freedom. Thus, the matrix \([ \tilde{A} ]\) is defined as follows:

**Linear Element**

\[ [ \tilde{A} ] = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \]

(3.204)

**Quadratic Element**

\[ [ \tilde{A} ] = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \end{bmatrix} \]

The vector \( \{ \tilde{d} \} \) can now be solved for in Eq. (3.203) and substituted into Eq. (3.200) such that the desired interpolation relation given by Eq. (3.197) is obtained where the set of interpolating functions is defined as follows:

\[ [ N ] = \{ \tilde{X} \}^T [ \tilde{A} ]^{-1} \]  

(3.205)
The solution of this equation gives the components of the shape function matrices as follows:

**Linear Element**

\[ N_i = \frac{1}{2} (1 + \tilde{c}_i \xi) \]

**Quadratic Element (no sum over \( i \))**

\[ \tilde{N}_i = \frac{1}{2} \tilde{c}_i^2 (1 + \tilde{c}_i \xi) + \left(1 - \frac{3}{2} \tilde{c}_i^2 \right)(1 - \xi^2) \]

Plots of each of these component shape functions for each node is given in Figure 3.9. In these plots, it is seen that the shape functions given by Eq. (3.206) have a unit value at their corresponding nodes and a zero value at the other nodes. Each of these curves can

**Figure 3.9**: Plots of shape function components for the (a) linear polynomial and for the (b) quadratic polynomial.
be obtained for the displacement field by applying a unitary value to the displacement
degree of freedom at the node of interest and a zero value to the remaining degrees of
freedom.

The shape functions and displacements can be used to compute the strains in the
element. For the one-dimensional bar case, the strains reduce to a single axial component.
Thus, Eq. (3.187) is reduced to the one-dimensional case as follows:

\[ \varepsilon_x = \frac{du}{dx} = [B]\{a\} \] (3.207)

The strain-displacement matrix can be written in the following form:

\[
\begin{bmatrix}
B
\end{bmatrix}
\begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x}
\end{bmatrix}
\]
(3.208)

The strain-displacement matrix can be written in the following form:

\[
\begin{array}{ccc}
\text{Linear Element} & & \text{Quadratic Element} \\
[B] = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x}
\end{bmatrix} & [B] = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x}
\end{bmatrix}
\end{array}
\]

The shape functions derived previously were defined in terms of the natural
coordinate system. Thus, using the chain rule, the required derivative of the shape
functions with respect to the global coordinate system are written in terms of the
derivative with respect to the natural coordinate system as follows:

\[ \frac{\partial N_i}{\partial x} = \frac{\partial N_i}{\partial \xi} \frac{\partial \xi}{\partial x} = G \frac{\partial N_i}{\partial \xi} \] (3.209)

where the required derivative of the shape functions can be written as follows:

\[
\begin{array}{cc}
\text{Linear Element} & \text{Quadratic Element} \\
\frac{dN_1}{d\xi} = \frac{1}{2} \tilde{c}_i & \frac{dN_1}{d\xi} = \frac{1}{2} \tilde{c}_i - \frac{3}{2} \tilde{c}_i^2 
\end{array}
\]
(3.210)

In order to evaluate Eq. (3.209) utilizing the shape functions defined in the natural
coordinate system, the Jacobian, \( J \), is required which gives the inverse transformation as
follows:

\[ \frac{\partial N_i}{\partial \xi} = J \frac{\partial N_i}{\partial x} = \frac{1}{G} \frac{\partial N_i}{\partial x} \] (3.211)

where, from the chain rule, the Jacobian is defined as follows:

\[ J = \frac{1}{G} = \frac{\partial x}{\partial \xi} \] (3.212)
Utilizing the definition of the coordinates given by Eq. (3.196), the Jacobian can be written as follows:

\[
J = \frac{\partial N_i}{\partial \xi_x} x_i
\]  
(3.213)

### 3.6.2 Two-Dimensional Quadrilateral Elements

Two-dimensional bar elements are defined here for interpolation through a standard procedure for the development of isoparametric finite elements (Taig, 1961; Irons, 1966). In this discussion, the shape functions are derived for both a four-node bi-linear interpolating element (Figure 3.7.1, c) and an eight-node bi-quadratic interpolating element (Figure 3.7.1, d). In labeling these elements, the first letter ‘C’ indicates a standard continuum stress/displacement element, the second pair ‘PE’ indicates a plane-strain quadrilateral element, and the final number indicates the number of nodes used to discretize the displacements.

The degrees of freedom for these elements are defined by a horizontal displacement, \(u_i\), and a vertical displacement, \(v_i\), at each node, \(i\). Thus, for an \(n\)-node element, the element can be represented by a vector containing the global coordinates for the element and by a vector containing the element degrees of freedom as follows:

\[
\{c\} = \{x_1 \ y_1 \ x_2 \ y_2 \ \cdots \ x_n \ y_n\}^T
\]  
(3.214)

\[
\{a\} = \{u_1 \ v_1 \ u_2 \ v_2 \ \cdots \ u_n \ v_n\}^T
\]  
(3.215)

The elements considered here are derived using isoparametric formulations such that the same shape functions are used to interpolate the coordinates of the nodes and the displacements:

\[
x = \begin{bmatrix} x \\ y \end{bmatrix} = [N]\{c\}
\]  
(3.216)

\[
u = \begin{bmatrix} u \\ v \end{bmatrix} = [N]\{a\}
\]  
(3.217)

where the matrix of shape functions is defined as follows:

\[
[N] = \begin{bmatrix}
N_1 & 0 & N_2 & 0 & \cdots & N_n & 0 \\
0 & N_1 & 0 & N_2 & \cdots & 0 & N_n
\end{bmatrix}
\]  
(3.218)

For the derivations that follow, the components of the coordinates and the components of the degrees of freedom are separated for each coordinate axes such that:
\begin{align}
\{c_x\} &= \{x_1 \ x_2 \ \cdots \ x_n\}^T \\
\{c_y\} &= \{y_1 \ y_2 \ \cdots \ y_n\}^T \\
\{a_u\} &= \{u_1 \ u_2 \ \cdots \ u_n\}^T \\
\{a_v\} &= \{v_1 \ v_2 \ \cdots \ v_n\}^T
\end{align}

For this decomposition, the interpolated values of the coordinates of the nodes and the displacements are written as follows:

\begin{align}
x &= \{N^x\}\{c_x\} \\
y &= \{N^y\}\{c_y\} \\
u &= \{N^x\}\{a_u\} \\
v &= \{N^y\}\{a_v\}
\end{align}

where the vector of shape functions is defined as follows:

\begin{align}
\{N^x\} &= \{N_1 \ N_2 \ \cdots \ N_n\}
\end{align}

In order to derive the shape functions, a natural coordinate system is used as shown in Figure 3.7.2 (c) such that a vector of reference nodal coordinates can be defined for the \(\xi\) coordinates and for the \(\eta\) coordinates as follows:

**Bi-Linear Element**

\begin{align}
\{\tilde{c}_x\} &= \{-1 \ +1 \ +1 \ -1\}^T \\
\{\tilde{c}_y\} &= \{-1 \ -1 \ +1 \ +1\}^T
\end{align}

**Bi-Quadratic Element**

\begin{align}
\{\tilde{c}_x\} &= \{-1 \ +1 \ +1 \ -1 \ 0 \ +1 \ 0 \ -1\}^T \\
\{\tilde{c}_y\} &= \{-1 \ -1 \ +1 \ +1 \ -1 \ 0 \ +1 \ 0\}^T
\end{align}

Utilizing this coordinate system, a polynomial is assumed for the discretization of the displacement fields such that:

\begin{align}
u &= \{\tilde{X}\}^T\{\tilde{a}_u\} \\
v &= \{\tilde{X}\}^T\{\tilde{a}_v\}
\end{align}
where the vector \( \{ \tilde{X} \} \) defines the order of the interpolation and the vectors \( \{ \tilde{d}_u \} \) and \( \{ \tilde{d}_v \} \) contains coefficients acting as generalized degrees of freedom for this polynomial.

For the four-node element, the interpolating polynomial is linear in \( \xi \) and in \( \eta \) such that these vectors take the following forms:

**Bi-Linear Element**
\[
\{ \tilde{X} \} = \{ 1 \ \xi \ \eta \ \xi \eta \}^T
\]
\[
\{ \tilde{d}_u \} = \{ \tilde{d}_{u1} \ \tilde{d}_{u2} \ \tilde{d}_{u3} \ \tilde{d}_{u4} \}^T
\]
\[
\{ \tilde{d}_v \} = \{ \tilde{d}_{v1} \ \tilde{d}_{v2} \ \tilde{d}_{v3} \ \tilde{d}_{v4} \}^T
\]

**Bi-Quadratic Element**
\[
\{ \tilde{X} \} = \{ 1 \ \xi \ \eta \ \xi^2 \ \eta^2 \ \xi^2 \eta \ \xi \eta^2 \}^T
\]
\[
\{ \tilde{d}_u \} = \{ \tilde{d}_{u1} \ \tilde{d}_{u2} \ \ldots \ \tilde{d}_{u8} \}^T
\]
\[
\{ \tilde{d}_v \} = \{ \tilde{d}_{v1} \ \tilde{d}_{v2} \ \ldots \ \tilde{d}_{v8} \}^T
\]

In order to write the generalized degrees of freedom, \( \{ \tilde{d}_u \} \) and \( \{ \tilde{d}_v \} \), in terms of the nodal degrees of freedom, \( \{ a_u \} \) and \( \{ a_v \} \), the following expression is used:

\[
\{ a_u \} = [ \tilde{A} ] \{ \tilde{d}_u \}
\]
\[
\{ a_v \} = [ \tilde{A} ] \{ \tilde{d}_v \}
\]

The matrix \([ \tilde{A} ]\) used in both of these relationships are identical and can be found by evaluating either Eq. (3.232) or (3.233) for each of the nodes as follows:

**Bi-Linear Element**
\[
[ \tilde{A} ] = \begin{bmatrix}
+1 & -1 & -1 & +1 \\
+1 & +1 & -1 & -1 \\
+1 & +1 & +1 & +1 \\
+1 & -1 & +1 & -1
\end{bmatrix}
\]

60
Bi-Quadratic Element

\[
\begin{bmatrix}
    +1 & -1 & -1 & +1 & +1 & -1 & -1 \\
    +1 & +1 & -1 & -1 & +1 & +1 & -1 \\
    +1 & +1 & +1 & +1 & +1 & +1 & +1 \\
    +1 & -1 & +1 & -1 & +1 & +1 & -1 \\
    +1 & 0 & -1 & 0 & 0 & +1 & 0 \\
    +1 & +1 & 0 & 0 & +1 & 0 & 0 \\
    +1 & 0 & +1 & 0 & 0 & +1 & 0 \\
    +1 & -1 & 0 & 0 & +1 & 0 & 0 \\
\end{bmatrix}
\]  

(3.243)

The vectors \( \{ \tilde{d}_u \} \) and \( \{ \tilde{d}_v \} \) can now be solved for in Eqs. (3.240) and (3.241) Substitution of the resulting vectors into Eqs. (3.232) and (3.233), the desired interpolation relation given by Eqs. (3.225) and (3.226) is obtained where the interpolating functions are defined as follows:

\[
\{ N^* \} = \{ \tilde{X} \}^T [ \tilde{A} ]^{-1}
\]  

(3.244)

For the four-node bar element, the solution of this equation gives the shape function vector as in Eq. (3.227) with components written as follows:

Bi-Linear Element

\[
N_i = f_{u_i} (\xi) f_{\eta_i} (\eta) \quad \text{(no sum over} \ i) \]  

(3.245)

Bi-Quadratic Element

\[
N_i = f_{u_i} (\xi) f_{\eta_i} (\eta) + f^*_{u_i} (\xi) f_{\eta_i} (\eta) + f_{u_i} (\xi) f^*_{\eta_i} (\eta) \quad \text{(no sum over} \ i) \]  

(3.246)

where these shape functions are written in terms of the following functions:

Bi-Linear Element

\[
f_{u_i} (s) = \frac{1}{2} \left( 1 + \tilde{c}_{u_i} s \right)
\]  

(3.247)

Bi-Quadratic Element

\[
f_{u_i} (s) = \frac{1}{2} \tilde{c}_{u_i}^2 \left( 1 + \tilde{c}_{u_i} s \right) \quad \text{(no sum over} \ i) \]  

(3.248)

\[
f^*_{u_i} (s) = \left( 1 - \frac{3}{2} \tilde{c}_{u_i}^2 \right) (1 - s^2)
\]  

(3.249)
As with the bar elements, the shape functions and displacements can be used to compute the strains in the element. For the case of a plane strain element, the two-dimensional strain matrix can be written in the following form:

\[
\{ \varepsilon \} = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x} \\ 0 \\ \frac{\partial}{\partial x} \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = [B] \{u\}
\]

(3.250)

The strain-displacement matrix can be written in the following form:

\[
[B] = \begin{bmatrix} B_1 & B_2 & \cdots & B_n \end{bmatrix}
\]

(3.251)

where the sub-matrices, \([B_i]\), are evaluated from the following expression:

\[
[B_i] = \begin{bmatrix} \frac{\partial N_i}{\partial x} & 0 \\ 0 & \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial y} & \frac{\partial N_i}{\partial x} \end{bmatrix}
\]

(3.252)

To avoid locking in isochoric deformations, the B matrix is modified for plane strain conditions according to the so-called B-Bar enhancement as introduced by Hughes (1980). This technique is a generalization of the mean-dilatation formulation of Nagtegaal et al. (1974) The main motivation is the development of a finite element scheme that properly accounts for the incompressibility constraint emanating from the volume-preserving nature of plastic flow. In this method, only the dilatational part of the displacement gradient is the independent variable such that the \([B_i]\) matrix is replaced by the \([\bar{B}_i]\) matrix which is defined as follows:

\[
[\bar{B}_i] = [B_i] - [B_{di}] + [\bar{B}_{di}]
\]

\[
= \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \\ B_2 & B_1 \end{bmatrix} - \frac{1}{3} \begin{bmatrix} B_1 & B_2 \\ B_2 & B_1 \\ 0 & 0 \end{bmatrix} + \frac{1}{3} \begin{bmatrix} \bar{B}_1 & \bar{B}_2 \\ \bar{B}_2 & \bar{B}_1 \\ 0 & 0 \end{bmatrix}
\]

(3.253)
where:

\[
\overline{B}_i = \frac{\int_{V_r}^{V} B_i \, dV}{\int_{V_r}^{V} dV}
\]  

(3.254)

The shape functions derived previously were defined in terms of the natural coordinate system. Thus, the required derivatives of the shape functions with respect to the global coordinate system must be written in terms of derivatives with respect to the natural coordinate:

\[
\left\{ \frac{\partial N_i}{\partial \xi} \right\} \left\{ \frac{\partial N_i}{\partial \eta} \right\} = \left[ G \right] \left\{ \frac{\partial N_i}{\partial \xi} \right\} \left\{ \frac{\partial N_i}{\partial \eta} \right\} \quad (3.255)
\]

where, from the chain rule, the transformation matrix is defined as follows:

\[
\left[ G \right] = \begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\
\frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y}
\end{bmatrix}
\]  

(3.256)

and the components of the vectors which define the required derivatives of the shape functions can be written as follows:

**Bi-Linear Element**

\[
\frac{\partial N_i}{\partial \xi} = g_{\xi_i} (\xi) f_{\eta_i} (\eta) \quad (\text{no sum over } i) \quad (3.257)
\]

\[
\frac{\partial N_i}{\partial \eta} = f_{\xi_i} (\xi) g_{\eta_i} (\eta) \quad (\text{no sum over } i) \quad (3.258)
\]

**Bi-Quadratic Element**

\[
\frac{\partial N_i}{\partial \xi} = g_{\xi_i} (\xi) f_{\eta_i} (\eta) + g_{\eta_i} (\xi) f_{\eta_i} (\eta) + f_{\xi_i} (\xi) g_{\eta_i} (\eta) \quad (\text{no sum over } i) \quad (3.259)
\]

\[
\frac{\partial N_i}{\partial \eta} = f_{\xi_i} (\xi) g_{\eta_i} (\eta) + f_{\xi_i} (\xi) g_{\eta_i} (\eta) + f_{\xi_i} (\xi) g_{\eta_i} (\eta) \quad (\text{no sum over } i) \quad (3.260)
\]

where these shape function derivatives are written in terms of previously defined functions, Eqs. (3.247) to (3.249), and the following functions:
Bi-Linear Element
\[ g_s(s) = \frac{1}{2} \hat{c}_s \]  
(3.261)

Bi-Quadratic Element
\[ g_s(s) = \frac{1}{2} \hat{c}_s \]
(3.262)
\[ g_s^*(s) = -2s \left(1 - \frac{3}{2} \hat{c}_s^2\right) \]  
(3.263)

In order to evaluate Eq. (3.255) utilizing the shape functions defined in the natural coordinate system, the Jacobian matrix, \( [J] \), is required which gives the inverse transformation as follows:
\[
\begin{bmatrix}
\frac{\partial N_i}{\partial \xi} \\
\frac{\partial N_i}{\partial \eta}
\end{bmatrix}
= [J]
\begin{bmatrix}
\frac{\partial N_i}{\partial x} \\
\frac{\partial N_i}{\partial y}
\end{bmatrix}
= [G]^{-1}
\begin{bmatrix}
\frac{\partial N_i}{\partial \xi} \\
\frac{\partial N_i}{\partial \eta}
\end{bmatrix}
\]  
(3.264)

where, from the chain rule, the Jacobian matrix is defined as follows:
\[
[J] =
\begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta}
\end{bmatrix}
\]  
(3.265)

Utilizing the definition of the coordinates given by Eq. (3.223) and (3.224), the Jacobian matrix can be written as follows:
\[
[J] =
\begin{bmatrix}
\frac{\partial N_i}{\partial x} & \frac{\partial N_i}{\partial y} \\
\frac{d \xi}{dx} & \frac{d \xi}{dy} \\
\frac{\partial N_i}{\partial \eta} & \frac{\partial N_i}{\partial \eta}
\end{bmatrix}
\begin{bmatrix}
x_i \\
y_i
\end{bmatrix}
= \begin{bmatrix}
J_{11} & J_{12} \\
J_{21} & J_{22}
\end{bmatrix}
\]  
(3.266)

Thus, the transformation matrix, \( [G] \), in Eq. (3.255) can be written as follows:
\[
[G] = [J]^{-1} = \frac{1}{J} \begin{bmatrix}
J_{22} & -J_{12} \\
-J_{21} & J_{11}
\end{bmatrix}
\]  
(3.267)
In this equation, \( J \) is the determinant of the Jacobian matrix and is given by the following expression:

\[
J = J_{11} J_{22} - J_{12} J_{21}
\]  

(3.268)

### 3.7 Conclusions

In this chapter, thermodynamically consistent theoretical formulations and the numerical implementation of a classical continuum plasticity model were presented. Following standard thermodynamics and using local state variables, a complete set of constitutive equations were derived where a local yield surface was used to determine the occurrence of plasticity and hardening conjugate forces (stress like terms) were defined as general functions of their corresponding hardening state variables (strain like terms). A fully implicit backward Euler scheme was developed and a set of governing equations were derived to be solved in a Newton-Raphson solution procedure. The next chapter couples damage with the plasticity framework presented here and gives the thermodynamically consistent theoretical formulations and the numerical implementation for the coupled damage-plasticity model. The framework developed will then be used to derive the gradient enhanced coupled damage-plasticity model.
CHAPTER 4: LOCAL COUPLED PLASTICITY – DAMAGE MODEL

4.1 INTRODUCTION

CHAPTER 3 presented the formulation of a local plasticity model. This type of model works well for fully ductile materials; however, for materials in general and brittle in particular, micro-cracks and micro-voids can develop which are not accounted for in plasticity. In classical fracture mechanics, macro-cracks are modeled discontinuously. Continuum damage mechanics, on the other hand, introduces a continuous damage variable which is used as a measure of micro-cracks and micro-voids. In the simplest case, this damage variable is introduced as a scalar. This scalar measure has been used to adequately solve many mechanics problems in the literature (e.g. Kachanov, 1958; Lemaitre, 1984; etc.). However, in reality, all materials have been shown to accumulate damage anisotropically, and a second order damage tensor is required to properly define the problem.

![Stress-strain curve for a material with coupled plasticity and damage denoting elastic and damage strains.](image)

**Figure 4.1**: Stress – strain curve for a material with coupled plasticity and damage denoting elastic and damage strains.
A simple plot of the uniaxial stress-strain behavior for a material with both coupled plasticity and damage is presented in Figure 4.1. As discussed in CHAPTER 3, plasticity does not begin to occur until after the stress reaches the critical value, $\sigma_{yp}$, at point $n_2$. However, as seen in this plot, the stress-strain curve begins to have a nonlinear behavior once it reaches a critical value, $\sigma_{yd}$, at point $n_1$. This is due to the accumulation of micro-cracks and micro-voids which reduce the elastic stiffness tensor from the original, undamaged elastic stiffness, $E$. After this point, damage begins to accumulate. Removal of the external loading conditions at a point before or at point $n_2$ will not return the state to its original state at point $n_0$ as not all of the micro-cracks and micro-voids will close; the state of the damaged material will follow a linear path defined by the damaged elastic stiffness modulus, $E_1$, to point $n_3$. Thus, even though the material does not experience plasticity, irrecoverable strains occur due to the damage. These strains are denoted as the inelastic damage strains, $\varepsilon^{id}$. The total recoverable part of the strain, $\varepsilon^e$, can be decomposed into an elastic strain due to the effective undamaged material, $\varepsilon^e$, and an additional elastic strain, $\varepsilon^{ed}$, due to the change in the elastic stiffness modulus (with closure of some cracks and voids).

Figure 4.2: Stress – strain curve for a material with coupled plasticity and damage denoting elastic and coupled plastic-damage strains.
Once the loading exceeds the critical threshold defined by the yield stress, $\sigma_{yp}$, the damaged material enters into a plastically loaded state of deformation (Figure 4.2). After loading up to point $n_5$, the elastic curve that the material will follow is defined by the damaged elastic stiffness modulus, $E_2$. The state will return to point $n_6$ such that the total elastic strain introduced previously as $\varepsilon^e$ is recovered. This strain is again decomposed into an elastic strain due to the effective undamaged material, $\tilde{\varepsilon}^e$, and an additional elastic strain, $\varepsilon^{ed}$, due to the change in the elastic stiffness modulus. However, now the irrecoverable strains include both an inelastic component due to damage, $\varepsilon^{id}$, and an inelastic component due to plasticity, $\varepsilon^p$. The total irrecoverable component of strain is denoted here as the inelastic damage and plastic strain, $\varepsilon^{pd}$.

The change in the damage surface can be explained in terms of the accumulation of micro-cracks and micro-voids with loading. Loading causes the micro-cracks and micro-voids to generate, to propagate, and to interact. The ease with which the micro-cracks are able to move determines the damage hardness of the material. With an increase in the micro-damage density, there begins to be more interactions between the micro-cracks and between the micro-voids such that damage increase becomes more difficult and the stress required to produce additional micro-damage increases. The material exhibits hardening due to the arresting of micro-cracks because of their respective interactions. A damage material model can be used to describe this behavior by defining the evolution of a damage tensor through a damage criterion such that a damage surface is defined as well as the change in size, shape, and position of the damage surface. In this work, a $J_2$ type of damage criterion is used with isotropic hardening corresponding to the change in the size of the damage surface.

The constitutive model is derived using consistent thermodynamics in a similar fashion as in CHAPTER 3 for a classical rate-independent continuum J2 plasticity model. Based on the first law of thermodynamics, the Helmholtz free energy is introduced to describe the current state of energy in the material (Malvern, 1969; Coussy, 1995), and is a function of the strain and the internal state variables under consideration.

### 4.2 Continuum Damage Mechanics and Thermodynamics

Continuum Damage Mechanics (CDM) allows one to develop constitutive equations within the concept of continuum mechanics such that there is a degradation of the material during loading due to micro-damage. In order to develop the model equations, CDM assumes that the real, damaged state of the material can be represented by a fictitious, effective undamaged state with a continuum damage measure, $\phi$, representing the micro-damage.

As for the plasticity model in CHAPTER 3, the thermodynamics of irreversible processes is followed where a local state consisting of state variables (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000) is introduced. A
thermodynamic potential is used to define state laws based on the state variables, and the evolution of the thermodynamic conjugate forces are obtained by assuming the physical existence of the dissipation potential at the macroscale and through the use of the theory of functions of several variables with both plastic and Lagrange multipliers.

In order to understand the basis for defining a damage measure, first consider a one-dimensional case in which a scalar damage measure (Kachanov, 1958) is used for transformation from the damaged state to the effective state. For the one-dimensional case, consider a damaged bar with a uniform cross-section of area $A$ subject to a uniaxial load, $T$, as shown in Figure 4.3 (a), such that the stress on the bar is defined as $\sigma = T/A$. This damaged bar contains defects such as micro-voids and micro-cracks, and the area of these defects in any given cross-section is denoted by $A^D$. The density of these defects is defined as the scalar damage measure, $\varphi$, and can be written as follows (Kachanov, 1958):

$$\varphi = \frac{A^D}{A} \quad (4.1)$$

The effective, undamaged bar is defined as a bar with a uniform cross-section of area $\bar{A}$ subject to the same uniaxial load, $T$, as shown in Figure 4.3 (b), such that the stress on the bar is defined by $\bar{\sigma} = T/\bar{A}$. The area of this bar is defined to be the net area of the damaged bar which resists the load, and can be written as the area of the damaged bar with the micro-damage removed:

$$\bar{A} = A - A^D \quad (4.2)$$

![Figure 4.3](image): Transformation from actual damaged state to effective undamaged state for the uniaxial bar.
such that the damage measure can be written in terms of the area of the damaged bar and the area of the effective bar as follows:

\[ \varphi = \frac{A - \tilde{A}}{A} \]  

(4.3)

Thus, if there is no damage in the bar \( (A^D = 0) \), the total area of the bar resists the load applied to the bar. This state corresponds to a bar with a damage measure of \( \varphi = 0 \). On the other hand, once the bar fractures, there is no area remaining to resist the applied load such that \( \tilde{A} = 0 \). This state of fracture corresponds to a bar with a damage measure of \( \varphi = 1 \). However, rupture will occur once the damage measure reaches a critical value, \( \varphi = \varphi_c \), which is smaller than one. For example, Lemaitre (1984) defined the critical value to be between 0.2 and 0.8 for metals.

This simple isotropic damage measure is often used to define the degradation of the material in three-dimensional applications by assuming that the degradation takes place uniformly in all directions such that a second-order isotropic damage measure can be written as follows:

\[ \Phi = \begin{bmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & \varphi \end{bmatrix} \]  

(4.4)

As engineering materials tend to have anisotropic material behavior, damage tends to develop differently in different directions. In order to capture this behavior, a different damage measure must be used for each of the directions such that a second-order anisotropic damage measure must be defined (e.g. Sidoroff, 1981; Cordebois & Sidoroff, 1982; Murakami & Ohno, 1981; Murakami, 1983; Krajcinovic, 1983; Voyiadjis & Kattan, 1992, 1993; Voyiadjis & Park, 1997, 1999; Voyiadjis & Deliktas, 2000; etc.).

In order to define this anisotropic measure, consider a representative volume element (RVE) of the damaged material such that each face of the RVE has a normal in the direction of a global coordinate system axis, \( \chi \), as shown in Figure 4.4 (a). For anisotropic damage, each face of this RVE will have a different damage distribution. Thus, a vector \( \rho \) can be used to represent the micro-damage density such that each component of the vector represents the density of the micro-damage on the \( i \)-th surface and can be written as follows (Voyiadjis & Venson, 1995):

\[ \rho_i = \frac{A^D_i}{A_i} = \frac{A_i - \tilde{A}_i}{A_i} \quad \text{(no sum over } i) \]  

(4.5)
where, for the $i$-th surface, $A_i$ is the total damaged area, $\tilde{A}_i$ is the effective net area which resists a load, and $A_i^D$ is the area of the micro-damage. For a general case of anisotropic damage, the damage measure can be written in terms of these damage densities such that (Voyiadjis & Venson, 1995; Voyiadjis et al., 1995):

$$\varphi = \sqrt{\rho \otimes \rho}$$

(4.6)

This damage tensor $\varphi$ is a real symmetric tensor such that the eigenvalues of this tensor are all real $(\hat{\varphi_1}, \hat{\varphi_2}, \hat{\varphi_3})$ and there always exists at least three real eigenvectors $(\hat{e^1}, \hat{e^2}, \hat{e^3})$. Thus, for an RVE consisting of a damage state defined by $\varphi$, there always exists a corresponding RVE rotated to the principal directions, such that the normals of the principal RVE are defined by the vectors $\hat{e^1}$, $\hat{e^2}$, and $\hat{e^3}$ as shown in Figure 4.4 (b). Thus, a damage tensor $\hat{\varphi}$ can be defined in the orthogonal principal directions as a diagonal tensor such that:

$$\hat{\varphi} = \begin{bmatrix} \hat{\varphi_1} & 0 & 0 \\ 0 & \hat{\varphi_2} & 0 \\ 0 & 0 & \hat{\varphi_3} \end{bmatrix}$$

(4.7)

In order to rotate the damage tensor from the principal directions to the global directions, an orthogonal transformation tensor $Q$ is used through the following equation:

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.4}
\caption{RVE’s in the global coordinate system (a) and in the principal directions (b)}
\end{figure}
\[ \varphi = Q^T \cdot \hat{\varphi} \cdot Q \]  

(4.8)

where the transformation tensor is written in terms of the components of the eigenvectors such that:

\[
\begin{bmatrix}
\hat{e}_1^1 & \hat{e}_2^1 & \hat{e}_3^1 \\
\hat{e}_1^2 & \hat{e}_2^2 & \hat{e}_3^2 \\
\hat{e}_1^3 & \hat{e}_2^3 & \hat{e}_3^3
\end{bmatrix}
\]

(4.9)

The inverse of this rotation, due to the properties of orthogonal tensors, can be written as follows:

\[ \hat{\varphi} = Q \cdot \varphi \cdot Q^T \]  

(4.10)

Thus, a tensor has been defined which can be used to represent the damage in a body. It will be shown in subsequent sections that the stresses and the strains in the actual configuration can be transformed to this fictitious undamaged configuration through the use of this damage tensor.

### 4.2.1 Stress Transformations

In order to demonstrate how stresses are transformed to the effective configuration, again consider the one-dimensional case in Figure 4.3. As the bars in both the damaged configuration and the effective undamaged configuration are subjected to the same uniaxial load, \( T \), the following equality holds:

\[ T = \sigma A = \tilde{\sigma} \tilde{A} \]  

(4.11)

Making use of the definition for the damage measure given in Eq. (4.3), the linear transformation relation from the actual Cauchy stress, \( \sigma \), to the effective Cauchy stress, \( \tilde{\sigma} \), is written as follows (Kachanov, 1958):

\[ \tilde{\sigma} = \frac{\sigma}{1 - \varphi} \]  

(4.12)

In the absence of damage, i.e. \( \varphi = 0 \), the stress in the undamaged configuration and the stress in the damaged configuration are identical; however, when the damage state approaches rupture, i.e. when \( \varphi \) approaches unity, the stress in the effective configuration becomes very large. This can be visualized by noting that, though the same load, \( T \), is applied in both configurations, the area in the effective configuration that this load acts upon is very small as the damage state approaches rupture.
For a general state of anisotropic damage, the Cauchy stress is transformed to the effective Cauchy stress through a linear transformation such that (Murakami & Ohno, 1981; Murakami, 1983):

\[ \tilde{\sigma} = M : \sigma \]  

(4.13)

where \( M \) is the fourth order damage effect tensor in terms of the second order damage tensor, \( \varphi \). This tensor can be written by transforming the damage effect tensor, \( \hat{M} \), which is defined with reference to the principal direction coordinate system:

\[ M = \mathbf{Q}^T \cdot \hat{M} \cdot \mathbf{Q} \]  

(4.14)

Eq. (4.14) allows the use of the diagonal form of the damage tensor as given in Eq. (4.7). Various forms for the principal damage effect tensor have been given in the literature. Sidoroff (1981), Cordebois & Sidoroff (1982), and Lee et al. (1986) expressed the components of this matrix in the following form:

\[
\begin{bmatrix}
\hat{M}
\end{bmatrix}_{ijkl} = \frac{\delta_{ik} \delta_{jl}}{\sqrt{(1 - \hat{\varphi}_{ik})(1 - \hat{\varphi}_{jl})}} \quad \text{(no sum over } i, j, k, l) \quad (4.15)
\]

Alternate forms for the components of this damage effect tensor have been presented by Voyiadjis & Park (1997) as follows:

\[
\begin{bmatrix}
\hat{M}
\end{bmatrix}_{ijkl} = \frac{\delta_{ik} \delta_{jl} \left[ (1 - \hat{\varphi}_{ij}) + (1 - \hat{\varphi}_{jk}) \right]}{2(1 - \hat{\varphi}_{ik})(1 - \hat{\varphi}_{jl})} \quad \text{(no sum over } i, j, k, l) \quad (4.16)
\]

\[
\begin{bmatrix}
\hat{M}
\end{bmatrix}_{ijkl} = \frac{2\delta_{ik} \delta_{jl}}{(1 - \hat{\varphi}_{ik}) + (1 - \hat{\varphi}_{jl})} \quad \text{(no sum over } i, j, k, l) \quad (4.17)
\]

The differences between these forms of the damage effect tensor are brought about by the symmetrization procedure used as discussed in Voyiadjis & Park (1997). In the rest of this work, it is assumed that the components of the damage effect tensor are as described by Eq. (4.17); however, similar formulations can be performed for the other representations. Thus, using this form of the principal damage tensor, the components of the term \( \partial \hat{M} / \partial \varphi \) are found by taking derivatives of the components given by Eq. (4.17) such that:

\[
\frac{\partial \begin{bmatrix}
\hat{M}
\end{bmatrix}_{ijkl}}{\partial \varphi_{ab}} = \frac{2\delta_{ia} \delta_{jb} \left( \delta_{ia} \delta_{kb} + \delta_{ja} \delta_{ib} \right)}{\left[ (1 - \hat{\varphi}_{ik}) + (1 - \hat{\varphi}_{jl}) \right]^2} \quad \text{(no sum over } i, j, k, l) \quad (4.18)
\]
As this model incorporates plasticity in addition to damage, it will be necessary in evaluating the yield criterion to define the deviatoric components of the effective stress. Given the Cauchy stress tensor and the effective Cauchy stress tensor, the deviatoric parts are defined here as follows:

\[ s = (1 - \frac{1}{3} \mathbf{1} \otimes \mathbf{1}) : \sigma \]  
\[ \tilde{s} = (1 - \frac{1}{3} \mathbf{1} \otimes \mathbf{1}) : \tilde{\sigma} \]  

Substituting the transformation relation, Eq. (4.13), into Eq. (4.20), a linear relationship between the Cauchy stress tensor and the effective deviatoric stress tensor is obtained such that:

\[ \tilde{s} = \mathbf{N} : \sigma \]  

where the fourth order tensor \( \mathbf{N} \) is a linear operator defined as follows:

\[ \mathbf{N} = \mathbf{M} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} : \mathbf{M} \]  

Utilizing Eq. (4.19) in Eq. (4.21), the following relationship is obtained for the effective deviatoric stress:

\[ \tilde{s} = \mathbf{M} : s + \frac{1}{2} \mathbf{M} : \mathbf{1} \otimes \mathbf{1} : \sigma - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} : \mathbf{M} : \sigma \]  

This equation cannot be manipulated to obtain a linear transformation between the deviatoric stress and the effective deviatoric stress, and it will thus be required to use Eq. (4.21) for the transformation of the deviatoric stress.

The isotropic hardening and kinematic hardening conjugate forces defined in Section 3.2.3 must also be written in terms of the effective configuration. As defined in Section 3.2.3, the isotropic hardening conjugate force represented by the scalar \( R \) measures the expansion or contraction of the yield surface in the stress space. As this conjugate force is a scalar, a transformation to the effective configuration is performed in a similar fashion as performed in Eq. (4.12) such that:

\[ \tilde{R} = \frac{R}{1 - \| \varphi \|} \]  

where \( \tilde{R} \) is the isotropic hardening conjugate force in the effective configuration. The norm of the damage tensor is used in this transformation as a scalar measure of damage, \( \varphi_{eq} \). The kinematic hardening conjugate force represented by the second-order tensor \( \mathbf{X} \) measures the movement and distortion of the yield surface in the stress space. The backstress conjugate force is a second-order tensor which can be linearly transformed using the same method as for the Cauchy stress such that:
\[ \tilde{X} = M : X \] (4.25)

where \( \tilde{X} \) is the backstress conjugate force in the effective configuration. It will be beneficial in the formulation of the yield condition to define the backstress tensor in terms of the fourth order tensor \( N \) from Eq. (4.22). As the backstress conjugate force is a deviatoric tensor, \( M \) can be replaced with \( N \) such that:

\[ \tilde{X} = N : X \] (4.26)

Given the damaged and the effective Cauchy stress tensor as well as the damaged and the effective backstress conjugate force, the damaged and the effective relative stress tensors are defined here as follows:

\[ \tilde{\xi} = s - \tilde{X} \] (4.27)

\[ \xi = s - X \] (4.28)

Substituting the transformation relations, Eq. (4.21) and (4.26), into Eq. (4.27), the following transformation of the relative stress tensor to the effective configuration is obtained:

\[ \tilde{\xi} = s - \tilde{X} = N : (\sigma - X) \] (4.29)

The norm of this effective relative stress will be used in the effective configuration yield condition and is defined as follows:

\[ \| \tilde{\xi} \| = \| s - \tilde{X} \| = \| N : (\sigma - X) \| \] (4.30)

### 4.2.2 Elastic Strain Transformations

Under uniaxial loading, the strain at a given stress has two parts: a recoverable elastic strain, and an irreversible plastic strain (Figure 4.2). The reversible part is related to the stress through the usual linear elastic equations using a damaged elastic stiffness tensor. It will be shown that this fourth order tensor can be defined as a function of the damage tensor, \( \varphi \), through the inverse of the damage effect tensor, \( M \). In this work, additive decomposition of the total observable strain, \( \varepsilon \), into its internal variable components is assumed:

\[ \varepsilon = \varepsilon^e + \varepsilon^{pd} \] (4.31)

where \( \varepsilon^e \) is the reversible thermo-elastic component of the strain and \( \varepsilon^{pd} \) is the irreversible component of the strain due to plasticity and damage. The elastic strain can
be further decomposed into an elastic strain corresponding to the undamaged configuration, $\varepsilon^e$, and an additional component due to the reduction of the elastic stiffness tensor, $\varepsilon^{ed}$, such that:

$$\varepsilon^e = \varepsilon^e + \varepsilon^{ed}$$  (4.32)

The total irrecoverable component of strain, $\varepsilon^{pd}$, is the irreversible part of the strain which remains when the external loads are removed and can be decomposed into an inelastic component due to damage, $\varepsilon^{id}$, and an inelastic component due to plasticity, $\varepsilon^p$, such that:

$$\varepsilon^{pd} = \varepsilon^p + \varepsilon^{id}$$  (4.33)

The transformation of the strains from the damaged state to the effective state in this work is derived through the use of the concept of elastic energy equivalence (Sidoroff, 1981). This concept assumes that the elastic energy in the damaged state and in the effective state are equivalent such that:

$$\frac{1}{2} \tilde{\sigma} : \tilde{\varepsilon}^e = \frac{1}{2} \sigma : \varepsilon^e$$  (4.34)

Substitution of Eq. (4.13) into this equation gives the transformation relation for the elastic strain from the damaged configuration to the effective configuration as follows:

$$\tilde{\varepsilon}^e = M^{-T} : \varepsilon^e$$  (4.35)

It is assumed that the following Hookean relation holds for both the damaged configuration and for the effective configuration:

$$\sigma = C^e : \varepsilon^e$$  (4.36)

$$\tilde{\sigma} = \tilde{C}^e : \tilde{\varepsilon}^e$$  (4.37)

where $C^e$ is the damaged elasticity modulus and $\tilde{C}^e$ is the effective, undamaged elasticity modulus. For isotropic elasticity, the effective, undamaged elasticity modulus is equivalent to that defined by Eq. (3.19) and is written here as follows:

$$\tilde{C}^e = \kappa^e I \otimes I + 2\mu^e \left( I - \frac{1}{3} I \otimes I \right)$$  (4.38)

Substituting Eqs. (4.36) and (4.37) into Eq. (4.34) and utilizing the transformation Eq. (4.35), the assumption of elastic energy equivalence gives the transformation relation between the damaged elastic tangent modulus $C^e$ and the effective elasticity modulus $\tilde{C}^e$ to be the following (Voyiadjis & Kattan, 1992, 1993):
\[ C^e = M^{-1} : \tilde{C}^e : M^{-T} \]  
(4.39)

where the inverse of the damage effect tensor is defined in terms of the principal damage effect tensor as:

\[ M^{-1} = Q^T \cdot \dot{Q}^T \cdot \dot{M}^{-1} \cdot Q \cdot Q \]  
(4.40)

As the principal damage effect tensor defined by the components in Eqs. (4.15) to (4.17) is a diagonal matrix, the components of its inverse can easily be written as follows:

\[
\left[ \dot{M}^{-1} \right]_{ijkl} = \frac{1}{2} \delta_{ik} \delta_{jl} \left[ (1 - \dot{\phi}_{ik}) + (1 - \dot{\phi}_{jl}) \right] 
\]

(no sum over \( i, j, k, l \))  
(4.41)

The components of the term \( \partial \dot{M}^{-1} / \partial \dot{\phi} \) are found by taking derivatives of the components given by Eq. (4.41) such that:

\[
\frac{\partial \left[ \dot{M}^{-1} \right]_{ijkl}}{\partial \dot{\phi}_{ab}} = -\frac{1}{2} \delta_{ia} \delta_{jb} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) 
\]

(no sum over \( i, j, k, l, a, b \))  
(4.42)

### 4.2.3 State Variables

The local coupled plasticity-damage model is defined through the use of the method of material local state identification. In this method, a model is developed such that the thermodynamic state at a given point in space and time is completely determined by a given set of state variables at that point in space and time. As this set of state variables does not include gradients for the local theory, the state at the given point is independent of the behavior surrounding the point; however, in CHAPTER 5, gradients will be introduced as state variables and the method of material nonlocal state identification will be followed to derive the thermodynamic equations.

The set of state variables are separated into a set of observable state variables and a set of internal state variables. The observable variables are those that can be measured and which appear regardless of the material phenomena. The observable state variables used here are the temperature denoted by the scalar \( T \), the total strain denoted by the second-order tensor \( \epsilon \), and the damage tensor denoted by the second-order tensor \( \phi \). For pure elasticity, this set of observable state variables entirely defines the point; however, for elasto-plasticity, the material has a history dependency which requires an additional set of internal state variables.

For this coupled damage-plasticity model, the internal state variables will consist of hardening variables as defined for plasticity in Eq. (3.2), as well as an additional hardening variable for damage, \( \kappa \). The hardening internal state variables are unitless,
strain like quantities and are accumulated into a set of plasticity related measures, $V^p$ and a set of damage related measures, $V^d$, as follows:

\[
V^p = [r, \alpha] \\
V^d = [\kappa]
\]

(4.43)
(4.44)

where the internal state variables considered here are the plasticity related variables presented in CHAPTER 3, and the damage related variable representing the flux of the isotropic hardening behavior denoted by the scalar $r$ which corresponds to the change in the size of the damage surface. Although there is only one hardening variable for the damage, the general form of a set $V^d$ is retained for derivations in CHAPTER 5.

### 4.2.4 Equations of State

In order to determine state laws which relate the internal state variable fluxes to their conjugate thermodynamic forces, a thermodynamic potential defined as the Helmholtz free energy is introduced which is a state function of a thermodynamic system (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000). This thermodynamic potential is used to describe the current state of energy in the material, and is a function of the observable state variables and the internal state variables under consideration:

\[
\psi = \psi\left(\varepsilon, T, \varepsilon^{pd}, \varepsilon', \Phi, V^p, V^d\right)
\]

(4.45)

However, as the strains are decomposed for this coupled plasticity-damage model in the same way as the plasticity model, this Helmholtz free energy is rewritten as follows:

\[
\psi = \psi\left(\varepsilon', T, \Phi, V^p, V^d\right)
\]

(4.46)

The Clausius-Duhem inequality can be written in the same form as given by Eq. (3.7); however, the time derivative of $\psi$ is now expanded based on the additional internal state variables as follows:

\[
\dot{\psi} = \frac{\partial \psi}{\partial \varepsilon'} \dot{\varepsilon'} + \frac{\partial \psi}{\partial T} \dot{T} + \frac{\partial \psi}{\partial \Phi} \dot{\Phi} + \frac{\partial \psi}{\partial V^p} \dot{V}^p + \frac{\partial \psi}{\partial V^d} \dot{V}^d
\]

(4.47)

Using this relationship along with the strain decomposition given by Eq. (4.31), the Clausius-Duhem inequality can be expanded in the following form:
\[
\sigma : \dot{\varepsilon}^{\text{irr}} + \left(\sigma - \rho \frac{\partial \psi}{\partial \varepsilon}\right) : \dot{\varepsilon}^e - \rho \left(\frac{\partial \psi}{\partial T} + s\right) \dot{T} \\
- \rho \frac{\partial \psi}{\partial \varphi} : \dot{\varphi} - \rho \frac{\partial \psi}{\partial \mathbf{V}^p} : \dot{\mathbf{V}}^p - \rho \frac{\partial \psi}{\partial \mathbf{V}^d} : \dot{\mathbf{V}}^d - \mathbf{q} \cdot \nabla T \geq 0
\] (4.48)

As the formulations in Section 3.2.2 were derived using the general set, \( \mathbf{V} \), of macroscopic measures of irreversible phenomena, the formulations for the equations of state do not need to be repeated here, and the thermo-elastic state laws are written as follows:

\[
\sigma = \rho \frac{\partial \psi}{\partial \epsilon^e} 
\] (4.49)

\[
s = -\frac{\partial \psi}{\partial T} 
\] (4.50)

\[
\mathbf{Y} = -\frac{\partial \psi}{\partial \varphi} 
\] (4.51)

From these state laws, the stress, \( \sigma \), and the enthalpy, \( s \), are defined as the conjugate forces corresponding to the state variables \( \epsilon^e \) and \( T \), respectively. Similarly, \( \mathbf{Y} \) is defined as the conjugate force corresponding to the damage measure, \( \varphi \), and sets of conjugate forces, \( \mathbf{A}^p \) and \( \mathbf{A}^d \), are defined which correspond to the hardening internal state variables:

\[
\mathbf{A}^p = [R, \mathbf{X}] 
\] (4.52)

\[
\mathbf{A}^d = [K] 
\] (4.53)

where the scalar \( R \) and the second-order tensor \( \mathbf{X} \) are defined as in Eq. (3.15); and the scalar \( K \) measures the expansion or contraction of the damage surface in the stress space. Whereas the internal state variables are unitless, strain like quantities, the thermodynamic conjugate forces are a set of stress like quantities that are related to the state variables as the stress is related to the strain. These conjugate forces are defined in the Clausius-Duhem inequality by the following sets of state laws:

\[
\mathbf{A}^p = \rho \frac{\partial \psi}{\partial \mathbf{V}^p} 
\] (4.54)

\[
\mathbf{A}^d = \rho \frac{\partial \psi}{\partial \mathbf{V}^d} 
\] (4.55)
4.2.5 Conjugate Forces

Since the internal state variables are selected independently of one another, one can express the analytical form of the Helmholtz free energy in terms of its internal state variables as:

\[
\rho \psi = \frac{1}{2} \varepsilon : C^e \varepsilon + W^p \left( V^p \right) + W^d \left( V^d \right) - \rho Ts
\]  

(4.56)

where the fourth-order tensor \( C^e \) is the damaged elastic tangent modulus and is in terms of the damage tensor \( \Phi \), the scalar \( \rho \) is the material density, and the superscripted “e,” “p,” and “d” imply terms associated with elasticity, plasticity, and damage, respectively. For this form of the Helmholtz free energy and from the state law Eq. (4.49), the stress applied to stretch or compress a body is defined to be proportional to the elastic strain thus produced in the form of a Hookean relationship as follows:

\[
\sigma = C^e : \varepsilon
\]

(4.57)

where the damaged elasticity tensor is defined by Eq. (4.39). In a similar fashion, from the state law Eq. (4.51), the relation between the damage measure flux and its corresponding conjugate force is written as follows:

\[
Y = \frac{1}{2} \varepsilon^T : \frac{\partial C^e}{\partial \Phi} : \varepsilon = \frac{1}{2} \sigma^T : \frac{\partial C^{-e}}{\partial \Phi} : \sigma
\]

(4.58)

where the derivative of the damaged stiffness tensor and the inverse damaged stiffness tensor with respect to the damage tensor is written as follows:

\[
\frac{\partial C^e}{\partial \Phi} = 2 M^{-1} : \tilde{C}^e : \frac{\partial M^{-T}}{\partial \Phi}
\]

(4.59)

\[
\frac{\partial C^{-e}}{\partial \Phi} = 2 M^{-T} : \tilde{C}^{-e} : \frac{\partial M^{-1}}{\partial \Phi}
\]

(4.60)

The energy terms, \( W^p \left( V^p \right) \), have been introduced in Section 3.2.3. In the same way, the term \( W^d \left( V^d \right) \) accounts for energy introduced into the system by the damage hardening such that:

\[
W^d \left( V^d \right) = W^\kappa \left( \kappa \right)
\]

(4.61)

In the same way as was done for the plasticity energy terms, power and exponential laws are used here to introduce the energy due to the damage isotropic hardening such that and can thus be selected from one of the following:
Power Laws
\[ W^\kappa(\kappa) = \frac{H_\kappa}{m_\kappa+1} \kappa^{m_\kappa+1} \] (4.62)

Exponential Laws
\[ W^\kappa(\kappa) = K_\kappa \left( \kappa + \frac{1}{\gamma_\kappa} e^{-\gamma_\kappa \kappa} - \frac{1}{\gamma_\kappa} \right) \] (4.63)

In these relationships, \( H_\kappa, m_\kappa, \) and \( K_\infty \) are positive material and geometrical dependent parameters. Utilizing the energy terms in the Helmholtz free energy, the state laws, Eq. (4.55), result in definitions for the hardening - thermodynamic conjugate forces as power and exponential relations of the corresponding state variables:

Power Laws
\[ K = H_\kappa r^{m_\kappa} \] (4.64)

Exponential Laws
\[ K = K_\infty \left( 1 - e^{-\gamma_\kappa \kappa} \right) \] (4.65)

The internal state variable - thermodynamic conjugate force relationships are defined based on the material being investigated and different relationships can be selected for the plasticity hardening laws and for the damage hardening laws. Though two typical models, the power and exponential laws, are used here, more complex models can be incorporated in the same manner; however, the analysis of the material model is beyond the scope of this work. This work is focused on the development of a formulation based on a general functional form of the thermodynamic conjugate forces. This allows the constitutive model to be developed without making an assumption as to the behavior of the material model such that the conjugate forces are written as a general function of their corresponding internal state variable:

\[ R = R(r) \] (4.66)
\[ X = X(\alpha) \] (4.67)
\[ K = K(\kappa) \] (4.68)

4.2.6 Dissipation Potential and Flow Rules

The evolution of the thermodynamic conjugate forces can be obtained through the evolution relations of the internal state variables, which are obtained by assuming the physical existence of the dissipation potential at the macroscale. The energy dissipation due to plasticity and damage are found by substituting the thermodynamic state laws into the Clausius-Duhem inequality and are thus given as the product of the thermodynamic conjugate forces with the respective flux variables as follows:
\[ \Pi = \sigma : \dot{\epsilon}^{pd} - Y : \dot{\phi} - \rho A^p \cdot \dot{V}^p - \rho A^d \cdot \dot{V}^d - q \cdot \frac{\nabla T}{T} \geq 0 \]  \hspace{1cm} (4.69)

The theory of functions of several variables is used here with a plastic Lagrange multiplier \( \hat{\lambda}^p \) and a damage Lagrange multiplier \( \hat{\lambda}^d \) to construct the objective function \( \Omega \) in the following form:

\[ \Omega = \Pi - F \dot{\lambda}^p - G \dot{\lambda}^d \]  \hspace{1cm} (4.70)

where \( F \) and \( G \) are the plastic potential and the damage potential and will be defined subsequently. In order to obtain the plastic strain rate and the damage tensor rate, the following condition is used to extremize the objective function:

\[
\frac{\partial \Omega}{\partial \sigma} = 0 \hspace{1cm} (4.71)
\]

\[
\frac{\partial \Omega}{\partial Y} = 0 \hspace{1cm} (4.72)
\]

From these conditions for the case when \( 0 \leq F \leq 0 \), the corresponding evolution equations for the plastic strain and for the damage tensor are given as follows:

\[
\dot{\epsilon}^{pd} = \frac{\partial F}{\partial \sigma} \dot{\lambda}^p + \frac{\partial G}{\partial \sigma} \dot{\lambda}^d \]  \hspace{1cm} (4.73)

\[
\dot{\phi} = -\frac{\partial F}{\partial Y} \dot{\lambda}^p - \frac{\partial G}{\partial Y} \dot{\lambda}^d \]  \hspace{1cm} (4.74)

Since the plastic strain rate will be developed in the current deformed and damaged configuration, its corresponding evolution equation will be a function of the damage measure. Similarly, the evolution equation of the conjugate force due to damage will be a function of the stress. The evolution equations for the plastic strain and the damage are interdependent (Voyiadjis & Deliktas, 2000), and therefore the two dissipative mechanisms shown above are implicitly interdependent through the stress and the conjugate forces due to damage. Note that, if \( F \leq 0 \), then \( \partial F / \partial \sigma = \partial F / \partial Y = 0 \), or if \( G \leq 0 \), then \( \partial G / \partial \sigma = \partial G / \partial Y = 0 \), and the evolution equations for the plastic strain and the damage become decoupled. Note that this coupled form of the total inelastic strains corresponds with the additive decomposition given by Eq. (4.33) such that:

\[
\dot{\epsilon}^p = \frac{\partial F}{\partial \sigma} \dot{\lambda}^p \]  \hspace{1cm} (4.75)

\[
\dot{\epsilon}^d = \frac{\partial G}{\partial \sigma} \dot{\lambda}^d \]  \hspace{1cm} (4.76)
In order to derive the evolution equations for the hardening state variables, the following conditions are used to extremize the objective function:

\[
\frac{\partial \Omega}{\partial \mathbf{A}^p} = 0 \quad \text{(4.77)}
\]

\[
\frac{\partial \Omega}{\partial \mathbf{A}^d} = 0 \quad \text{(4.78)}
\]

From this conditions for the case when \( F \geq 0 \) and \( G \geq 0 \), the corresponding set of evolution equations for the hardening state variables are given as follows:

\[
\dot{\mathbf{V}}^p = -\frac{\partial F}{\partial \mathbf{A}^p} \dot{\lambda}^p \quad \text{(4.79)}
\]

\[
\dot{\mathbf{V}}^d = -\frac{\partial G}{\partial \mathbf{A}^d} \dot{\lambda}^d \quad \text{(4.80)}
\]

The following loading-unloading conditions known as the Kuhn-Tucker conditions (Kuhn & Tucker, 1951) must be enforced:

\[
\dot{\lambda}^p \geq 0; \quad f \leq 0; \quad \dot{\lambda}^p f = 0 \quad \text{(4.81)}
\]

\[
\dot{\lambda}^d \geq 0; \quad g \leq 0; \quad \dot{\lambda}^d g = 0 \quad \text{(4.82)}
\]

### 4.2.7 Yield Condition and Damage Condition

Associative plasticity can be used here to derive the evolution equations for the constitutive model such that the plastic potential, \( F \), is set equal to the yield criterion, \( f \). In the effective, undamaged configuration, the yield criterion can be written as follows:

\[
F = f = \|\hat{\xi}\| - \sqrt{\frac{2}{3}} \left[ \mathbf{\sigma} + \hat{\mathbf{R}} \right] \leq 0 \quad \text{(4.83)}
\]

where \( \hat{\mathbf{R}} \) is the effective isotropic hardening conjugate force defined by Eq. (4.24), and \( \hat{\xi} \) is the effective relative stress tensor defined by Eq. (4.29). Utilizing the relations developed for the transformation of stresses in Section 4.2.1, specifically Eqs. (4.24) and (4.30), the yield criterion can be written in terms of the damaged state such that:

\[
F = f = \|\mathbf{N} \cdot (\mathbf{\sigma} - \mathbf{X})\| - \sqrt{\frac{2}{3}} \left[ \mathbf{\sigma} + \frac{\mathbf{R}}{1 - \|\varphi\|} \right] \leq 0 \quad \text{(4.84)}
\]

Similarly, associative damage can be used here to derive the evolution equations for the constitutive model such that the damage potential, \( G \), is set equal to the damage
criterion, \( g \). The damage criterion is written in the same form as the Von Mises yield criterion presented in the previous section such that:

\[
G = g = \|\mathbf{Y}\| - \sqrt{\frac{2}{3}} \left[ \sigma_{\text{yd}} + K \right] = 0
\]  

(4.85)

where \( \sigma_{\text{yd}} \) is the initial damage threshold at which damage begins to occur. The normals to the plastic potential and to the damage potential can now be defined as given in APPENDIX B.1, allowing the evolution equations of the internal state variables to be defined. Thus, the complete set of constitutive equations for the local coupled plasticity-damage model have been derived and are summarized as follows:

**Yield Criterion and Damage Criterion**

\[
F = f = \|\mathbf{N} : (\mathbf{\sigma} - \mathbf{X})\| - \sqrt{\frac{2}{3}} \left[ \sigma_{\text{yp}} + \frac{R}{1 - \|\mathbf{\varphi}\|} \right] \leq 0
\]

(4.86)

\[
G = g = \|\mathbf{Y}\| - \sqrt{\frac{2}{3}} \left[ \sigma_{\text{yd}} + K \right] = 0
\]

(4.87)

**State Laws**

\[
\mathbf{\sigma} = \mathbf{C}^e : (\mathbf{\varepsilon} - \mathbf{\varepsilon}^{\text{pl}})
\]

(4.88)

\[
\mathbf{Y} = \frac{1}{3} \mathbf{\sigma}^T : \frac{\partial \mathbf{C}^{-e}}{\partial \mathbf{\varphi}} : \mathbf{\sigma}
\]

(4.89)

\[
R = R(r)
\]

(4.90)

\[
\mathbf{X} = \mathbf{X}(\alpha)
\]

(4.91)

\[
K = K(\kappa)
\]

(4.92)

**State Variable Evolution Equations**

\[
\dot{\varepsilon}^{\text{pl}} = f_\sigma \dot{\lambda}^p + g_\sigma \dot{\lambda}^d
\]

(4.93)

\[
\dot{\mathbf{\varphi}} = -f_X \dot{\lambda}^p - g_X \dot{\lambda}^d
\]

(4.94)

\[
\dot{r} = -f_\alpha \dot{\lambda}^p
\]

(4.95)

\[
\dot{\alpha} = f_\alpha \dot{\lambda}^p
\]

(4.96)

\[
\dot{\kappa} = -g_{\kappa} \dot{\lambda}^d
\]

(4.97)

**Kuhn-Tucker Conditions**

\[
\dot{\lambda}^p \geq 0; \quad f \leq 0; \quad \dot{\lambda}^p f = 0
\]

(4.98)

\[
\dot{\lambda}^d \geq 0; \quad g \leq 0; \quad \dot{\lambda}^d g = 0
\]

(4.99)
4.2.8 Plasticity and Damage Consistency Conditions

At a plastic state where \( f = 0 \), the consistency condition \( \dot{f} = 0 \) results from the loading-unloading conditions of Eq. (4.81). Thus, as the yield criterion is a function of the effective Cauchy stress, the backstress, the isotropic hardening, and the damage tensor, the consistency condition can be expanded in terms of the conjugate forces:

\[
\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial R} : \dot{R} + \frac{\partial f}{\partial X} : \dot{X} + \frac{\partial f}{\partial \phi} : \dot{\phi} = 0
\]  
(4.100)

As the conjugate forces have been defined as general functions of the state variables as shown in Eqs. (4.90) and (4.91), the consistency condition can be rewritten in terms of the flux variables as follows:

\[
\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial R} \frac{\partial R(r)}{\partial r} : \dot{r} + \frac{\partial f}{\partial X} \frac{\partial X(\alpha)}{\partial \alpha} : \dot{\alpha} + \frac{\partial f}{\partial \phi} : \dot{\phi} = 0
\]  
(4.101)

After substituting the normals to the yield surface as defined in APPENDIX B.1 and the evolution equations for the internal state variables as defined in Eqs. (4.93) to (4.96), the consistency condition is expanded and can be written in the following form:

\[
H^{pp} \dot{\lambda}^p + H^{pd} \dot{\lambda}^d \equiv B^p
\]  
(4.102)

where:

\[
H^{pp} = f^p_h \frac{\partial R(r)}{\partial r} + f^p_\sigma \frac{\partial X(\alpha)}{\partial \alpha} : f_\sigma + f_\phi : f_X
\]  
(4.103)

\[
H^{pd} = f_\phi : g_X
\]  
(4.104)

\[
B^p = f_\sigma \dot{\sigma}
\]  
(4.105)

At a damage state where \( g = 0 \), the consistency condition \( \dot{g} = 0 \) results from the loading-unloading conditions of Eq. (4.82). Thus, as the damage criterion is a function of the Cauchy stress, the damage isotropic hardening, and the damage measure, the consistency condition can be expanded in terms of the conjugate forces:

\[
\dot{g} = \frac{\partial g}{\partial \sigma} : \dot{\sigma} + \frac{\partial g}{\partial K} \dot{K} + \frac{\partial g}{\partial \phi} : \dot{\phi} = 0
\]  
(4.106)

As the hardening conjugate force has been defined as a general function of the state variable as shown in Eq. (4.92), the consistency condition can be rewritten in terms of the flux variables as follows:
\[
\dot{g} = \frac{\partial g}{\partial \sigma} : \dot{\sigma} + \frac{\partial g}{\partial K} \frac{\partial K}{\partial \kappa} \dot{\kappa} + \frac{\partial g}{\partial \phi} \dot{\phi} = 0 \quad (4.107)
\]

After substituting the normals to the damage surface as defined in APPENDIX B.1 and the evolution equations for the internal state variables as defined in Eqs. (4.93), (4.94), and (4.97), the consistency condition is expanded and can be written in the following form:

\[
H^{dp} \dot{\lambda}^p + H^{dd} \dot{\lambda}^d \equiv B^d \quad (4.108)
\]

where:

\[
H^{dp} = g_{,\sigma} : f_Y
\quad (4.109)
\]

\[
H^{dd} = g_{,\kappa} \frac{\partial K}{\partial \kappa} + g_{,\phi} : g_Y
\quad (4.110)
\]

\[
B^d = g_{,\sigma} : \dot{\sigma}
\quad (4.111)
\]

The plastic multiplier and the damage multiplier can be solved from the linear system of equations given by Eqs. (4.102) and (4.108) such that:

\[
\begin{bmatrix}
\dot{\lambda}^p \\
\dot{\lambda}^d
\end{bmatrix} = \frac{1}{H} \begin{bmatrix}
H^{dd} & -H^{pd} \\
-H^{dp} & H^{pp}
\end{bmatrix} \begin{bmatrix}
B^p \\
B^d
\end{bmatrix}
\quad (4.112)
\]

where:

\[
H = H^{pp} H^{dd} - H^{pd} H^{dp}
\quad (4.113)
\]

Using this solution, the plastic and damage multipliers can be written in terms of the incremental stress as follows:

\[
\dot{\lambda}^p = \frac{1}{H} \left( H^{dd} f_{,\sigma} - H^{pd} g_{,\sigma} \right) : \dot{\sigma}
\quad (4.114)
\]

\[
\dot{\lambda}^d = \frac{1}{H} \left( -H^{dp} f_{,\sigma} + H^{pp} g_{,\sigma} \right) : \dot{\sigma}
\quad (4.115)
\]

In order to write these multipliers in terms of the incremental strain, the incremental form of the Hookean stress is used in the following form which is found by differentiating Eq. (4.88):

\[
\dot{\sigma} = C^e : (\dot{\varepsilon} - \dot{\varepsilon}^{pd}) + \dot{C}^e : (\varepsilon - \varepsilon^{pd})
\quad (4.116)
\]

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where the incremental damaged elastic stiffness tensor is found by differentiating Eq. (4.39). The resulting equation is given in APPENDIX B.1 and is rewritten here as follows:

\[
\dot{C}^e = \frac{\partial C^e}{\partial \phi} : \dot{\phi} = 2C^e : M^T : \frac{\partial M^{-T}}{\partial \phi} : \dot{\phi} \quad \text{(4.117)}
\]

Thus, the incremental stress can be written in the following form:

\[
\dot{\sigma} = C^e \left( \dot{\varepsilon} - \varepsilon^{pd} \right) + C^e : Z : \dot{\phi} \quad \text{(4.118)}
\]

where the fourth-order tensor \( Z \) is defined as follows:

\[
Z = 2M^T : \frac{\partial M^{-T}}{\partial \phi} : \left( \varepsilon - \varepsilon^{pd} \right) = C^{-e} : \frac{\partial C^e}{\partial \phi} : \left( \varepsilon - \varepsilon^{pd} \right) \quad \text{(4.119)}
\]

Using Eq. (4.118) in the consistency conditions, Eqs. (4.101) and (4.107), and following the same procedure as for the derivation of Eqs. (4.102) and (4.108), the following system of equations are obtained:

\[
\begin{align*}
 h^{pp} \lambda^p + h^{pd} \lambda^d &\equiv b^p \\
 h^{dp} \lambda^p + h^{dd} \lambda^d &\equiv b^d
\end{align*} \quad \text{(4.120) and (4.121)}
\]

where:

\[
\begin{align*}
 h^{pp} &= H^{pp} + f_{a} : C^e : f_{a} + f_{a} : C^e : Z : f_{Y} \\
 h^{dd} &= H^{dd} + g_{a} : C^e : g_{a} + g_{a} : C^e : Z : g_{Y} \\
 h^{pd} &= H^{pd} + f_{a} : C^e : g_{a} + f_{a} : C^e : Z : g_{Y} \\
 h^{dp} &= H^{dp} + g_{a} : C^e : f_{a} + g_{a} : C^e : Z : f_{Y} \\
 b^p &= f_{a} : C^e : \dot{\varepsilon} \\
 b^d &= g_{a} : C^e : \dot{\varepsilon}
\end{align*} \quad \text{(4.122-4.127)}
\]

The plastic multiplier and the damage multiplier can be solved from the linear system of equations given by Eqs. (4.120) and (4.121) such that:

\[
\begin{bmatrix}
\dot{\lambda}^p \\
\dot{\lambda}^d
\end{bmatrix} = \frac{1}{h} \begin{bmatrix}
 h^{dd} & - h^{pd} \\
 - h^{dp} & h^{pp}
\end{bmatrix} \begin{bmatrix}
b^p \\
b^d
\end{bmatrix}
\quad \text{(4.128)}
\]
where:

\[
H = h^{pp}h^{dd} - h^{pd}h^{dp}
\]  

(4.129)

Using this solution, the plastic and damage multipliers are written in terms of the incremental strain as follows:

\[
\dot{\lambda}^p = \frac{1}{h} \left( h^{dd}f_{\sigma} - h^{pd}g_{\sigma} \right) : C^e : \dot{\epsilon}
\]  

(4.130)

\[
\dot{\lambda}^d = \frac{1}{h} \left( -h^{dp}f_{\sigma} + h^{pp}g_{\sigma} \right) : C^e : \dot{\epsilon}
\]  

(4.131)

### 4.2.9 Elasto-Plastic-Damage Tangent Modulus

It is desired to obtain the elasto-plastic-damage tangent modulus which relates the incremental stress and the total incremental strain. It will be shown that this modulus can be derived in terms of an elastic continuum modulus which relates the incremental stress and the incremental elastic strain. In order to obtain these relations, the relation between the incremental stress and the incremental damage measure must be obtained. This relation is derived by substituting the incremental multipliers written in terms of the incremental stress, Eqs. (4.114) and (4.115), into the evolution equation for the damage measure, Eq. (4.94):

\[
\dot{\phi} = T : \dot{\sigma}
\]  

(4.132)

where:

\[
T = -\frac{1}{H} \left( f_{\gamma} \otimes \left( H^{dd}f_{\sigma} - H^{pd}g_{\sigma} \right) + g_{\gamma} \otimes \left( -H^{dp}f_{\sigma} + H^{pp}g_{\sigma} \right) \right)
\]  

(4.133)

Using this relation in the incremental form of the Hookean stress-strain relation, Eq. (4.118), a Hookean type relationship for the incremental stress can be obtained as follows:

\[
\dot{\sigma} = D^e : \left( \dot{\epsilon} - \dot{\epsilon}^{pd} \right) = D^e : \dot{\epsilon}^e
\]  

(4.134)

where the elastic continuum tangent modulus, \( D^e \), is defined by the following expression:
Using the evolution of the plastic strain, Eq. (4.93), along with the incremental multipliers defined in terms of the incremental stress defined by Eqs. (4.114) and (4.115), Eq. (4.134) becomes the constitutive law as follows:

\[ \dot{\sigma} = D^{epd} : \dot{\varepsilon} \]  

(4.136)

where the elastic-plastic-damage continuum tangent modulus, \( D^{epd} \), is defined by the following expression:

\[
D^{epd} = \begin{cases} 
D^{-e} & \text{if } \dot{\lambda}^p = 0; \dot{\lambda}^d = 0 \\
D^{-e} + \frac{f_\sigma \otimes f_\sigma}{H^{pp}} & \text{if } \dot{\lambda}^p > 0; \dot{\lambda}^d = 0 \\
D^{-e} + \frac{g_\sigma \otimes g_\sigma}{H^{dd}} & \text{if } \dot{\lambda}^p = 0; \dot{\lambda}^d > 0 \\
D^{-e} + f_\sigma \otimes \left( \frac{H^{dd}}{H} f_\sigma - \frac{H^{pd}}{H} g_\sigma \right) - g_\sigma \otimes \left( \frac{H^{dp}}{H} f_\sigma - \frac{H^{pp}}{H} g_\sigma \right) & \text{if } \dot{\lambda}^p > 0; \dot{\lambda}^d > 0 
\end{cases}
\]

(4.137)

It should be noted that, in order to avoid spurious loading-unloading at yield due to the abrupt transition from elasticity to plasticity (Belytschko et al., 2000), a consistent tangent modulus will be derived in a subsequent section.

### 4.2.10 Uniaxially Loaded Bar

In order to better understand the equations, the model developed in this chapter is reduced here to a one-dimensional, uniaxially loaded bar, with the assumption of isotropic damage. For the isotropic case of damage, the damage tensor is denoted by the diagonal matrix given in Eq. (4.4). As the damage tensor does not need to be rotated to obtain a diagonal matrix, the transformation matrix is defined as the identity tensor, i.e. \( Q = I \). This also means that the damage effect tensor is the principal damage effect tensor such that \( \hat{M} = \hat{M} \). Thus, for isotropic damage, the principal damage effect tensor defined by Eqs. (4.15) to (4.17) and the corresponding inverse of the principal damage effect tensor are reduced to the following:
\[
[M]_{ijkl} = \left[ \dot{M} \right]_{ijkl} = \frac{\delta_{ik} \delta_{jl}}{(1 - \varphi)} \quad (4.138)
\]
\[
[M]^{-1}_{ijkl} = \left[ \dot{M} \right]^{-1}_{ijkl} = (1 - \varphi) \delta_{ik} \delta_{jl} \quad (4.139)
\]

This also allows the following stress and elastic strain transformation laws which can be applied for Eqs. (4.13), (4.21), (4.24), (4.26), and (4.35):

\[
\hat{\sigma} = \frac{\sigma}{1 - \varphi} \quad (4.140)
\]
\[
\hat{s} = \frac{s}{1 - \varphi} \quad (4.141)
\]
\[
\hat{R} = \frac{R}{1 - \varphi} \quad (4.142)
\]
\[
\hat{X} = \frac{X}{1 - \varphi} \quad (4.143)
\]
\[
\hat{\varepsilon}^e = (1 - \varphi) \varepsilon^e \quad (4.144)
\]

Additionally, the transformation of the elastic stiffness tensor, Eq. (4.39), can be written as follows:

\[
C^e = (1 - \varphi)^2 \hat{C}^e \quad (4.145)
\]

Comparing Eq. (4.144) with the decomposition of the total elastic strain, Eq. (4.32), it is seen that the assumption of additive decomposition of the total elastic strain holds and that the additional component of the strain due to the reduction of the elastic stiffness tensor is found to be the following:

\[
\varepsilon^\text{ed} = \varphi \varepsilon^e \quad (4.146)
\]

For this loading case, as there are no shear stresses or shear strains, the Cauchy stress tensor is written in symmetric vector form in terms of axial components and reduced to be in terms of a single axial component:

\[
\{ \sigma \} = \begin{bmatrix} \sigma_{11} \\ 0 \\ 0 \end{bmatrix} \quad (4.147)
\]

Utilizing the relation given by Eq. (3.79) for the effective, undamaged configuration, the effective elastic strains can be written as follows:
From the transformation laws, Eqs. (4.140) and (4.144), the elastic strains in the damaged configuration are written in a similar form:

\[
\begin{align*}
\{\varepsilon_{11}^e\} &= \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu \\ -\nu & 1 & -\nu \\ -\nu & -\nu & 1 \end{bmatrix} \begin{bmatrix} \sigma_{11} \end{bmatrix} = \begin{bmatrix} \tilde{\varepsilon}_{11}^e \\ -\nu \tilde{\varepsilon}_{11}^e \end{bmatrix} \\
\{\varepsilon_{22}^e\} &= \begin{bmatrix} \varepsilon_{11}^e + \varepsilon_{11}^p \\ -\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p \\ -\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p \end{bmatrix} \\
\{\varepsilon_{33}^e\} &= \frac{1}{E (1 - \nu^2)} \begin{bmatrix} 1 & -\nu & -\nu \\ -\nu & 1 & -\nu \\ -\nu & -\nu & 1 \end{bmatrix} \begin{bmatrix} \sigma_{11} \end{bmatrix} = \begin{bmatrix} \tilde{\varepsilon}_{11}^e \\ -\nu \tilde{\varepsilon}_{11}^e \end{bmatrix}
\end{align*}
\] (4.149)

The plastic strain tensor and the backstress flux tensor conjugate force are used from Eqs. (3.80) and (3.82), and the total strain is rewritten here as follows:

\[
\begin{align*}
\{\varepsilon_{11}\} &= \left\{ \frac{\varepsilon_{11}^e + \varepsilon_{11}^p}{\varepsilon_{11}^e} \right\} \\
\{\varepsilon_{22}\} &= \left\{ -\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p \right\} \\
\{\varepsilon_{33}\} &= \left\{ -\nu \varepsilon_{11}^e - \frac{1}{2} \varepsilon_{11}^p \right\}
\end{align*}
\] (4.150)

Utilizing the definition of a deviatoric tensor, the effective relative stress tensor used in the yield condition and given by Eq. (4.27) can be written in the following form:

\[
\begin{align*}
\{\xi_{11}\} &= \left\{ \frac{2}{3} \sigma_{11}^e - X_{11} \right\} \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \\
\{\xi_{22}\} &= \left\{ \frac{2}{3} \sigma_{11}^e - X_{11} \right\} \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \\
\{\xi_{33}\} &= \frac{1}{1 - \nu^2} \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}
\end{align*}
\] (4.151)

The damage conjugate force, Eq. (4.89), can also be written for the 1D, isotropic damage case as follows:

\[
Y = -\frac{\sigma_{11}^2}{E (1 - \nu^2)^3}
\] (4.152)

The yield condition given by Eq. (4.86) and the damage condition given by Eq. (4.87) can now be written for the uniaxial loading case as follows:

\[
f = \sqrt{3} \left( \frac{\sigma_{11} - \frac{\nu}{2} X_{11}}{1 - \nu^2} - \sigma_{\nu} - \frac{R}{1 - \nu^2} \right) \leq 0
\] (4.153)

\[
g = \frac{\sigma_{11}^2}{E (1 - \nu^2)^3} - \sqrt{3} \left( \sigma_{\nu} + K \right) \leq 0
\] (4.154)
If plasticity occurs with loading, i.e. if $\dot{\lambda}^p > 0$, then the normals to the yield surface which will be required to compute the inverse elasto-plastic-damage modulus can be written as follows:

\[
\{ f_{\sigma} \} = \left\{ \frac{x}{\| x \|} = \frac{\sqrt{3}}{1 - \varphi} \begin{pmatrix} 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} \right\}
\] (4.155)

\[
f_{,y} = \sqrt{\frac{3}{2}} \left( \left| \sigma_{11} - \frac{3}{2} X_{11} \right| - R \right) \frac{E (1 - \varphi)^2}{\sigma_{11}^2} = -\sqrt{\frac{3}{2}} \frac{\sigma_{yp}}{Y}
\] (4.156)

\[
f_{,\sigma} = \sqrt{\frac{3}{2}} \left( \left| \sigma_{11} - \frac{3}{2} X_{11} \right| - \frac{R}{(1 - \varphi)^2} \right) = \sqrt{\frac{3}{2}} \frac{\sigma_{yp}}{1 - \varphi}
\] (4.157)

\[
f_{,r} = -\sqrt{\frac{3}{2}} \frac{1}{(1 - \varphi)}
\] (4.158)

\[
\{ f_{,x} \} = -\frac{1}{2} \{ f_{,\sigma} \}
\] (4.159)

Note that the second parts of Eqs. (4.156) and (4.157) were derived by using the following relationship which is from the yield surface and is valid when $f = 0$:

\[
\sigma_{yp} = \sqrt{\frac{3}{2}} \left( \left| \sigma_{11} - \frac{3}{2} X_{11} \right| - \frac{R}{1 - \varphi} \right)
\] (4.160)

If damage occurs with loading, i.e. if $\dot{\lambda}^d > 0$, then the normals to the damage surface which will be required to compute the inverse elasto-plastic-damage modulus can be written as follows:

\[
\{ g_{,\sigma} \} = \frac{2 \sigma_{11}}{E (1 - \varphi)^3} \begin{pmatrix} 1 \\ -\nu \\ -\nu \end{pmatrix}
\] (4.161)

\[
g_{,y} = -1
\] (4.162)

\[
g_{,\sigma} = \frac{-\sigma_{11}^2}{E (1 - \varphi)^4} = \frac{Y}{(1 - \varphi)}
\] (4.163)

\[
g_{,x} = -\sqrt{\frac{3}{2}}
\] (4.164)

The relation between the increment of the uniaxial stress and the increment of uniaxial strain can be found from the inverse of the constitutive relation, Eq. (4.137):
The inverse elastic-plastic-damage modulus is written in terms of the inverse elastic continuum modulus. The desired component of this modulus if found from Eq. (4.135) and can be written here as follows:

\[
D^{-e}_{1111} \sigma_{11} = \dot{\epsilon}_{11}
\]  

\[
(4.165)
\]

\[
D^{-e}_{1111} = \begin{cases}
\frac{1}{E(1-\varphi)^2} & \text{if } \dot{\lambda}^p = 0; \dot{\lambda}^d = 0 \\
\frac{1}{E(1-\varphi)^2} - \frac{4\sigma_{yp}}{3(1-\varphi)\sigma_{11}} \frac{1}{H^{pp}} & \text{if } \dot{\lambda}^p > 0; \dot{\lambda}^d = 0 \\
\frac{1}{E(1-\varphi)^2} + \frac{4\sigma_{11}^2}{E^2(1-\varphi)^6} \frac{1}{H^{dd}} & \text{if } \dot{\lambda}^p = 0; \dot{\lambda}^d > 0 \\
\frac{1}{E(1-\varphi)^2} - \left( \frac{4\sigma_{yp}}{3(1-\varphi)\sigma_{11}} \frac{H^{dd}}{H} - \frac{4\sqrt{3}\sigma_{yp}}{E(1-\varphi)^3} \frac{H^{pd}}{H} \right) & \text{if } \dot{\lambda}^p > 0; \dot{\lambda}^d > 0 \\
\left( \frac{2\sqrt{3}\sigma_{11}}{E(1-\varphi)^4} \frac{H^{dp}}{H} - \frac{4\sigma_{11}^2}{E^2(1-\varphi)^6} \frac{H^{pp}}{H} \right) & \text{if } \dot{\lambda}^p > 0; \dot{\lambda}^d > 0
\end{cases}
\]

(4.166)

where the hardening coefficients are defined as follows:

\[
H^{pp} = \frac{2}{3(1-\varphi)^2} \frac{\partial R(r)}{\partial r} + \frac{2}{(1-\varphi)^2} \frac{\partial X_{11}}{\partial \alpha_{11}} - \frac{2}{3} \frac{\sigma_{yp}^2}{(1-\varphi)Y}
\]

(4.167)

\[
H^{pd} = -\sqrt{3} \frac{\sigma_{yp}}{1-\varphi}
\]

(4.168)

\[
H^{dp} = -\sqrt{3} \frac{\sigma_{yp}}{1-\varphi}
\]

(4.169)

\[
H^{dd} = \frac{2}{3} \frac{\partial K(\kappa)}{\partial \kappa} \frac{Y}{(1-\varphi)}
\]

(4.170)

\[
H = H^{pp} H^{dd} - H^{pd} H^{dp}
\]

(4.171)

The desired component of the elasto-plastic-damage modulus can now be found from Eq. (4.137) as follows:
Thus, from Eq. (4.165), the relation between the total incremental strain and the uniaxial stress is given as follows:

$$\bar{\sigma}_{11} = \frac{1}{D_{1111}^{eqd}} \dot{\varepsilon}_{11}$$  \hspace{1cm} (4.173)

4.3 Rate Boundary Value Problem

In the analysis of a small deformation rate boundary value problem (see 2D example, Figure 4.5), the body has a plastic region, $V_p$, and an elastic region outside of this zone. Additionally, the body has a damage region $V_d$ which may be in either or both the elastic and plastic domains. The region which overlaps both the plastic region and the damaged region is denoted by $V_{p_d}$. $V$ denotes the total domain.

The rate boundary value problem in the strong form is described by the following governing equations:

**Equilibrium equation:**

$$\nabla \cdot \bar{\sigma} + b = 0$$  \hspace{1cm} (4.174)

**Applied tractions boundary condition**

$$n \cdot \bar{\sigma} + \bar{t} = 0 \text{ on } \Gamma_t$$  \hspace{1cm} (4.175)

**Applied displacements boundary condition**

$$u = \bar{u} \text{ on } \Gamma_u$$  \hspace{1cm} (4.176)
where $\Gamma_r$ is the boundary over which tractions, $\hat{t}$, are applied, $\Gamma_u$ is the boundary over which displacements, $\hat{u}$, are applied, and $b$ are body forces. In this local model using finite elements, only the equilibrium equation is required in order to obtain a unique solution of the boundary value problem. The weak form of the equilibrium equation can be written by multiplying Eq. (3.129) by a virtual displacement rate vector, $\delta \hat{u}$, and integrating. The equilibrium equation is integrated over the entire body:

$$\int_v \delta \hat{u} \cdot (\nabla \cdot \hat{\sigma} + \dot{\hat{b}}) dV = 0 \quad (4.177)$$

Integrating by parts the weak form of the equilibrium equation gives the following:

$$\int_v \delta \hat{u} \cdot bdV + \int_{\Gamma_r} \delta \hat{u} \cdot \dot{\hat{t}} d\Gamma =$$

$$\int_v \delta \varepsilon : C^e : (\dot{\varepsilon} - f_{\sigma} \dot{\lambda}^p - g_{\sigma} \dot{\lambda}^d - Z : (f_{\gamma} \dot{\lambda}^p + g_{\gamma} \dot{\lambda}^d)) dV \quad (4.178)$$

### 4.4 Integration Algorithm

In the solution procedure, a linearized form of the governing equation given by Eq. (4.178) is solved within an incremental iterative Newton-Raphson solution procedure for

![Figure 4.5](image)

**Figure 4.5**: A general boundary value problem consisting of a body with a plastic region, $V_{\lambda^p}$, a damage region, $V_{\lambda^d}$, a damaged-plastic region, $V_{\lambda^p\lambda^d}$, and an elastic region, $V_e$. 

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the increment of strain over the time increment $\Delta t_j$ such that:

$$\varepsilon_j = \varepsilon_0 + \Delta t_j \varepsilon = \varepsilon_0 + \Delta \varepsilon_j$$

(4.179)

where the subscripted $j$'s and 0 indicate that the variable is computed at iteration $j$ and at the previously converged state, respectively; and the symbol $\Delta$ denotes a total increment from the previously converged state to the iteration, $j$. The increments of the plastic multiplier, $\Delta \lambda_j^p$, and the damage multiplier, $\Delta \lambda_j^d$, are then computed, and the state of the material is updated such that:

$$\varepsilon_j^{pd} = \varepsilon_0^{pd} + \Delta \varepsilon_j^{pd}$$

(4.180)

$$\phi_j = \phi_0 + \Delta \phi_j$$

(4.181)

$$r_j = r_0 + \Delta r_j$$

(4.182)

$$\alpha_j = \alpha_0 + \Delta \alpha_j$$

(4.183)

$$\kappa_j = \kappa_0 + \Delta \kappa_j$$

(4.184)

The stress and the damage measure for this integration scheme are also defined at iteration $j$ as follows:

$$\sigma_j = C_j^e : (\varepsilon_j - \varepsilon_j^{pd}) = \sigma_0 + C_j^e : (\Delta \varepsilon_j - \Delta \varepsilon_j^{pd}) + C_j^e : Z_j : \Delta \phi_j$$

(4.185)

$$Y_j = \sigma_j^T : \left( \frac{\partial C_j^{-e}}{\partial \phi} \right)_j : \sigma_j$$

(4.186)

where the damaged elastic stiffness tensor can be defined in incremental form as follows:

$$C_j^e = C_0^e + \Delta C_j^e$$

(4.187)

The integration scheme used here enforces that $f_j = 0$ and $g_j = 0$ at the end of the time step:

$$F_j = f_j = \| N_j : (\sigma_j - X_j) \| - \sqrt{\frac{2}{3}} \left[ \sigma_{p} \frac{R_j}{1 - \| \phi_j \|} \right] \leq 0$$

(4.188)

$$G_j = g_j = \| Y_j \| - \sqrt{\frac{2}{3}} \left[ \sigma_{yd} + K_j \right] \equiv 0$$

(4.189)

where the deviatoric damage measure tensor is defined as follows:

$$N_j = M_j - \frac{1}{3} I \otimes I : M_j = I^D : M_j$$

(4.190)
and the conjugate forces are defined as functions of the state variables such that:

\[
R_j = R(r_j) \quad (4.191)
\]

\[
X_j = X(\alpha_j) \quad (4.192)
\]

\[
K_j = K(\kappa_j) \quad (4.193)
\]

In order to address this type of problem, a return mapping algorithm is used. This algorithm has an initial elastic-predictor step, followed by a plastic-damage-corrector step. In the elastic-predictor step, the incremental strains are assumed to be elastic with no damage such that an initial trial stress and an initial trial damage conjugate force can be computed as:

\[
\sigma_{j}^{trial} = \sigma_0 + C_0^e : \Delta \varepsilon_j \quad (4.194)
\]

\[
Y_{j}^{trial} = \sigma_j^{trial} : \left( \frac{\partial C^{-e}}{\partial \varepsilon} \right)_0 : \sigma_j^{trial} \quad (4.195)
\]

The trial state \((\sigma_j^{trial}, Y_j^{trial}, \varepsilon_j^{pd}, \varphi_j, r_j, \alpha_j, \kappa_j)\) is then used in a trial yield criterion and a trial damage criterion to decide whether an elastic point enters the plastic and/or damage regimes or whether a plastic or damage point elastically unloads. For the case when \(f_{trial} \leq 0\) and \(g_{trial} \leq 0\), the integration point is assumed to be elastic with no additional damage and the current state \((\sigma_j, Y_j, \varepsilon_j^{pd}, \varphi_j, r_j, \alpha_j, \kappa_j)\) is set to the trial state \((\sigma_j^{trial}, Y_j^{trial}, \varepsilon_j^{pd}, \varphi_j, r_j, \alpha_j, \kappa_j)\). Alternatively, when \(f_{trial} > 0\), the current state resulting from this trial state lies outside of the yield surface. Plasticity has occurred and the state has to be returned to the yield surface. Similarly, when \(g_{trial} > 0\), the current state resulting from this trial state lies outside of the damage surface. Damage has occurred and the state has to be returned to the damage surface. Using the definition of the Cauchy stress from Eq. (4.185) along with the definition of the trial stress, Eq. (4.194), the Cauchy stress is corrected as follows:

\[
\sigma_j = \sigma_j^{trial} + \Delta C_j^e : \Delta \varepsilon_j - C_j^e : \Delta \varepsilon_j^{pd} + C_j^e : Z_j : \Delta \varphi_j \quad (4.196)
\]

Thus, the correction to the stress during the corrector phase is defined as:

\[
\Delta \sigma_j = \Delta C_j^e : \Delta \varepsilon_j - C_j^e : \Delta \varepsilon_j^{pd} + C_j^e : Z_j : \Delta \varphi_j \quad (4.197)
\]

While the trial stress is computed based upon the increment of the total strain, this inelastic corrector is computed based upon the increments of the plastic multiplier and the damage multiplier which are computed from the integration scheme used. In this scheme, the increment of the multipliers are set to zero \((\Delta \lambda_j^{p(0)} = 0; \Delta \lambda_j^{d(0)} = 0)\), and, at
each iteration, \( k \), the plastic and damage multipliers are incremented by \( d\lambda_j^{p(k)} \) and \( d\lambda_j^{d(k)} \), respectively, such that:

\[
\begin{align*}
\Delta\lambda_j^{p(k+1)} &= \Delta\lambda_j^{p(k)} + d\lambda_j^{p(k)} \\
\Delta\lambda_j^{d(k+1)} &= \Delta\lambda_j^{d(k)} + d\lambda_j^{d(k)}
\end{align*}
\]  

(4.198)  

(4.199)

This increment is computed by using a linearized form of the nonlinear equation, \( f(\Delta\lambda_j^p, \Delta\lambda_j^d) \), such that:

\[
f^{(k)} + \frac{df^{(k)}}{d\Delta\lambda_j^p} d\lambda_j^{p(k)} + \frac{df^{(k)}}{d\Delta\lambda_j^d} d\lambda_j^{d(k)} = 0
\]

(4.200)

This iterative procedure is followed until the state computed from the plastic multiplier and the damage multiplier converges. This occurs when the stress has returned to both the yield surface and to the damage surface.

### 4.4.1 Fully Implicit Backward Euler Scheme

An implicit backward Euler scheme as presented in Belytschko et al. (2000) is used for the integration of the constitutive model. This type of integration scheme is implicit (computed at time \( j \)) in the plasticity multiplier, the damage multiplier, the plastic strain, the damage measure, the hardening variables, and the plastic flow direction. The integration scheme is defined by Eqs. (4.180) to (4.189), where the increments of the state variables are written as follows:

\[
\Delta\sigma_j = f_{\sigma_j} \Delta\lambda_j^p + g_{\sigma_j} \Delta\lambda_j^d
\]  

(4.201)

\[
\Delta\varphi_j = -f_{\chi_j} \Delta\lambda_j^p - g_{\chi_j} \Delta\lambda_j^d
\]  

(4.202)

\[
\Delta r_j = -f_{r_j} \Delta\lambda_j^p
\]  

(4.203)

\[
\Delta\alpha_j = f_{\alpha_j} \Delta\lambda_j^p
\]  

(4.204)

\[
\Delta\kappa_j = -f_{\kappa_j} \Delta\lambda_j^d
\]  

(4.205)

The increment of the elastic stiffness tensor is also defined here as follows:

\[
\Delta C_j^e = \left( \frac{\partial C_j^e}{\partial \varphi} \right)_j : \Delta\varphi_j = 2 C_j^e : M_j^T : \left( \frac{\partial M_j^{-T}}{\partial \varphi} \right)_j : \Delta\varphi_j
\]

(4.206)

Thus, the correction to the stress during the corrector phase can be written as follows:
\[ \Delta \sigma_j = -C^\varepsilon_j : \Delta \varepsilon_{pd}^{j} + \left( \frac{\partial C^\varepsilon}{\partial \varphi} \right)_j : \left( \varepsilon_j + \Delta \varepsilon_j - \varepsilon_{pd}^{j} \right) : \Delta \varphi_j \] (4.207)

It can be seen that the problem defined by this model can be entirely defined by solving for three unknowns, \( \Delta \sigma_j \), \( \Delta \lambda_j^p \), and \( \Delta \lambda_j^d \), through the use of the following three nonlinear equations defined from Eqs. (4.201), (4.188), and (4.189):

\[
a_j = -\varepsilon_{pd}^{j} + \varepsilon_0^{j} + f_{\sigma_j} \Delta \lambda_j^p + g_{\sigma_j} \Delta \lambda_j^d = 0 \] (4.208)

\[
f_j = \| \mathbf{N}_j : (\sigma_j - \mathbf{X}_j) \| - \sqrt{2} \left[ \sigma_{yp} + \frac{R_j}{1 - \| \varphi_j \|} \right] \leq 0 \] (4.209)

\[
g_j = \| \mathbf{Y}_j \| - \sqrt{2} \left[ \sigma_{yd} + K_j \right] \equiv 0 \] (4.210)

Making use of Eq. (4.197), these three equations can be linearized as in Eq. (4.200) such that, for each iteration \( k \), the following equations hold:

\[
a_j^{(k)} + C^{-\varepsilon_j^{(k)}} : d\sigma_j^{(k)} - C^{-\varepsilon_j^{(k)}} : \left( \frac{\partial C^\varepsilon}{\partial \varphi} \right)^{(k)}_j : \left( \varepsilon_j^{(k)} + d\varepsilon_j^{(k)} - \varepsilon_{pd}^{(k)} \right) : d\varphi_j^{(k)} \
+ df_{\sigma_j}^{(k)} \Delta \lambda_j^p^{(k)} + f_{\sigma_j}^{(k)} d\lambda_j^p^{(k)} + g_{\sigma_j}^{(k)} \Delta \lambda_j^d^{(k)} + g_{\sigma_j}^{(k)} d\lambda_j^d^{(k)} = 0 \] (4.211)

\[
f_j^{(k)} + f_{\sigma_j}^{(k)} : d\sigma_j^{(k)} + f_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + f_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} = 0 \] (4.212)

\[
g_j^{(k)} + g_{\sigma_j}^{(k)} : d\sigma_j^{(k)} + g_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + g_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} = 0 \] (4.213)

where:

\[
d\varphi_j^{(k)} = -\left( f_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + df_{\lambda_j^p}^{(k)} \Delta \lambda_j^p^{(k)} + g_{\lambda_j^p}^{(k)} d\lambda_j^d^{(k)} + dg_{\lambda_j^p}^{(k)} \Delta \lambda_j^d^{(k)} \right) \] (4.214)

The increments of the normals to the yield surface and to the damage surface can be expanded in terms of the increments of the unknowns such that:

\[
df_{\sigma_j}^{(k)} = f_{\sigma_j}^{(k)} : d\sigma_j^{(k)} + f_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + f_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} \] (4.215)

\[
df_{\lambda_j^p}^{(k)} = f_{\lambda_j^p}^{(k)} : d\sigma_j^{(k)} + f_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + f_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} \] (4.216)

\[
dg_{\sigma_j}^{(k)} = g_{\sigma_j}^{(k)} : d\sigma_j^{(k)} + g_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + g_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} \] (4.217)

\[
dg_{\lambda_j^p}^{(k)} = g_{\lambda_j^p}^{(k)} : d\sigma_j^{(k)} + g_{\lambda_j^p}^{(k)} d\lambda_j^p^{(k)} + g_{\lambda_j^d}^{(k)} d\lambda_j^d^{(k)} \] (4.218)
The first and second derivatives of the yield condition and of the damage condition in Eqs. (4.211) to (4.218) are given in APPENDIX B.1 and are evaluated at time step $j$ and at iteration $k$. After substituting Eq. (4.214), (4.215), (4.216), (4.217), and (4.218) into Eq. (4.211), the increment of the stress can be solved for such that:

$$d\sigma_j^{(k)} = -A_j^{(k)} : a_j^{(k)} - A_j^{p(k)} : A_j^{p(k)} d\lambda_j^{p(k)} - A_j^{d(k)} : A_j^{d(k)} d\lambda_j^{d(k)}$$  \hspace{1cm} (4.219)$$

where:

$$A_j^{-l(k)} = C_j^{-l(k)} + f_{,\sigma_\sigma_j} \Delta \lambda_j^{p(k)} + g_{,\sigma_\sigma_j} \Delta \lambda_j^{d(k)} + C_j^{-l(k)} \left( \frac{\partial C^e}{\partial \phi} \right)_j^{(k)} \left( \epsilon_j^{(k)} + d\epsilon_j^{(k)} - \epsilon_j^{pd(k)} \right) \left( f_{,\lambda_\lambda_j} \Delta \lambda_j^{p(k)} + g_{,\lambda_\lambda_j} \Delta \lambda_j^{d(k)} \right)$$  \hspace{1cm} (4.220)$$

$$A_j^{p(k)} = f_{,\lambda} + f_{,\lambda \lambda_j} \Delta \lambda_j^{p(k)} + g_{,\lambda \lambda_j} \Delta \lambda_j^{d(k)} + C_j^{-l(k)} \left( \frac{\partial C^e}{\partial \phi} \right)_j^{(k)} \left( \epsilon_j^{(k)} + d\epsilon_j^{(k)} - \epsilon_j^{pd(k)} \right) \left( f_{,\lambda_\lambda_j} \Delta \lambda_j^{p(k)} + g_{,\lambda_\lambda_j} \Delta \lambda_j^{d(k)} \right)$$  \hspace{1cm} (4.221)$$

$$A_j^{d(k)} = g_{,\lambda} + f_{,\lambda \lambda_j} \Delta \lambda_j^{p(k)} + g_{,\lambda \lambda_j} \Delta \lambda_j^{d(k)} + C_j^{-l(k)} \left( \frac{\partial C^e}{\partial \phi} \right)_j^{(k)} \left( \epsilon_j^{(k)} + d\epsilon_j^{(k)} - \epsilon_j^{pd(k)} \right) \left( g_{,\lambda_\lambda_j} \Delta \lambda_j^{p(k)} + g_{,\lambda_\lambda_j} \Delta \lambda_j^{d(k)} \right)$$  \hspace{1cm} (4.222)$$

This increment of stress can now be substituted into the linearized yield condition, Eq. (4.212), which can then be written in the following form:

$$h_j^{p(k)} d\lambda_j^{p(k)} + h_j^{pd(k)} d\lambda_j^{d(k)} \equiv b_j^{p(k)}$$  \hspace{1cm} (4.223)$$

where:

$$h_j^{p(k)} = f_{,\lambda} + f_{,\lambda \lambda_j} \Delta \lambda_j^{p(k)}$$  \hspace{1cm} (4.224)$$

$$h_j^{pd(k)} = f_{,\lambda} + f_{,\lambda \lambda_j} \Delta \lambda_j^{d(k)}$$  \hspace{1cm} (4.225)$$

$$b_j^{p(k)} = f_{,\lambda} - f_{,\lambda \lambda_j} : a_j^{(k)}$$  \hspace{1cm} (4.226)$$

The increment of stress can also be substituted into the linearized damage condition, Eq. (4.213), which can then be written in the following form:
where:

\[
h_j^{d_p(k)} = g^{(k)}_{,\sigma_j} : A_j^{(k)} : \mathbf{a}_j^{(k)} - g^{(k)}_{,a_j} \quad (4.228)
\]

\[
h_j^{d_d(k)} = g^{(k)}_{,\sigma_j} : A_j^{(k)} : \mathbf{a}_j^{(k)} - g^{(k)}_{,a_j} \quad (4.229)
\]

\[
b_j^{d_d(k)} = g^{(k)}_{,\sigma_j} : A_j^{(k)} : \mathbf{a}_j^{(k)} \quad (4.230)
\]

The plastic multiplier and the damage multiplier can be solved from the linear system of equations given by Eqs. (4.120) and (4.121) such that:

\[
\begin{bmatrix}
    d\lambda_j^{p(k)} \\
    d\lambda_j^{d(k)}
\end{bmatrix} = \frac{1}{h_j^{(k)}} \begin{bmatrix}
    h_j^{d_d(k)} & -h_j^{p_d(k)} \\
    -h_j^{d_p(k)} & h_j^{p_p(k)}
\end{bmatrix} \begin{bmatrix}
    b_j^{p(k)} \\
    b_j^{d(k)}
\end{bmatrix} \quad (4.231)
\]

where:

\[
h_j^{(k)} = h_j^{p_p(k)} h_j^{d_d(k)} - h_j^{p_d(k)} h_j^{d_p(k)} \quad (4.232)
\]

Using this solution, the plastic and damage multipliers are written as follows:

\[
d\lambda_j^{p(k)} = \frac{1}{h_j^{(k)}} \left( h_j^{d_d(k)} \left( f_j^{(k)} - f_{,\sigma_j}^{(k)} : A_j^{(k)} : \mathbf{a}_j^{(k)} \right) - h_j^{p_d(k)} \left( g_j^{(k)}_{,\sigma_j} : A_j^{(k)} : \mathbf{a}_j^{(k)} \right) \right) \quad (4.233)
\]

\[
d\lambda_j^{d(k)} = \frac{1}{h_j^{(k)}} \left( -h_j^{d_p(k)} \left( f_j^{(k)} - f_{,\sigma_j}^{(k)} : A_j^{(k)} : \mathbf{a}_j^{(k)} \right) + h_j^{p_p(k)} \left( g_j^{(k)}_{,\sigma_j} : A_j^{(k)} : \mathbf{a}_j^{(k)} \right) \right) \quad (4.234)
\]

Thus, the increments of the unknown stress and the unknown plastic and damage multipliers have been derived at iteration \( k \). Using Eqs. (4.219), (4.233), and (4.234), the unknowns are updated as follows:

\[
\Delta\lambda_j^{p(k+1)} = \Delta\lambda_j^{p(k)} + d\lambda_j^{p(k)} \quad (4.235)
\]

\[
\Delta\lambda_j^{d(k+1)} = \Delta\lambda_j^{d(k)} + d\lambda_j^{d(k)} \quad (4.236)
\]

\[
\sigma_j^{(k+1)} = \sigma_j^{(k)} + d\sigma_j^{(k)} \quad (4.237)
\]

Using the increments of the damage and plastic multiplier, the increments of the yield surface normals and the damage surface normals are computed using Eqs. (4.215), (4.216), (4.217), and (4.218). Using the resulting matrices, the state variables are updated as follows:
\[ \varepsilon_j^{\text{eq}(k+1)} = \varepsilon_j^{\text{eq}(k)} + f_{e,\sigma_j}^k \Delta \varepsilon_j^{\text{eq}(k)} + \frac{df_{e,\sigma_j}^k}{d\varepsilon_j^{\text{eq}(k)}} \Delta \varepsilon_j^{\text{eq}(k)} + g_{e,\sigma_j}^k d \lambda_j^{d(k)} + dg_{e,\sigma_j}^k d \lambda_j^{d(k)} \] (4.238)

\[ \phi_j^{(k+1)} = \phi_j^{(k)} - f_{\phi,\sigma_j}^k \Delta \phi_j^{(k)} - \frac{df_{\phi,\sigma_j}^k}{d\phi_j^{(k)}} \Delta \phi_j^{(k)} - g_{\phi,\sigma_j}^k d \lambda_j^{d(k)} - dg_{\phi,\sigma_j}^k d \lambda_j^{d(k)} \] (4.239)

\[ f_j^{(k+1)} = f_j^{(k)} - f_{f,\sigma_j}^k d \lambda_j^{p(k)} \] (4.240)

\[ a_j^{(k+1)} = a_j^{(k)} + f_{a,\sigma_j}^k d \lambda_j^{p(k)} + df_{a,\sigma_j}^k d \lambda_j^{d(k)} \] (4.241)

\[ \kappa_j^{(k+1)} = \kappa_j^{(k)} - f_{\kappa,\sigma_j}^k d \lambda_j^{d(k)} \] (4.242)

The Newton iteration procedure is repeated until convergence is obtained by checking \( a_j, f_j, \) and \( g_j \) from Eqs. (4.208) to (4.210).

### 4.4.2 Consistent Tangent Operator

The trial stress can be used to predict if an integration point has entered the plastic and/or damage regime, and the internal state variables can then be updated using the integration scheme. In order to obtain proper quadratic convergence, the choice of a tangent operator must be consistent with the integration scheme. The consistent tangent operator is defined as follows (e.g. Simo & Taylor, 1985):

\[ C_{jg}^{\text{eq}} = \left( \frac{d\sigma}{d\varepsilon} \right)_j \] (4.243)

Following the procedure given in Belytschko et al. (2000), the following set of equations are used which corresponds to the integration scheme of the previous section:

\[ d\sigma_j = C_j^e : (d\varepsilon_j - d\varepsilon_j^{\text{eq}}) + C_j^\phi : d\phi_j \] (4.244)

\[ d\varepsilon_j^{\text{eq}} = df_{\varepsilon,\sigma_j}^p \Delta \varepsilon_j^{p} + f_{\varepsilon,\sigma_j}^p d \lambda_j^{e} + dg_{\varepsilon,\sigma_j}^p d \lambda_j^{d} \] (4.245)

\[ d\phi_j = -df_{\phi,\sigma_j}^p \Delta \phi_j^{p} - f_{\phi,\sigma_j}^p d \lambda_j^{e} - dg_{\phi,\sigma_j}^p d \lambda_j^{d} \] (4.246)

\[ df_j = f_{\sigma,\sigma_j}^p : d\sigma_j + f_{\lambda,\lambda_j}^e d \lambda_j^{e} + f_{\lambda,\lambda_j}^d d \lambda_j^{d} = 0 \] (4.247)

\[ dg_j = g_{\sigma,\sigma_j}^p : d\sigma_j + g_{\lambda,\lambda_j}^e d \lambda_j^{e} + g_{\lambda,\lambda_j}^d d \lambda_j^{d} = 0 \] (4.248)

where the increments of the yield surface normal and damage surface normal required in these equations are defined by evaluating the normals in the previous section at time step \( j \). These equations are substituted into Eqs. (4.245) and (4.246), and the resulting equations are then substituted into Eq. (4.244). The resulting equation can be solved for the increment of the stress such that:

\[ d\sigma_j = A_j d\varepsilon_j - d\lambda_j^p A_j^p - d\lambda_j^d A_j^d \] (4.249)

where:
The plastic multiplier and the damage multiplier can be solved from the linear system of equations given by Eqs. (4.253) and (4.257) such that:

\[
\begin{pmatrix}
\frac{d\lambda_j^p}{d\lambda_j^d} \\
\frac{d\lambda_j^d}{d\lambda_j^d}
\end{pmatrix} = \frac{1}{h_j} \begin{pmatrix} h_j^{dd} & -h_j^{dp} \\ -h_j^{dp} & h_j^{pp} \end{pmatrix} \begin{pmatrix} b_j^p \\ b_j^d \end{pmatrix}
\]

(4.261)

where:

\[
h_j = h_j^{pp} h_j^{dd} - h_j^{pd} h_j^{dp}
\]

(4.262)
Using this solution, the plastic and damage multipliers are written in terms of the incremental strain as follows:

\[ d\lambda^p_j = \frac{1}{h_j}\left(h^{dd}_j f_{\sigma_j} - h^{pd}_j g_{\sigma_j}\right) : C^e_j : d\varepsilon_j \]  
(4.263)

\[ d\lambda^d_j = \frac{1}{h_j}\left(-f_{\sigma_j} h^{dp}_j + g_{\sigma_j} h^{pp}_j\right) : C^e_j : d\varepsilon_j \]  
(4.264)

Substituting the above relations in Eq. (4.249) gives the algorithmic relation between the increment of the stress and the elastic strain as follows:

\[ d\sigma_j = C_{\text{alg}}^e : d\varepsilon_j \]  
(4.265)

where \( C_{\text{alg}}^e \) is the algorithmic stiffness operator and is defined as follows:

\[ C_{\text{alg}}^e = A_j - \frac{1}{h_j} A_j : \left(A_j^d \otimes \left(h^{dd}_j f_{\sigma_j} - h^{pd}_j g_{\sigma_j}\right) + A_j^d \otimes \left(-f_{\sigma_j} h^{dp}_j + g_{\sigma_j} h^{pp}_j\right)\right) : C^e_j \]  
(4.266)

In the next section, an algebraic form of the governing equation is formulated using the integration scheme which can be solved within an incremental iterative Newton-Raphson solution.

### 4.5 Finite Element Formulation

In order to solve a boundary value problem, the finite element approach is adopted in this work such that the displacement field is discretized. The algorithm requires a weak satisfaction of the equilibrium condition such that:

\[ \int_V \delta u : (\nabla \cdot \sigma + \mathbf{b}_j) dV = 0 \]  
(4.267)

Using integration by parts for the weak form of the equilibrium equation, and substituting the algorithmic relation Eq. (3.182), the governing equation is written as follows:

\[ \int_V \delta \varepsilon : C_{\text{alg}}^e : d\varepsilon_j dV = \int_V \delta \mathbf{u} : \mathbf{b}_j dV + \int_{\Gamma} \delta \mathbf{u} : \mathbf{t}_j d\Gamma - \int_V \delta \varepsilon : \sigma_j dV \]  
(4.268)

Note that this equation is enforced over the entire body, including the plastic domain, the damage domain, and the elastic domain. In the right hand side of the governing equations, the stress at iteration \( j \) must be known. As seen from the integration scheme,
for each integration point in an inelastic state, the backward Euler elastic predictor-inelastic corrector algorithm is used to compute the stress. The governing equation can be linearized consistently and solved within an incremental iterative Newton-Raphson solution procedure.

The displacement is discretized using a set of displacement nodal degrees of freedom contained in the vector \( \{ a_j \} \). As the governing equation only involves first order derivatives of the displacement field (i.e. strains), the discretization procedure for the displacement field only requires \( C^0 \) continuous interpolation functions. The interpolating relation and the strain-displacement relation are defined in the plasticity chapter by Eqs. (3.186) and (3.187), respectively. Using these discretization, the weak form of the equilibrium equation defined by Eq. (4.268) becomes:

\[
\{ \delta a \}^T \int \left[ B^T \left[ C_{alg}^j \right] B \right] \{ da \} \, dV = \{ \delta a \}^T \left( \int \left[ \{ N \}^T \{ b_j \} \right] \, dV + \int \left[ \{ N \}^T \{ \dot{t}_j \} \right] \, d\Gamma - \int \left[ \{ B \}^T \{ \sigma_j \} \right] \, dV \right) \tag{4.269}
\]

As this governing equation must be admissible for any variation in \( \{ \delta a \} \), this equation can be written as a set of algebraic equations:

\[
[K_{aa}] \{ da \} = [f_e] + [f_a] + [f_b] \tag{4.270}
\]

where the sub-matrices are defined as follows:

**Diagonal matrices**

\[
[K_{aa}] = \int \left[ B^T \left[ C_{alg}^j \right] B \right] \, dV \tag{4.271}
\]

**External force vector and body force vector**

\[
[f_e] = \int \left[ \{ N \}^T \{ \dot{t}_j \} \right] \, d\Gamma \tag{4.272}
\]

\[
[f_b] = \int \left[ \{ N \}^T \{ b_j \} \right] \, dV \tag{4.273}
\]

**Vector of nodal forces (equivalent to internal stresses)**

\[
[f_a] = -\int \left[ B^T \left[ \sigma_j \right] \right] \, dV \tag{4.274}
\]

Thus, the weak form of the governing equation has been written in terms of a stiffness matrix, a vector of degrees of freedom, and a vector of residuals in the standard form used by finite elements. These matrices and vectors can be computed for the elements.
which discretize a body and accumulated into global matrices and vectors for the entire body. A finite element procedure is then followed to solve the equations. The problem defined by this set of equations is nonlinear as the stiffness and the load residuals are a function of the body deformation. The degrees of freedom thus cannot automatically be solved from the system of equations. An iterative procedure is thus required to obtain the degrees of freedom such that the left-hand side of the governing equations is in equilibrium with the load vector residuals of the right-hand side. A typical procedure, which is not discussed here but is readily available from the commercial finite element program ABAQUS using the user subroutine UEL, is the Newton-Raphson method; however, other methods such as the modified Newton-Raphson may be used.

4.6 CONCLUSIONS

In this chapter, the framework of continuum damage mechanics was presented and used to develop a plasticity model coupled with damage through thermodynamically consistent theoretical formulations. The numerical implementation for this coupled model was also given. Following standard thermodynamics and using local state variables, a complete set of constitutive equations were derived where a local yield surface was used to determine the occurrence of plasticity and a local damage surface was used to determine the occurrence of damage. Hardening conjugate forces (stress like terms) for both plasticity and damage were defined as general functions of their corresponding hardening state variables (strain like terms). A fully implicit backward Euler scheme was developed and a set of governing equations were derived to be solved in a Newton-Raphson solution procedure. The next chapter takes this framework and introduces gradient enhancements into the plasticity condition and into the damage condition and proved the numerical implementation for this gradient enhanced coupled damage-plasticity model.
CHAPTER 5: GRADIENT ENHANCED COUPLED PLASTICITY –
DAMAGE MODEL

5.1 INTRODUCTION

The constitutive model for the gradient theory is derived using consistent thermodynamics in a similar fashion as in CHAPTER 4 for the classical rate-independent continuum J2 plasticity model coupled with damage. Based on the first law of thermodynamics, the Helmholtz free energy is introduced to describe the current state of energy in the material (Malvern, 1969; Coussy, 1995), and is a function of the strain and the internal state variables under consideration.

In this work, it is assumed that the solid can be modeled as rate independent and can be considered to be deforming quasi-statically and isothermally. The gradient enhanced constitutive model is derived using consistent thermodynamics in the same fashion as a classical rate-independent continuum J2 plasticity model (e.g. Doghri, 1993; Simo & Hughes, 1998; Belytschko et al., 2000) coupled with a continuum damage model (e.g. Kachanov, 1958; Lee et al., 1985; Voyiadjis & Kattan, 1992, 1993; Voyiadjis & Deliktas, 2000).

5.2 GRADIENT-ENHANCED CONTINUUM MECHANICS AND THERMODYNAMICS

The gradient enhanced constitutive model is derived using consistent thermodynamics in the same fashion as a classical rate-independent continuum J2 plasticity model (e.g. Doghri, 1993; Simo & Hughes, 1998; Belytschko et al., 2000) coupled with a continuum damage model (e.g. Kachanov, 1958; Lee et al., 1985; Voyiadjis & Kattan, 1992, 1993; Voyiadjis & Deliktas, 2000). Based on the first law of thermodynamics, the Helmholtz free energy is introduced to describe the current state of energy in the material (Malvern, 1969; Coussy, 1995), and is a function of the strain and the internal state variables under consideration.

As opposed to the previously derived models in CHAPTER 3 and CHAPTER 4, the thermodynamics of irreversible processes followed here will introduce a non-local state consisting of state variables (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000) and the corresponding gradients of the state variables. The gradients of the state variables introduce a spatial dependence of the state. A thermodynamic potential is used which allows the state laws to be defined based on the state variables. The evolution of the thermodynamic conjugate forces are then obtained by assuming the physical existence of the dissipation potential at the macroscale and through the use of the theory of functions of several variables with both plastic and Lagrange multipliers.
The model presented here follows consistent thermodynamics for small strain, rate-independent materials; however, gradients are incorporated in the constitutive model by the introduction of nonlocal measures into the plasticity potential function and yield criterion and into the damage potential function and damage criterion.

5.2.1 State Variables

The nonlocal coupled plasticity-damage model is derived through the use of the method of material nonlocal state identification. In this method, a model is developed such that the thermodynamic state at a given point in space and time is completely determined by a given set of state variables at that point in space and time. As this set of state variables include gradients for the nonlocal theory, the state at the given point is dependent on the behavior surrounding the point, i.e. the state is nonlocal.

The set of state variables are separated into a set of observable state variables and a set of internal state variables. The observable variables are those that can be measured and which appear regardless of the material phenomena. The observable state variables used here are the temperature denoted by the scalar $T$, the total strain denoted by the second-order tensor $\varepsilon$, and the damage tensor denoted by the second-order tensor $\varphi$. For pure elasticity, this set of observable state variables entirely defines the point; however, for elasto-plasticity, the material has a history dependency which requires an additional set of internal state variables.

For this coupled damage-plasticity model, the internal state variables will consist of hardening variables as defined for plasticity in Eq. (3.2), as well as an additional hardening variable for damage, $\kappa$. The hardening internal state variables are unitless, strain like quantities and are accumulated into a set of plasticity related measures, $V^p$, and a set of damage related measures, $V^d$, as follows:

$$ V^p = [r, \alpha] $$
$$ V^d = [\kappa] $$

where the internal state variables considered here are the plasticity related variables presented in CHAPTER 3 and the damage related variables presented in CHAPTER 4.

In this proposed work, the macroscale internal state variable and the corresponding gradient term are assumed to be independent internal state variables with respect to each other with different physical interpretations and initial conditions which allows these two different physical phenomena to be identified separately. Since stresses and strains are macro-variables that are computed using the internal state variables of the material, gradient effects are not introduced directly through the strains and stresses by introducing gradient dependent, nonlocal measures of the stress and strain (Voyiadjis & Dorgan,
Similarly, as the damage measure is a macro-variable similar to the strain, nonlocal measures of $\varphi$ are not introduced in this work.

The form of the "nonlocal" measures used in this work is justified from the discussion of approximating the nonlocal integral equation. The nonlocal integral introduces long-range microstructural interaction by assuming the variable response at a material point is dependent on the state of its neighborhood in addition to the state of the point itself (Pijaudier-Cabot & Bažant, 1987; Bažant & Pijaudier-Cabot, 1988). Integral equations have been investigated by a number of researchers whereby the components of the stress and strain fields are expressed by an averaging integral (e.g. Kunin, 1968; Eringen & Edelen, 1972; Bažant, 1984; Bažant, & Chang, 1984; Bažant et al., 1984; Pijaudier-Cabot & Bažant, 1987; Bažant & Pijaudier-Cabot, 1988). The integral form of the nonlocal internal state variable is approximated by using a truncated Taylor expansion of the weighted average at the position of the local counterpart over a surrounding volume at a small distance from the point (Mühlhaus & Aifantis, 1991). A coefficient is introduced through this method that incorporates a length scale into the formulation. This length scale may not be constant, and, for the case of gradient plasticity, may be expressed as a variable dependent on the accumulated plastic strain, dislocation spacing, grain size, etc. (Voyiadis & Abu Al-Rub, 2005).

Bammann & Aifantis (1989), Aifantis (1999), Voyiadis et al. (2001a,b), and Voyiadis & Dorgan (2001) investigated the use of gradient enhanced measures as in Eq. (2.19) to describe nonlocal behavior of damage and plastic hardening through the damage and plasticity potential functions. With regard to using gradients to describe the non-local behavior of the material, the measures $\bar{\varphi}$, $\bar{\alpha}$, and $\bar{\kappa}$ (which are not necessarily internal state variables) are used to characterize the nonlocal kinematic and isotropic hardening for plasticity and the nonlocal isotropic hardening for damage, respectively, and are given such that (Mühlhaus & Aifantis, 1991):

\begin{align*}
\bar{\varphi} &= r + c_r \nabla^2 r \\
\bar{\alpha} &= \alpha + c_\alpha \nabla^2 \alpha \\
\bar{\kappa} &= \kappa + c_\kappa \nabla^2 \kappa
\end{align*}

(5.3) \hspace{2cm} (5.4) \hspace{2cm} (5.5)

The coefficients $c_r$, $c_\alpha$, and $c_\kappa$ introduce material length scales and are defined as in Eq. (2.19) to be a constant proportional to an internal characteristic length squared. For kinematic hardening, the constant $c_\alpha$ weights each component of the gradient tensor identically. Nonlocal measures of the thermodynamic conjugate forces are assumed to have the same form:

\begin{align*}
\bar{R} &= R + c_r \nabla^2 R \\
\bar{X} &= X + c_\alpha \nabla^2 X \\
\bar{K} &= K + c_\kappa \nabla^2 K
\end{align*}

(5.6) \hspace{2cm} (5.7) \hspace{2cm} (5.8)
These nonlocal conjugate forces will be introduced into the yield criterion and the damage criterion. It will be shown that the computation of the Laplacian of a conjugate force requires the corresponding flux variable, its gradient, and its Laplacian. Thus, four additional sets of state variables are defined and are written as follows:

\[
\nabla \nabla p = [\nabla r, \nabla \alpha] \\
\nabla^2 \nabla p = [\nabla^2 r, \nabla^2 \alpha] \\
\nabla \nabla d = [\nabla \kappa] \\
\nabla^2 \nabla d = [\nabla^2 \kappa]
\]

In order to provide a justification for introducing a variable and its corresponding gradients as internal state variables, as an example, consider the Hamiltonian of a dynamical system which is written as \( H(x,p) \), where \( x \) is the position vector and \( p \) is the velocity or momentum vector. The quantities \( x \) and \( p \) are called state variables and are certainly treated as independent variables, even though the Hamiltonian form of the equations of motion are given as:

\[
\dot{x}(t) = \nabla_p (x,p) \\
\dot{p}(t) = -\nabla_x (x,p)
\]

For another example, consider the calculus of variation problem of minimizing the functional given as:

\[
I(y) = \int_a^b f(x,y(x),y'(x)) \, dx
\]

which is subject to \( y(a) = A, \; y(b) = B \). The standard assumptions are that \( F \) is of class \( C^0 \), and solutions \( y \) are sought in \( C^2 \). A necessary condition of a \( C^2 \) function \( y \) in order that it minimize the functional \( I \) is that \( y \) satisfies the Euler-Lagrange equation:

\[
\frac{\partial}{\partial x} F_y(x,y(x),y'(x)) = F_y(x,y(x),y'(x))
\]

The standard notation for the general first-order nonlinear partial differential equation in two variables is \( F_y(x,u,p,q) = 0 \), where \( p = \nabla_x u(x,y) \) and \( q = \nabla_y u(x,y) \). This partial differential equation is solved by first solving the following characteristic equations:
\[
\dot{x}(t) = F_p(x, y, u, p, q) \tag{5.17}
\]
\[
\dot{y}(t) = F_q(x, y, u, p, q) \tag{5.18}
\]
\[
\dot{u}(t) = pF_p(x, y, u, p, q) + qF_q(x, y, u, p, q) \tag{5.19}
\]
\[
\dot{p}(t) = -F_x(x, y, u, p, q) - pF_u(x, y, u, p, q) \tag{5.20}
\]
\[
\dot{q}(t) = -F_y(x, y, u, p, q) - qF_u(x, y, u, p, q) \tag{5.21}
\]

A final example is given directly by the following chain rule:

\[
\frac{\partial F(x, y(x))}{\partial x} = \frac{\partial F(x, y)}{\partial x} + \frac{\partial F(x, y)}{\partial y} \frac{\partial y}{\partial x} \tag{5.22}
\]

As demonstrated by the preceding examples, it is mathematically correct to assume a quantity and its gradient to be independent state variables, and this is readily extended to a quantity and its corresponding Laplacian.

### 5.2.2 Stress Transformations

For this gradient enhanced state, modified transformation equations are required in order to transform the yield condition from the effective configuration to the damaged configuration. The transformation of the effective stress and of the effective deviatoric stress defined by Eqs. (4.13) and (4.21), respectively, are not modified by the gradient enhancements. For the plasticity hardening conjugate forces used in the yield condition, rather than transform both the conjugate force and its Laplacian, the nonlocal measure of these hardening conjugate forces defined by Eqs. (5.6) and (5.7) are transformed. As the nonlocal conjugate force for isotropic hardening is a scalar, a transformation to the effective configuration is performed in a similar fashion as performed in Eq. (4.24) such that:

\[
\tilde{R} = \frac{R}{1 - \|\varphi\|} = \frac{R + c_x \nabla^2 R}{1 - \|\varphi\|} \tag{5.23}
\]

where \(\tilde{R}\) is the nonlocal measure of the isotropic hardening conjugate force in the effective configuration. The norm of the damage tensor is used in this transformation as a scalar measure of damage, \(\varphi_{eq}\). The nonlocal measure of the backstress conjugate force is a second-order tensor which can be linearly transformed using the same method as for the deviatoric Cauchy stress as performed in Eq. (4.26) such that:

\[
\tilde{X} = N : \vec{X} = N : \left( X + c_x \nabla^2 X \right) \tag{5.24}
\]
Given the damaged and the effective Cauchy stress tensor as well as the nonlocal measures of the damaged and the effective backstress conjugate force, the damaged and the effective relative stress tensors are defined here in terms of the nonlocal measures as follows:

\[
\tilde{\xi} = \tilde{s} - \tilde{X}
\]

\[
\xi = s - X
\]

such that the transformation of the relative stress tensor to the effective configuration is written as follows:

\[
\tilde{\xi} = \tilde{s} - \tilde{X} = N : (\sigma - \bar{X})
\]  

(5.25)  

(5.26)  

(5.27)

The norm of this effective relative stress will be used in the effective configuration yield condition and is defined as follows:

\[
\|\tilde{\xi}\| = \|\tilde{s} - \tilde{X}\| = \|N : (\sigma - \bar{X})\|
\]

(5.28)

5.2.3 Equations of State

In order to determine state laws which relate the internal state variable fluxes to their conjugate thermodynamic forces, a thermodynamic potential defined as the Helmholtz free energy is introduced which is a state function of a thermodynamic system (Malvern, 1969; Lemaitre & Chaboche, 1994; Coussy, 1995; Doghri, 2000). This thermodynamic potential is used to describe the current state of energy in the material, and is a function of the observable state variables and the internal state variables under consideration:

\[
\psi = \psi \left( \epsilon, T, \epsilon^{nd}, \epsilon^p, \varphi, \nabla \nabla \nabla \nabla \epsilon_p, \nabla^2 \epsilon_p, \nabla^d \nabla \nabla^d, \nabla^2 \nabla^d \right)
\]

(5.29)

However, as the strains are decomposed for this coupled plasticity-damage model, this Helmholtz free energy can be rewritten as follows:

\[
\psi = \psi \left( \epsilon^e, T, \varphi, \nabla \nabla \nabla \epsilon_p, \nabla^2 \epsilon_p, \nabla \nabla \nabla \nabla \nabla \nabla^d, \nabla^2 \nabla^d \right)
\]

(5.30)

The Clausius-Duhem inequality can be written in the same form as given by Eq. (3.7) ; however, the time derivative of \( \psi \) is now expanded based on the additional internal state variables as follows:
\[
\psi = \frac{\partial \psi}{\partial \varepsilon} : \dot{\varepsilon} + \frac{\partial \psi}{\partial T} : \dot{T} + \frac{\partial \psi}{\partial \phi} : \dot{\phi} + \frac{\partial \psi}{\partial \nabla V_p} : \dot{V}_p + \frac{\partial \psi}{\partial \nabla V_d} : \dot{V}_d + \frac{\partial \psi}{\partial \nabla^2 V_p} : \nabla^2 \dot{V}_p + \frac{\partial \psi}{\partial \nabla^2 V_d} : \nabla^2 \dot{V}_d
\]  
(5.31)

Using this relationship along with the strain decomposition given by Eq. (4.31), the
Clausius-Duhem inequality can be expanded in the following form:

\[
\sigma : \dot{\varepsilon}^p + \left( \sigma - \rho \frac{\partial \psi}{\partial \varepsilon} \right) : \dot{\varepsilon} - \rho \left( \frac{\partial \psi}{\partial T} + s \right) : \dot{T} - \rho \frac{\partial \psi}{\partial \phi} : \dot{\phi} - \rho \frac{\partial \psi}{\partial \nabla V_p} : \nabla \dot{V}_p - \rho \frac{\partial \psi}{\partial \nabla^2 V_p} : \nabla^2 \dot{V}_p - \rho \frac{\partial \psi}{\partial \nabla V_d} : \nabla \dot{V}_d - \rho \frac{\partial \psi}{\partial \nabla^2 V_d} : \nabla^2 \dot{V}_d \geq 0
\]  
(5.32)

As the formulations in Section 4.2.4 were derived using the general sets, \( V_p \) and \( V_d \), of macroscopic measures of irreversible phenomena, the formulations for the equations of state do not need to be repeated here, and the thermo-elastic state laws are rewritten as follows:

\[
\sigma = \rho \frac{\partial \psi}{\partial \varepsilon} \]  
(5.33)

\[
s = -\frac{\partial \psi}{\partial T} \]  
(5.34)

\[
Y = -\frac{\partial \psi}{\partial \phi} \]  
(5.35)

From these state laws, the stress, \( \sigma \), and the enthalpy, \( s \), are defined as the conjugate forces corresponding to the state variables \( \varepsilon, T \), respectively. Similarly, \( Y \) is defined as the conjugate force corresponding to the damage measure, \( \phi \), and sets of conjugate forces, \( A_p \) and \( A_d \), are defined which correspond to the hardening internal state variables:

\[
A^p = [R, X] \]  
(5.36)

\[
A^d = [K] \]  
(5.37)

where the scalar \( R \) and the second-order tensor \( X \) are the plasticity hardening conjugate forces as defined in Eq. (3.15); and the scalar \( K \) is the damage hardening conjugate force as defined in Eq. (4.53). Whereas the internal state variables are unitless, strain like quantities, the thermodynamic conjugate forces are a set of stress like quantities that are
related to the state variables as the stress is related to the strain. These conjugate forces are defined in the Clausius-Duhem inequality by the following sets of state laws:

\[ \mathbf{A}^p = \rho \frac{\partial \psi}{\partial \mathbf{N}^p} \]  
\[ \mathbf{A}^d = \rho \frac{\partial \psi}{\partial \mathbf{N}^d} \]  

Additionally, sets of conjugate forces are defined which correspond to the gradient state variables given by Eqs. (5.9) to (5.12) such that:

\[ \nabla \mathbf{A}^p = \left[ \nabla \mathbf{R}, \nabla \mathbf{X} \right] \]  
\[ \nabla^2 \mathbf{A}^p = \left[ \nabla^2 \mathbf{R}, \nabla^2 \mathbf{X} \right] \]  
\[ \nabla \mathbf{A}^d = \left[ \nabla \mathbf{K} \right] \]  
\[ \nabla^2 \mathbf{A}^d = \left[ \nabla^2 \mathbf{K} \right] \]

These conjugate forces are defined in the Clausius-Duhem inequality by the following sets of state laws:

\[ \nabla \mathbf{A}^p = \rho \frac{\partial \psi}{\partial \nabla \mathbf{N}^p} \]  
\[ \nabla^2 \mathbf{A}^p = \rho \frac{\partial \psi}{\partial \nabla^2 \mathbf{N}^p} \]  
\[ \nabla \mathbf{A}^d = \rho \frac{\partial \psi}{\partial \nabla \mathbf{N}^d} \]  
\[ \nabla^2 \mathbf{A}^d = \rho \frac{\partial \psi}{\partial \nabla^2 \mathbf{N}^d} \]

### 5.2.4 Conjugate Forces

Since the internal state variables are selected independently of one another, one can express the analytical form of the Helmholtz free energy in terms of its internal state variables as:

\[ \rho \psi = \frac{\mu}{2} \mathbf{\varepsilon}^e : \mathbf{C}^e : \mathbf{\varepsilon}^e + W^p \left( \mathbf{V}^p, \nabla \mathbf{V}^p, \nabla^2 \mathbf{V}^p \right) + W^d \left( \mathbf{V}^d, \nabla \mathbf{V}^d, \nabla^2 \mathbf{V}^d \right) - \rho T s \]

where the fourth-order tensor \( \mathbf{C}^e \) is the damaged elastic tangent modulus and is in terms of the damage tensor \( \varphi \), the scalar \( \rho \) is the material density, and the superscripted “\( e \),” “\( p \),” and “\( d \)” imply terms associated with elasticity, plasticity, and damage, respectively.
As presented in Section 4.2.5, for this form of the Helmholtz free energy and from the state laws Eq. (5.33) and (5.35), equations for the stress and the damage conjugate force can be written here as follows:

\[
\sigma = \mathbf{C}^{e} : \varepsilon^{e} \tag{5.49}
\]

\[
\mathbf{Y} = \frac{1}{2} \varepsilon^{T} \cdot \frac{\partial \mathbf{C}^{e}}{\partial \phi} : \varepsilon^{e} = \frac{1}{2} \mathbf{\sigma}^{T} : \frac{\partial \mathbf{C}^{-e}}{\partial \phi} : \mathbf{\sigma} \tag{5.50}
\]

where the damaged elasticity tensor is defined by Eq. (4.39) and the derivative of the damaged elasticity tensor and its inverse with respect to the damage tensor are defined by Eqs. (4.59) and (4.60), respectively.

The terms \( W^{p} \left( \mathbf{V}^{P}, \nabla \mathbf{V}^{P}, \nabla^{2} \mathbf{V}^{P} \right) \) and \( W^{d} \left( \mathbf{V}^{d}, \nabla \mathbf{V}^{d}, \nabla^{2} \mathbf{V}^{d} \right) \) account for energy introduced into the system by the hardening terms and their corresponding gradient terms. It can be assumed that the energy introduced by the hardening terms is uncoupled such that:

\[
W^{p} \left( \mathbf{V}^{P}, \nabla \mathbf{V}^{P}, \nabla^{2} \mathbf{V}^{P} \right) = W^{r} \left( r \right) + W^{\nabla r} \left( \nabla r \right) + W^{\nabla^{2} r} \left( \nabla^{2} r \right) + W^{a} \left( \mathbf{a} \right) + W^{\nabla a} \left( \nabla \mathbf{a} \right) + W^{\nabla^{2} a} \left( \nabla^{2} \mathbf{a} \right) \tag{5.51}
\]

\[
W^{d} \left( \mathbf{V}^{d}, \nabla \mathbf{V}^{d}, \nabla^{2} \mathbf{V}^{d} \right) = W^{\kappa} \left( \kappa \right) + W^{\nabla \kappa} \left( \nabla \kappa \right) + W^{\nabla^{2} \kappa} \left( \nabla^{2} \kappa \right) \tag{5.52}
\]

Thus, based on the definition for these hardening energy terms and the state laws given by Eqs. (5.38) and (5.39), definitions for the hardening - thermodynamic conjugate force can now be obtained. The internal state variable - thermodynamic conjugate force relationships are defined based on the material being investigated and different relationships can be selected for the plasticity hardening laws and for the damage hardening laws. Though two typical models, the power and exponential laws, are used here to introduce the isotropic and kinematic hardening relations, more complex models can be incorporated in the same manner; however, the analysis of the material model is beyond the scope of this work. This work is focused on the development of a formulation based on a general functional form of the thermodynamic conjugate forces. This allows the constitutive model to be developed without making an assumption as to the behavior of the material model such that the conjugate forces are written as a general function of their corresponding internal state variable:

\[
R = R \left( r \right) \tag{5.53}
\]

\[
\mathbf{X} = \mathbf{X} \left( \mathbf{a} \right) \tag{5.54}
\]

\[
K = K \left( \kappa \right) \tag{5.55}
\]

Defining explicit forms for the energy terms due to the gradient state variables would place constraints on the gradients. Rather than enforce a constraint which may or may not
be realistic, expressions for the conjugate force gradients are directly derived based on the resulting expressions for the corresponding conjugate forces, such that the following expressions for the gradient conjugate forces are used:

\[
\nabla R = \frac{\partial R(r)}{\partial r} \nabla r
\]

\[
\nabla^2 R = \frac{\partial^2 R(r)}{\partial r^2} \nabla r \cdot \nabla r + \frac{\partial R(r)}{\partial r} \nabla^2 r
\]

\[
\nabla X = \frac{\partial X(a)}{\partial a} : \nabla a
\]

\[
\nabla^2 X = \frac{\partial^2 X(a)}{\partial a \partial a} : \nabla a \cdot \nabla a + \frac{\partial X(a)}{\partial a} : \nabla^2 a
\]

\[
\nabla K = \frac{\partial K(\kappa)}{\partial \kappa} : \nabla \kappa
\]

\[
\nabla^2 X = \frac{\partial^2 K(\kappa)}{\partial \kappa \partial \kappa} : \nabla \kappa \cdot \nabla \kappa + \frac{\partial K(\kappa)}{\partial \kappa} : \nabla^2 \kappa
\]

Thus, based on the material model defined by Eqs. (5.53) to (5.55), the gradient conjugate forces will be readily available without introducing additional models for the gradients.

### 5.2.5 Dissipation Potential and Flow Rules

The evolution of the thermodynamic conjugate forces can be obtained through the evolution relations of the internal state variables, which are obtained by assuming the physical existence of the dissipation potential at the macroscale. The energy dissipation due to plasticity and damage are found by substituting the thermodynamic state laws into the Clausius-Duhem inequality and are thus given as the product of the thermodynamic conjugate forces with the respective flux variables as follows:

\[
\Pi = \sigma : \dot{\varepsilon}^{pd} - Y : \dot{\phi} - \rho A^p : \dot{\dot{V}}^p - \rho \nabla A^p : \nabla \dot{V}^p - \rho \nabla^2 A^p : \nabla^2 \dot{V}^p
\]

\[
- \rho A^d : \dot{\dot{V}}^d - \rho \nabla A^d : \nabla \dot{V}^d - \rho \nabla^2 A^d : \nabla^2 \dot{V}^d - q \cdot \frac{\nabla T}{T} \geq 0
\]

The theory of functions of several variables is used here with a plastic Lagrange multiplier \( \dot{\lambda}^p \) and a damage Lagrange multiplier \( \dot{\lambda}^d \) to construct the objective function \( \Omega \) in the following form:

\[
\Omega = \Pi - F \dot{\lambda}^p - G \dot{\lambda}^d
\]
where $F$ and $G$ are the plastic potential and the damage potential and will be defined subsequently. In order to obtain the plastic strain rate and the damage tensor rate, the following condition is used to extremize the objective function:

\[
\frac{\partial \Omega}{\partial \sigma} = 0 \quad (5.64)
\]

\[
\frac{\partial \Omega}{\partial Y} = 0 \quad (5.65)
\]

From these conditions for the case when $F \geq 0$ and $G \geq 0$, the corresponding evolution equations for the plastic strain and for the damage tensor are given as follows:

\[
\dot{\varepsilon}^{pd} = \frac{\partial F}{\partial \sigma} \dot{\lambda}^{p} + \frac{\partial G}{\partial \sigma} \dot{\lambda}^{d} \quad (5.66)
\]

\[
\dot{\phi} = -\frac{\partial F}{\partial Y} \dot{\lambda}^{p} - \frac{\partial G}{\partial Y} \dot{\lambda}^{d} \quad (5.67)
\]

Since the plastic-damage strain rate will be developed in the current deformed and damaged configuration, its corresponding evolution equation will be a function of the damage measure. Similarly, the evolution equation of the conjugate force due to damage will be a function of the stress. The evolution equations for the inelastic strain and the damage are interdependent (Voyiatjis & Deliktas, 2000), and therefore the two dissipative mechanisms shown above are implicitly interdependent through the stress and the conjugate forces due to damage. Note that, if $F \leq 0$, then $\frac{\partial F}{\partial Y} = \frac{\partial F}{\partial \sigma} = 0$, or if $G \leq 0$, then $\frac{\partial G}{\partial Y} = \frac{\partial G}{\partial \sigma} = 0$, and the evolution equations for the inelastic strain and the damage become decoupled.

In order to derive the evolution equations for the hardening state variables, the following conditions are used to extremize the objective function:

\[
\frac{\partial \Omega}{\partial \chi^{p}} = 0 \quad (5.68)
\]

\[
\frac{\partial \Omega}{\partial \chi^{d}} = 0 \quad (5.69)
\]

From these conditions for the case when $F \geq 0$ and $G \geq 0$, the corresponding set of evolution equations for the hardening state variables are given as follows:

\[
\dot{\chi}^{p} = -\frac{\partial F}{\partial \chi^{p}} \dot{\lambda}^{p} \quad (5.70)
\]

\[
\dot{\chi}^{d} = -\frac{\partial G}{\partial \chi^{d}} \dot{\lambda}^{d} \quad (5.71)
\]
As in the discussion in the previous section on defining the gradient conjugate forces, the evolution equations for the gradients of the internal state variables are defined directly by operating on Eqs. (5.70) and (5.71) such that the following expressions are used:

\[ \nabla \dot{\lambda}^p = -\nabla \left( \frac{\partial F}{\partial A^p} \right) \dot{A}^p - \frac{\partial F}{\partial A^p} \nabla \dot{\lambda}^p \]  
(5.72)

\[ \nabla^2 \dot{\lambda}^p = -\nabla^2 \left( \frac{\partial F}{\partial A^p} \right) \dot{A}^p - 2\nabla \left( \frac{\partial F}{\partial A^p} \right) \cdot \nabla \dot{\lambda}^p - \frac{\partial F}{\partial A^p} \nabla^2 \dot{\lambda}^p \]  
(5.73)

\[ \nabla \dot{\lambda}^d = -\nabla \left( \frac{\partial G}{\partial A^d} \right) \dot{A}^d - \frac{\partial G}{\partial A^d} \nabla \dot{\lambda}^d \]  
(5.74)

\[ \nabla^2 \dot{\lambda}^d = -\nabla^2 \left( \frac{\partial G}{\partial A^d} \right) \dot{A}^d - 2\nabla \left( \frac{\partial G}{\partial A^d} \right) \cdot \nabla \dot{\lambda}^d - \frac{\partial G}{\partial A^d} \nabla^2 \dot{\lambda}^d \]  
(5.75)

In order to determine the gradients and Laplacians of the normals to the plastic potential, consider a point in the plastic domain (Figure 4.5) such that \( F = 0 \) at this point. If it is assumed that the surrounding area has also entered into the plastic regime \( (F = 0) \), then the gradient and Laplacian of the yield condition at this point can be assumed to be zero \( (\nabla F = 0; \nabla^2 F = 0) \) and the following simplifications can be utilized:

\[ \nabla \left( \frac{\partial F}{\partial A^p} \right) = \frac{\partial (\nabla F)}{\partial A^p} = 0 \]  
(5.76)

\[ \nabla^2 \left( \frac{\partial F}{\partial A^p} \right) = \frac{\partial (\nabla^2 F)}{\partial A^p} = 0 \]  
(5.77)

A similar argument can be made for a point in the damage domain in order to obtain the following additional simplifications:

\[ \nabla \left( \frac{\partial G}{\partial A^d} \right) = \frac{\partial (\nabla G)}{\partial A^d} = 0 \]  
(5.78)

\[ \nabla^2 \left( \frac{\partial G}{\partial A^d} \right) = \frac{\partial (\nabla^2 G)}{\partial A^d} = 0 \]  
(5.79)

Thus, the evolution equations for gradients of the internal state variables are simplified to the following expressions:

\[ \nabla \dot{\lambda}^p = -\frac{\partial F}{\partial A^p} \nabla \dot{\lambda}^p \]  
(5.80)

\[ \nabla^2 \dot{\lambda}^p = -\frac{\partial F}{\partial A^p} \nabla^2 \dot{\lambda}^p \]  
(5.81)
\[ \nabla \dot{\mathbf{V}}^d = - \frac{\partial G}{\partial \mathbf{A}^d} \nabla \dot{\mathbf{A}}^d \]  
(5.82)

\[ \nabla \hat{\nabla} \dot{\mathbf{V}}^d = - \frac{\partial G}{\partial \mathbf{A}^d} \nabla^2 \dot{\mathbf{A}}^d \]  
(5.83)

The following loading-unloading conditions known as the Kuhn-Tucker conditions (Kuhn & Tucker, 1951) must be enforced:

\[ \hat{\lambda} \geq 0 ; \quad f \leq 0 ; \quad \hat{\lambda} f = 0 \]  
(5.84)

\[ \dot{\lambda}^d \geq 0 ; \quad g \leq 0 ; \quad \dot{\lambda}^d g = 0 \]  
(5.85)

### 5.2.6 Yield Condition and Damage Condition

Associative plasticity can be used here to derive the evolution equations for the constitutive model such that the plastic potential, \( F \), is set equal to the yield criterion, \( f \). In the effective, undamaged configuration, the gradient enhanced yield criterion can be written as follows:

\[ F = f = \sqrt{\frac{2}{3}} - \sqrt{\frac{2}{3}} \left[ \sigma_{y_p} + \tilde{\sigma} \right] \leq 0 \]  
(5.86)

where \( \tilde{\sigma} \) is the nonlocal measure of the effective isotropic hardening conjugate force defined by Eq. (5.23), and \( \xi \) is the effective relative stress tensor defined by Eq. (5.27). Utilizing the relations developed for the transformation of stresses in Section 5.2.2, specifically Eqs. (5.23) and (5.28), the yield criterion can be written in terms of the damaged state such that:

\[ F = f = \left\| \mathbf{N} \cdot (\sigma - \overline{\mathbf{X}}) \right\| - \sqrt{\frac{2}{3}} \left[ \sigma_{y_p} + \tilde{\sigma} \right] \leq 0 \]  
(5.87)

Similarly, associative damage can be used here to derive the evolution equations for the constitutive model such that the damage potential, \( G \), is set equal to the damage criterion, \( g \). The damage criterion is written in the same form as the Von Mises yield criterion presented in the previous section such that:

\[ G = g = \left\| \mathbf{Y} \right\| - \sqrt{\frac{2}{3}} \left[ \sigma_{y_d} + \tilde{\sigma} \right] \leq 0 \]  
(5.88)

where \( \sigma_{y_d} \) is the initial damage threshold at which damage begins to occur. The normals to the plastic potential and to the damage potential can now be defined as given in APPENDIX B.2, allowing the evolution equations of the internal state variables to be
defined. Thus, the complete set of constitutive equations for the gradient enhanced coupled plasticity-damage model have been derived and are summarized as follows:

**Yield Criterion and Damage Criterion**

\[
F = f = \|N : (\sigma - X - c_X V^2 X)\| - \sqrt{\frac{2}{3}} \left[ \sigma_{yp} + \frac{R + c_r V^2 R}{1 - \|\varphi\|} \right] \leq 0 \quad (5.89)
\]

\[
G = g = \|Y\| - \sqrt{\frac{2}{3}} \left[ \sigma_{yd} + K + c_k V^2 K \right] \equiv 0 \quad (5.90)
\]

**State Laws**

\[
Y = \frac{1}{2} \sigma^T : \frac{\partial C^{-e}}{\partial \varphi} : \sigma \quad (5.91)
\]

\[
R = R(r) ; \quad \nabla^2 R = \frac{\partial^2 R(r)}{\partial r^2} \nabla r \cdot \nabla r + \frac{\partial R(r)}{\partial r} \nabla^2 r \quad (5.93)
\]

\[
X = X(\alpha) ; \quad \nabla^2 X = \frac{\partial^2 X(\alpha)}{\partial \alpha \partial \alpha} : \nabla \alpha \cdot \nabla \alpha + \frac{\partial X(\alpha)}{\partial \alpha} : \nabla^2 \alpha \quad (5.94)
\]

\[
K = K(\kappa) ; \quad \nabla^2 K = \frac{\partial^2 K(\kappa)}{\partial \kappa^2} : \nabla \kappa + \frac{\partial K(\kappa)}{\partial \kappa} \nabla^2 \kappa \quad (5.95)
\]

**State Variable Evolution Equations**

\[
\dot{e}^{pl} = f_\sigma \dot{\lambda}^p + g_\sigma \dot{\lambda}^d \quad (5.96)
\]

\[
\dot{\varphi} = -f_X \dot{\lambda}^p - g_X \dot{\lambda}^d \quad (5.97)
\]

\[
\dot{r} = -f_r \dot{\lambda}^p ; \quad \nabla \dot{r} = -f_r \nabla \dot{\lambda}^p ; \quad \nabla^2 \dot{r} = -f_r \nabla^2 \dot{\lambda}^p \quad (5.98)
\]

\[
\dot{\alpha} = f_\sigma \dot{\lambda}^p ; \quad \nabla \dot{\alpha} = f_\sigma \nabla \dot{\lambda}^p ; \quad \nabla^2 \dot{\alpha} = f_\sigma \nabla^2 \dot{\lambda}^p \quad (5.99)
\]

\[
\dot{\kappa} = -g_\kappa \dot{\lambda}^d ; \quad \nabla \dot{\kappa} = -g_\kappa \nabla \dot{\lambda}^d ; \quad \nabla^2 \dot{\kappa} = -g_\kappa \nabla^2 \dot{\lambda}^d \quad (5.100)
\]

**Kuhn-Tucker Conditions**

\[
\dot{\lambda}^p \geq 0 ; \quad f \leq 0 ; \quad \dot{\lambda}^p f = 0 \quad (5.101)
\]

\[
\dot{\lambda}^d \geq 0 ; \quad g \leq 0 ; \quad \dot{\lambda}^d g = 0 \quad (5.102)
\]

**5.2.7 Plasticity and Damage Consistency Conditions**

At a plastic state where \( f = 0 \), the consistency condition \( \dot{f} = 0 \) results from the loading-unloading conditions of Eq. (5.101). Thus, as the yield criterion is a function of the effective Cauchy stress, the backstress and its Laplacian, the isotropic hardening and its Laplacian, and the damage tensor, the consistency condition can be expanded in terms of the conjugate forces:
\[
\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial R} \dot{R} + \frac{\partial f}{\partial \nabla^2 R} \nabla^2 R + \frac{\partial f}{\partial X} \dot{X} + \frac{\partial f}{\partial \nabla^2 X} : \nabla^2 \dot{X} + \frac{\partial f}{\partial \phi} : \dot{\phi} \equiv 0
\] (5.103)

As the conjugate forces have been defined as functions of the state variables as shown in Eqs. (5.93) and (5.94), the consistency condition can be rewritten in terms of the flux variables as follows:

\[
\dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial \phi} : \dot{\phi} \\
+ \frac{\partial f}{\partial R} \dot{R} + \frac{\partial f}{\partial \nabla^2 R} \left( \frac{\partial \nabla^2 R}{\partial R} \dot{R} + \frac{\partial \nabla^2 R}{\partial \nabla r} \nabla \dot{r} + \frac{\partial \nabla^2 R}{\partial \nabla^2 r} \nabla^2 \dot{r} \right) \\
+ \frac{\partial f}{\partial X} : \dot{X} + \frac{\partial f}{\partial \nabla^2 X} \left( \frac{\partial \nabla^2 X}{\partial X} : \dot{X} + \frac{\partial \nabla^2 X}{\partial \nabla X} \nabla \dot{X} + \frac{\partial \nabla^2 X}{\partial \nabla^2 X} : \nabla^2 \dot{X} \right) = 0
\] (5.104)

Note that the derivatives of the Laplacian conjugate forces with respect to their corresponding state variables and gradient state variables are also needed and can be computed such that:

\[
\frac{\partial \nabla^2 R}{\partial r} = \frac{\partial^3 R}{\partial r^3} \nabla \dot{r} + \frac{\partial^2 R}{\partial r^2} \nabla^2 \dot{r}
\] (5.105)

\[
\frac{\partial \nabla^2 R}{\partial \nabla r} = 2 \frac{\partial^2 R}{\partial r^2} \nabla \dot{r}
\] (5.106)

\[
\frac{\partial \nabla^2 R}{\partial \nabla^2 r} = \frac{\partial R}{\partial \nabla r}
\] (5.107)

\[
\frac{\partial \nabla^2 X}{\partial \alpha} = \frac{\partial^3 X}{\partial \alpha \dot{\alpha} \dot{\alpha} \dot{\alpha}} : \nabla \dot{\alpha} + \frac{\partial^2 X}{\partial \alpha \dot{\alpha} \dot{\alpha}} : \nabla^2 \dot{\alpha}
\] (5.108)

\[
\frac{\partial \nabla^2 X}{\partial \nabla \alpha} = 2 \frac{\partial^2 X}{\partial \alpha \dot{\alpha} \dot{\alpha}} : \nabla \dot{\alpha}
\] (5.109)

\[
\frac{\partial \nabla^2 \dot{X}}{\partial \alpha \dot{\alpha}} = \frac{\partial \dot{X}}{\partial \alpha \dot{\alpha}}
\] (5.110)

The incremental form of the Hookean stress-strain relation, Eq. (5.91), is also used in the consistency condition and can be written in the following form:

\[
\dot{\sigma} = C^e : (\dot{\epsilon} - \dot{\epsilon}^{\text{old}}) + \dot{C}^e : (\dot{\epsilon} - \dot{\epsilon}^{\text{old}})
\] (5.111)

where the incremental damaged elastic stiffness tensor is found by differentiating Eq. (4.39). The resulting equation is given in APPENDIX B.1 and is rewritten here as follows:
\[
\dot{C}^e = \frac{\partial C^e}{\partial \phi} : \dot{\phi} = 2C^e : M^T : \frac{\partial M^{-T}}{\partial \phi} : \dot{\phi}
\]

(5.112)

Thus, the incremental stress can be written in the following form:

\[
\dot{\sigma} = C^e : (\dot{\varepsilon} - \varepsilon^{pd}) + C^e : Z : \dot{\phi}
\]

(5.113)

where the fourth-order tensor \( Z \) is defined as follows:

\[
Z = 2M^T : \frac{\partial M^{-T}}{\partial \phi} : (\varepsilon - \varepsilon^{pd}) = C^e : \frac{\partial C^e}{\partial \phi} : (\varepsilon - \varepsilon^{pd})
\]

(5.114)

After substituting these derivatives, the normals to the yield surface as defined in APPENDIX B.2, the evolution equations for the internal state variables as defined in Eqs. (5.96) to (5.99), and the incremental Hookean stress-strain relation, Eq. (5.111), the consistency condition is expanded and can be written in the following form:

\[
h_1^{pp} \dot{\lambda}^p + h_2^{pp} \cdot \nabla \dot{\lambda}^p + h_3^{pp} \nabla^2 \dot{\lambda}^p + h^{pd} \dot{\lambda}^p = b^p
\]

(5.115)

where:

\[
h_1^{pp} = f_\sigma : C^e : f_\sigma + (f_\phi + f_\sigma : C^e : Z) : f_Y
\]

\[
+ f_\sigma^2 \left( \frac{\partial R(r)}{\partial r} + c_R \frac{\partial^3 R(r)}{\partial r^3} \nabla r \cdot \nabla r + c_R \frac{\partial^2 R(r)}{\partial r^2} \nabla^2 r \right)
\]

(5.116)

\[
h_2^{pp} = 2c_R f_\sigma^2 \frac{\partial^2 R(r)}{\partial r^2} \nabla r + 2c_X f_\sigma : \frac{\partial X(\alpha)}{\partial \alpha} : \nabla \alpha : f_\sigma
\]

(5.117)

\[
h_3^{pp} = c_R f_\sigma^2 \frac{\partial R(r)}{\partial r} + c_X f_\sigma : \frac{\partial X(\alpha)}{\partial \alpha} : f_\sigma
\]

(5.118)

\[
h^{pd} = f_\sigma : C^e : g_\sigma + (f_\phi + f_\sigma : C^e : Z) : g_Y
\]

(5.119)

\[
b^p = f_\sigma : C^e : \dot{k}
\]

(5.120)

At a damage state where \( g = 0 \), the consistency condition \( \dot{g} = 0 \) results from the loading-unloading conditions of Eq. (5.102). Thus, as the damage criterion is a function of the Cauchy stress, the damage isotropic hardening and its Laplacian, and the damage measure, the consistency condition can be expanded in terms of the conjugate forces as follows:
\[
\dot{g} = \frac{\partial g}{\partial \sigma} : \dot{\sigma} + \frac{\partial g}{\partial K} \dot{K} + \frac{\partial g}{\partial \nabla^2 K} \nabla^2 \dot{K} + \frac{\partial g}{\partial \phi} : \dot{\phi} = 0
\]  

(5.121)

As the hardening conjugate force has been defined as a general function of the state variable as shown in Eq. (5.95), the consistency condition can be rewritten in terms of the flux variables as follows:

\[
\dot{g} = \frac{\partial g}{\partial \sigma} : \dot{\sigma} + \frac{\partial g}{\partial \phi} : \dot{\phi} 
+ \frac{\partial g}{\partial K} \frac{\partial K}{\partial \kappa} \dot{\kappa} + \frac{\partial g}{\partial \nabla^2 K} \left( \frac{\partial \nabla^2 K}{\partial \kappa} \dot{\kappa} + \frac{\partial \nabla^2 K}{\partial \nabla \kappa} \nabla \dot{\kappa} + \frac{\partial \nabla^2 K}{\partial \nabla^2 \kappa} \nabla^2 \dot{\kappa} \right) = 0
\]

(5.122)

Note that the derivatives of the Laplacians with respect to their corresponding state variables and gradient state variables are also needed and can be computed such that:

\[
\frac{\partial \nabla^2 K}{\partial \kappa} = \frac{\partial^2 K(\kappa)}{\partial \kappa^3} \nabla \kappa \cdot \nabla \kappa + \frac{\partial^2 K(\kappa)}{\partial \kappa^2} \nabla^2 \kappa 
\]

(5.123)

\[
\frac{\partial \nabla^2 K}{\partial \nabla \kappa} = 2 \frac{\partial^2 K(\kappa)}{\partial \kappa^2} \nabla \kappa 
\]

(5.124)

\[
\frac{\partial \nabla^2 K}{\partial \nabla^2 \kappa} = \frac{\partial K(\kappa)}{\partial \kappa} 
\]

(5.125)

After substituting these derivatives, the normals to the yield surface as defined in APPENDIX B.2, the evolution equations for the internal state variables as defined in Eqs. (5.96), (5.97), and (5.100), and the incremental Hookean stress-strain relation, Eq. (5.113), the consistency condition is expanded and can be written in the following form:

\[
h^{dp} \dot{\lambda}^p + h^{dd}_1 \dot{\lambda}^d + h^{dd}_2 \nabla \dot{\lambda}^d + h^{dd}_3 \nabla^2 \dot{\lambda}^d = b^d
\]

(5.126)

where:

\[
h^{dp} = g_\sigma : C^e : f_\sigma + \left( g_\sigma : C^e : Z + g_\phi \right) : f_N
\]

(5.127)

\[
h^{dd}_1 = g_\sigma : C^e : g_\sigma + \left( g_\sigma : C^e : Z + g_\phi \right) : g_N
\]

(5.128)

\[
h^{dd}_2 = 2 c_k g_{g,\kappa} \frac{\partial^2 K(\kappa)}{\partial \kappa^2} \nabla \kappa
\]

(5.129)

\[
h^{dd}_3 = c_k g_{g,\kappa} \frac{\partial K(\kappa)}{\partial \kappa}
\]

(5.130)
\[ b^d = g \cdot : C : \dot{\varepsilon} \]  

(5.131)

5.3 RATE BOUNDARY VALUE PROBLEM

In the analysis of a 3D small deformation plasticity rate boundary value problem, the body has a plastic region, \( V_{p} \), and an elastic region outside of this zone. Additionally, the body has a damage region \( V_{d} \) which may be in either or both the elastic and plastic domains. \( V \) denotes the total domain.

The rate boundary value problem in the strong form is described by the following governing equations:

**Equilibrium equation:**
\[ \nabla \cdot \sigma + \dot{b} = 0 \]  

(5.132)

**Applied tractions boundary condition**
\[ n \cdot \sigma + \dot{t} = 0 \text{ on } \Gamma \]  

(5.133)

**Applied displacements boundary condition**
\[ u = \dot{u} \text{ on } \Gamma_u \]  

(5.134)

where \( \Gamma \) is the boundary over which tractions, \( \dot{t} \), are applied, \( \Gamma_u \) is the boundary over which displacements, \( \dot{u} \), are applied, and \( b \) are body forces. As shown previously, the gradient dependent yield criterion and damage criterion are given as:

\[ F = f = \| N : (Q - X - c_h \nabla^2 X) \| - \sqrt{\frac{2}{3}} \left[ \sigma_{yp} + \frac{R + c_h \nabla^2 R}{1 - \| \phi \|} \right] \leq 0 \]  

(5.135)

\[ G = g = \| Y \| - \sqrt{\frac{2}{3}} \left[ \sigma_{yd} + K + c_h \nabla^2 K \right] \equiv 0 \]  

(5.136)

In a local model using finite elements, only the equilibrium equation is required to obtain a unique solution of the boundary value problem. In this work, the constitutive model contains a set of differential equations that involve macroscale second order gradients for both the plastic and damage multipliers. In order to solve such a higher order problem, additional equations are required. This is done by satisfying both the yield consistency condition and the damage consistency conditions in the weak form. The weak form of the equilibrium equation and of the consistency conditions can be written by multiplying the equations respectively by a virtual displacement rate vector, \( \delta \dot{u} \), a virtual plastic multiplier rate vector, \( \delta \dot{\lambda}^p \), and a virtual plastic multiplier rate vector, \( \delta \dot{\lambda}^d \), and integrating. The equilibrium equation is integrated over the entire body, the plasticity
consistency condition is integrated over the plastic region, and the damage consistency condition is integrated over the damage region:

\[
\int_V \delta \mathbf{u} \cdot (\nabla \cdot \mathbf{\sigma} + \mathbf{b}) \, dV = 0
\](5.137)

\[
\int_V \delta \dot{\lambda}^p \dot{f} \, dV = 0
\](5.138)

\[
\int_V \delta \dot{\lambda}^d \dot{g} \, dV = 0
\](5.139)

Substitution of the consistency conditions derived in the previous section into the weak form of the consistency conditions above, and integrating by parts the weak form of the equilibrium equation given above, the following governing equations are obtained:

\[
\int_V \delta \mathbf{\varepsilon} : \mathbf{C} : \left( \dot{\mathbf{\varepsilon}} - f_{\sigma} \dot{\lambda}^p - g_{\sigma} \dot{\lambda}^d - \mathbf{Z} \left( f_{\lambda} \dot{\lambda}^p + g_{\lambda} \dot{\lambda}^d \right) \right) \, dV - \int_{\Gamma} \delta \mathbf{u} \cdot \mathbf{b} \, d\Gamma = 0
\](5.140)

\[
\int_{V^p} \delta \dot{\lambda}^p \left( f_{\lambda} \cdot \mathbf{C} : \dot{\mathbf{\varepsilon}} - h_{\lambda \lambda} \dot{\lambda}^p - h_{\lambda \lambda} \cdot \nabla \dot{\lambda}^p - h_{\lambda \lambda} \nabla^2 \dot{\lambda}^p - h_{\lambda \lambda} \cdot \nabla^2 \dot{\lambda}^p - h_{\lambda \lambda} \nabla^2 \dot{\lambda}^p \right) \, dV = 0
\](5.141)

\[
\int_{V^d} \delta \dot{\lambda}^d \left( g_{\lambda} \cdot \mathbf{C} : \dot{\mathbf{\varepsilon}} - h_{\lambda \lambda} \dot{\lambda}^p - h_{\lambda \lambda} \cdot \nabla \dot{\lambda}^p - h_{\lambda \lambda} \nabla^2 \dot{\lambda}^p - h_{\lambda \lambda} \cdot \nabla^2 \dot{\lambda}^p - h_{\lambda \lambda} \nabla^2 \dot{\lambda}^p \right) \, dV = 0
\](5.142)

As the governing equations are now differential equations, an algebraic solution for these multipliers can no longer be obtained, and a finite element solution will be used. In order to solve the boundary value problem, a multifield approach is adopted such that the plastic and damage multipliers are discretized in addition to the displacement field. Since the degrees of freedom are increased, the two additional governing equations given by Eqs. (5.141) and (5.142) are required to obtain a solution.

**5.4 Integration Algorithm**

In this section, the integration scheme for the gradient enhanced constitutive model is presented. In order to solve the boundary value problem, a multifield approach is adopted such that the plastic and damage multipliers are discretized in addition to the displacement field. In the solution procedure, linearized forms of the governing equations given by Eqs. (5.140) to (5.142) are solved within an incremental iterative Newton-Raphson solution procedure for the increments of strain, plastic multiplier, and damage multiplier over the time increment \( \Delta t_j \) such that:

\[
\mathbf{\varepsilon}_j = \mathbf{\varepsilon}_0 + \Delta t_j \mathbf{\varepsilon} = \mathbf{\varepsilon}_0 + \Delta \mathbf{\varepsilon}_j
\]

\[
\Delta \dot{\lambda}^p_j = \Delta t_j \dot{\lambda}^p
\]
\[ \Delta \lambda_j^d = \Delta t_j d \lambda^d \]  

(5.145)

where the subscripted \( j \)'s and 0 indicate that the variable is computed at iteration \( j \) and at the previously converged state, respectively; and the symbol \( \Delta \) denotes a total increment from the previously converged state to the iteration, \( j \). The increments of the plastic multiplier, \( \Delta \lambda_j^p \), and of the damage multiplier, \( \Delta \lambda_j^d \), are then used to update the state of the material such that:

\[
\begin{align*}
\epsilon_j^p &= \epsilon_j^p + \Delta \epsilon_j^p \\
r_j &= r_0 + \Delta r_j ;
\end{align*}
\]

(5.146)

\[
\begin{align*}
\nabla r_j &= \nabla r_0 + \Delta \nabla r_j \\
\nabla^2 r_j &= \nabla^2 r_0 + \Delta \nabla^2 r_j ;
\end{align*}
\]

(5.98)

\[
\begin{align*}
\alpha_j &= \alpha_0 + \Delta \alpha_j ;
\end{align*}
\]

(5.98)

\[
\begin{align*}
\kappa_j &= \kappa_0 + \Delta \kappa_j ;
\end{align*}
\]

(5.98)

The increments of the plastic multiplier, \( \Delta \lambda_j^p \), and of the damage multiplier, \( \Delta \lambda_j^d \), are then used to update the state of the material such that:

\[
\begin{align*}
\sigma_j &= C_j^e : (\epsilon_j - \epsilon_j^{\text{red}}) = \sigma_0 + C_j^e : (\Delta \epsilon_j - \Delta \epsilon_j^{\text{red}}) + C_j^e : Z_j : \Delta \phi_j,
\end{align*}
\]

(5.147)

\[
Y_j = \sigma_j \frac{\partial C_j^e}{\partial \phi_j} : \sigma_j
\]

(5.148)

where the damaged elastic stiffness tensor can be defined in incremental form as follows:

\[
C_j^e = C_0^e + \Delta C_j^e
\]

(5.149)

The integration scheme used here enforces that \( f_j = 0 \) and \( g_j = 0 \) at the end of the time step:

\[
\begin{align*}
F_j = f_j &= \left\| N_j : (\sigma_j - X_j - c_K \nabla^2 X_j) \right\| - \sqrt{\frac{2}{3}} \left[ \sigma_{sp} + \frac{R_j + c_K \nabla^2 R_j}{1 - \| \phi_j \|} \right] \leq 0, \\
G_j = g_j &= \left\| Y_j \right\| - \sqrt{\frac{2}{3}} \left[ \sigma_d + 2 c_K \nabla^2 K_j \right] = 0
\end{align*}
\]

(5.150)

(5.151)

where the deviatoric damage measure tensor is defined as follows:

\[
N_j = M_j - \frac{1}{2} I \otimes I : M_j = I^D : M_j
\]

(5.152)

and the conjugate forces are defined as functions of the state variables such that:
\[ R_j = R(r_j); \quad \nabla^2 R_j = \frac{\partial^2 R(r_j)}{\partial r^2} \nabla r_j \cdot \nabla r_j + \frac{\partial R(r_j)}{\partial r} \nabla^2 r_j \quad (5.153) \]

\[ X_j = X(a_j); \quad \nabla^2 X_j = \frac{\partial^2 X(a_j)}{\partial a \partial a} : \nabla a_j \cdot \nabla a_j + \frac{\partial X(a_j)}{\partial a} : \nabla^2 a_j \quad (5.154) \]

\[ K_j = K(\kappa_j); \quad \nabla^2 K_j = \frac{\partial^2 K(\kappa_j)}{\partial \kappa^2} : \nabla \kappa_j + \frac{\partial K(\kappa_j)}{\partial \kappa} : \nabla^2 \kappa_j \quad (5.155) \]

As the plastic and damage multipliers are available from the nodal degrees of freedom, a return mapping algorithm is not required; however, in order to compute the stress and the damage conjugate force, an initial elastic-predictor step is used to determine if the point is loaded elastically or plastically and with or without damage. This is then followed by a plastic-damage-corrector. In determining the state of the material, the internal state variables are updated using the multipliers through Eqs. (5.146), and the initial trial stress and the initial trial damage conjugate force are computed as follows:

\[ \sigma_{j}^{\text{trial}} = \sigma_0 + C_\varepsilon^{\varepsilon} : \Delta \varepsilon_j \quad (5.156) \]

\[ Y_{j}^{\text{trial}} = \sigma_{j}^{\text{trial}} : \left( \frac{\partial C^{\varepsilon}}{\partial \phi} \right) : \sigma_{j}^{\text{trial}} \quad (5.157) \]

The trial state \( \left( \sigma_{j}^{\text{trial}}, Y_{j}^{\text{trial}}, \varepsilon_{j}^{\text{pd}}, \phi_j, r_j, a_j, \kappa_j \right) \) is then used in a trial yield criterion and a trial damage criterion to decide whether an elastic point enters the plastic and/or damage regimes or whether a plastic or damage point elastically unloads. For the case when \( f_{\text{trial}} \leq 0 \) and \( g_{\text{trial}} \leq 0 \), the integration point is assumed to be elastic with no additional damage and the current state \( \left( \sigma_j, Y_j, \varepsilon_{j}^{\text{pd}}, \phi_j, r_j, a_j, \kappa_j \right) \) is set to the trial state \( \left( \sigma_{j}^{\text{trial}}, Y_{j}^{\text{trial}}, \varepsilon_{j}^{\text{pd}}, \phi_j, r_j, a_j, \kappa_j \right) \). Alternatively, when \( f_{\text{trial}} > 0 \), the current state resulting from this trial state lies outside of the yield surface. Plasticity has occurred and the stress has to be corrected to the yield surface. Similarly, when \( g_{\text{trial}} > 0 \), the current state resulting from this trial state lies outside of the damage surface. Damage has occurred and the state has to be corrected to the damage surface. Using the definition of the Cauchy stress from Eq. (5.147) along with the definition of the trial stress, Eq. (5.156), the Cauchy stress is corrected as follows:

\[ \sigma_j = \sigma_{j}^{\text{trial}} + \Delta C_j^{\varepsilon} : \Delta \varepsilon_j - C_j^{\varepsilon} : \Delta \varepsilon_{j}^{\text{pd}} + C_j^{\varepsilon} : Z_j : \Delta \phi_j \quad (5.158) \]

Thus, the correction to the stress during the corrector phase is defined as:

\[ \Delta \sigma_j = \Delta C_j^{\varepsilon} : \Delta \varepsilon_j - C_j^{\varepsilon} : \Delta \varepsilon_{j}^{\text{pd}} + C_j^{\varepsilon} : Z_j : \Delta \phi_j \quad (5.159) \]
5.4.1 Fully Implicit Backward Euler Scheme

As with the implicit backward Euler scheme presented in Belytschko et al. (2000), the solution of the system of equations is implicit (computed at time $j$) in the plastic strain, the damage measure, the hardening variables, and the plastic flow direction. The solution scheme is defined by Eqs. (5.146) to (5.149), where the increments of the state variables are written as follows:

$$
\Delta \epsilon_{j}^{pd} = f_{\sigma} \Delta \lambda_{j}^{p} + g_{\sigma} \Delta \lambda_{j}^{d}
$$

$$
\Delta \phi_{j} = -f_{\lambda} \Delta \lambda_{j}^{p} - g_{\lambda} \Delta \lambda_{j}^{d}
$$

$$
\Delta r_{j} = -f_{\lambda^{p}} \Delta \lambda_{j}^{p}, \quad \Delta \nabla r_{j} = -f_{\lambda^{p}} \Delta \nabla \lambda_{j}^{p}, \quad \Delta \nabla^{2} r_{j} = -f_{\lambda^{p}} \Delta \nabla^{2} \lambda_{j}^{p}
$$

$$
\Delta \alpha_{j} = f_{\sigma} \Delta \lambda_{j}^{p}, \quad \Delta \nabla \alpha_{j} = f_{\sigma} \Delta \nabla \lambda_{j}^{p}, \quad \Delta \nabla^{2} \alpha_{j} = f_{\sigma} \Delta \nabla^{2} \lambda_{j}^{p}
$$

$$
\Delta \kappa_{j} = -f_{\kappa} \Delta \lambda_{j}^{d}, \quad \Delta \nabla \kappa_{j} = -f_{\kappa} \Delta \nabla \lambda_{j}^{d}, \quad \Delta \nabla^{2} \kappa_{j} = -f_{\kappa} \Delta \nabla^{2} \lambda_{j}^{d}
$$

The increment of the elastic stiffness tensor is also defined here as follows:

$$
\Delta C_{j}^{e} = \left( \frac{\partial C^{e}}{\partial \phi} \right)_{j} : \Delta \phi_{j} = 2C_{j}^{e} : \left( \frac{\partial M^{-T}}{\partial \phi} \right)_{j} : \Delta \phi_{j}
$$

Thus, the correction to the stress during the corrector phase can be written as follows:

$$
\Delta \sigma_{j} = -C_{j}^{e} : \Delta \epsilon_{j}^{pd} + \left( \frac{\partial C^{e}}{\partial \phi} \right)_{j} : (\epsilon_{j} + \Delta \epsilon_{j} - \epsilon_{j}^{pd}) : \Delta \phi_{j}
$$

Given the increments of strain, plastic multiplier, and damage multiplier from the solution of the global equations, it can be seen that the problem defined by this model can be entirely defined by solving for the increment of the stress, $\Delta \sigma_{j}$.

5.4.2 Consistent Tangent Operator

The trial stress can be used to predict if an integration point has entered the plastic and/or damage regime, and the internal state variables can then be updated using the integration scheme. In order to obtain proper quadratic convergence, the choice of a tangent operator must be consistent with the integration scheme. The consistent tangent operator is defined as follows (e.g. Simo & Taylor, 1985):

$$
C_{j}^{lg} = \left( \frac{d \sigma}{d \epsilon} \right)_{j}
$$
In Sections 4.4.2 and 3.5.2, this tangent operator has been derived for the local plasticity model and for the local plasticity-damage model, respectively. In the derivation, the incremental stress and the incremental plastic and damage multipliers are taken as unknowns. The governing equilibrium equation was linearized and solved within an incremental iterative Newton-Raphson solution procedure as discussed in Sections 3.6 and 4.5. From the Newton-Raphson solution, increments of the total strain are obtained, and increments of the stress and multipliers are solved for using the integration scheme.

For the solution of the gradient model, the governing equations will include the plasticity and damage consistency conditions in addition to the equilibrium equation. These governing equations will be linearized and solved within an incremental iterative Newton-Raphson solution procedure, from which increments of the total increments of strain and increments of the plastic and damage multiplier are obtained. Increments of the stress are then solved for using the integration scheme. Thus, the only unknown in the integration scheme is the stress. In order to derive the tangent operator, the following set of equations are used which corresponds to the integration scheme of the previous section:

\[
\begin{align*}
\sigma_j &= C^e_j \left( \varepsilon_j - \varepsilon_j^{pd} \right) + C^e_j : Z_j : \phi_j \\
\varepsilon_j^{pd} &= f_{\sigma_j} \Delta \lambda_j^p + f_{\sigma_j} d \lambda_j^p + g_{\sigma_j} \Delta \lambda_j^d + g_{\sigma_j} d \lambda_j^d \\
\phi_j &= -f_X \Delta \lambda_j^p - f_X d \lambda_j^p - g_X \Delta \lambda_j^d - g_X d \lambda_j^d 
\end{align*}
\]

where the increments of the normals to the yield surface and to the damage surface can be expanded in terms of the increments of the unknown stress such that:

\[
\begin{align*}
df_{\sigma_j} &= f_{\sigma_j} : d\sigma_j \\
df_{X_j} &= f_{X_j} : d\sigma_j \\
dg_{\sigma_j} &= g_{\sigma_j} : d\sigma_j \\
dg_{X_j} &= g_{X_j} : d\sigma_j 
\end{align*}
\]

The required normals to the yield surface and the damage surface are defined by evaluating the normals in APPENDIX B.2 at time step \( j \). The increments of the normals are substituted into Eqs. (5.169) and (5.170), and the resulting equations are then substituted into Eq. (5.168). The resulting equation can then be solved for algorithmic relation for the increment of stress:

\[
\begin{align*}
d\sigma_j &= D^e : \left( \varepsilon_j - f_{\sigma_j} d \lambda_j^p - g_{\sigma_j} d \lambda_j^d \right) + D^e : Z_j : \left( -f_X d \lambda_j^p - g_X d \lambda_j^d \right) 
\end{align*}
\]
Thus, in order to obtain proper convergence, the elastic stiffness tensor $C^e$ should be replaced by $D^e$ in the governing equations. In the next section, an algebraic form of the governing equations is formulated using the integration scheme which can be solved within an incremental iterative Newton-Raphson solution.

### 5.5 Mixed Finite Element Formulation

In order to solve a boundary value problem, a multifield finite element approach is adopted such that the plastic and damage multipliers are discretized in addition to the displacement field. Since the degrees of freedom are increased, two additional governing equations (i.e. the weak forms of the consistency conditions) are required to obtain a solution. Thus, utilizing the integration scheme defined in the previous section, the algorithm requires the following weak satisfaction of the equilibrium condition and of the consistency conditions such that:

\[
\begin{align*}
\int_V \delta u : \left( \nabla \sigma + b \right) dV &= 0 \quad (5.177) \\
\int_{V^p} \delta \lambda^p A f^p dV &= 0 \quad (5.178) \\
\int_{V^d} \delta \lambda^d A g^d dV &= 0 \quad (5.179)
\end{align*}
\]

Note that the last equations are written in terms of the total increment from the previous time step to the current time step ($\Delta f^p = f_j^p - f_0^p; \Delta g^d = g_j^d - g_0^d$). However, at the end of a converged time step, it is enforced that the yield criterion be zero in the plastic domain, $V^p$, and that the damage criterion be zero in the damage domain, $V^d$. Thus, the weak form of the consistency conditions can be written as follows:

\[
\begin{align*}
\int_{V^p} \delta \lambda^p f_j^p dV &= 0 \quad (5.180) \\
\int_{V^d} \delta \lambda^d g_j^d dV &= 0 \quad (5.181)
\end{align*}
\]

Using integration by parts for the weak form of the equilibrium equation, and substituting the algorithmic relation Eq. (5.175), the governing equations are written as follows:
\[
\int_{V}^{\delta \varepsilon} : D_{j}^{e} \left( d\varepsilon - f_{\sigma_{j}} d\lambda^{p} - g_{\sigma_{j}} d\lambda^{d} - Z_{j} \left( f_{\gamma_{j}} d\lambda^{p} + g_{\gamma_{j}} d\lambda^{d} \right) \right) dV
\]
\[
= \int_{V}^{\delta u} : b_{j} dV + \int_{\Gamma}^{\delta u} : \hat{t}_{j} d\Gamma - \int_{V}^{\delta \varepsilon} : \sigma_{j} dV
\]
\[
\int_{V}^{\delta \lambda^{p}} \left( -f_{\sigma_{j}} : D_{j}^{e} : d\varepsilon + h_{1}^{pp} d\lambda^{p} + h_{2}^{pp} \cdot d\nabla \lambda^{p} + h_{3}^{pp} d\nabla^{2} \lambda_{j}^{p} + h_{4}^{pd} d\lambda^{d} \right) dV = \int_{V}^{\delta \lambda^{p}} f_{j} dV
\]
\[
\int_{V}^{\delta \lambda^{d}} \left( -g_{\sigma_{j}} : D_{j}^{e} : d\varepsilon + h_{1}^{dp} d\lambda^{p} + h_{2}^{dp} d\lambda^{d} + h_{3}^{dp} \cdot d\nabla \lambda^{d} + h_{4}^{dd} d\nabla^{2} \lambda_{j}^{d} \right) dV = \int_{V}^{\delta \lambda^{d}} g_{j} dV
\]

where the coefficients defined by Eqs. (5.116) to (5.119) and Eqs. (5.127) to (5.130) are used here and are evaluated at time \( t = j \).

In the right hand side of the governing equations, the stress at iteration \( j \) must be known. As seen from the integration scheme, for each integration point in a plastic or damage state, the backward Euler elastic predictor-inelastic corrector algorithm is used to compute this stress.

Note that the governing equations are written over three different domains. The first governing equation is enforced over the entire body, including both the plastic domain and the damage domain as well as the elastic domain and the undamaged domain; the second governing equation is enforced over only the plastic domain; the third governing equation is enforced over only the damage domain. Note that these three domains can and will overlap, such that a body can have any or all of the following regions: (1) elastic undamaged, (2) elastic damaged, (3) plastic undamaged, and (4) plastic damaged.

In order to enforce the governing equations as given by Eqs. (5.182) to (5.184), different meshes must be used for each equation. The first equation would be enforced over the entire body; the second equations would be solved only over the plastic domain; and the third equation would be solved only over the damage domain. Thus, a method to check where each of the equations are to be enforced (i.e. what part of the body is plastic or what part of the body is damaged) would have to be developed. In the plastic domain at the nodal points, it is enforced that \( d\lambda^{p} \geq 0 \) in the plastic domain and \( f \leq 0 \) in the elastic domain. In the damage domain at the nodal points, it is enforced that \( d\lambda^{d} \geq 0 \) in the damage domain and \( g \leq 0 \) in the undamaged domain.

Alternatively, if the same mesh is to be used for all of the governing equations, i.e. the equations are to be integrated over the total domain \( V \), then it is enforced that \( f_{\sigma_{j}} = 0 \), \( f_{\gamma_{j}} = 0 \), \( f_{j} = 0 \), and \( d\lambda^{p} = 0 \) in the elastic domain and that \( g_{\sigma_{j}} = 0 \), \( g_{\gamma_{j}} = 0 \), \( g_{j} = 0 \), and \( d\lambda^{d} = 0 \) in the undamaged domain. The governing equations can then be solved across the entire body (Pamin, 2004; de Borst et al., 1995).
As the governing equations involve both the gradient and the Laplacian of the plastic multiplier and of the damage multiplier degrees of freedom, the discretization procedure for the plastic and damage multipliers requires higher order interpolation functions such as the Hermitian shape functions. Thus, a mixed finite element solution is used whereby different interpolation functions are used for the multiplier degrees of freedom and the displacement degrees of freedom.

For the displacement degrees of freedom, the governing equations only involve first order derivatives of the displacement field (i.e. strains), and so the discretization procedure for the displacement field only requires $C^0$ continuous interpolation functions. The displacement is discretized using a set of displacement nodal degrees of freedom contained in the vector $\{a_j\}$ such that the interpolating relation is defined as follows:

$$\mathbf{u}_j = [N]\{a_j\}$$  \hspace{1cm} (5.185)

where $[N]$ contains the set of $C^0$ continuous interpolating shape functions. By taking appropriate derivatives of Eq. (3.186), strains can be obtained through the following strain-displacement relation:

$$\mathbf{e}_j = \nabla [N]\{a_j\} = [B]\{a_j\}$$  \hspace{1cm} (5.186)

The derivation of the shape functions, $[N]$, and the strain-displacement matrix, $[B]$, have been shown for one-dimensional and two-dimensional elements in Sections 3.6.1 to 3.6.2, as well as the B-Bar method which is used to avoid locking in isochoic deformations.

For the multiplier degrees of freedom, the governing equations involve up to second order derivatives of the multiplier field, and so the discretization requires a cubic polynomial. To this end, the multipliers are discretized using a set of nodal degrees of freedom contained in the vectors $\{\Lambda^p_j\}$ and $\{\Lambda^d_j\}$ such that the interpolating relation is defined as follows:

$$\lambda^p_j = [h]\{\Lambda^p_j\}$$  \hspace{1cm} (5.187)

$$\lambda^d_j = [h]\{\Lambda^d_j\}$$  \hspace{1cm} (5.188)

where $[h]$ contains a set of Hermitian interpolating shape functions. These shape functions are derived from a cubic polynomial and are $C^1$ continuous. By taking appropriate derivatives of Eqs. (5.187) and (5.188), the gradient and Laplacian multipliers can be obtained through the following relations:
\[\nabla \Lambda_j^p = \nabla [h] \{ \Lambda_j^p \} = [p] \{ \Lambda_j^p \} \quad (5.189)\]
\[\nabla \Lambda_j^d = \nabla [h] \{ \Lambda_j^d \} = [p] \{ \Lambda_j^d \} \quad (5.190)\]
\[\nabla^2 \Lambda_j^p = \nabla^2 [h] \{ \Lambda_j^p \} = [q] \{ \Lambda_j^p \} \quad (5.191)\]
\[\nabla^2 \Lambda_j^d = \nabla^2 [h] \{ \Lambda_j^d \} = [q] \{ \Lambda_j^d \} \quad (5.192)\]

The derivation of the shape functions, \([h]\), and the gradient and Laplacian shape functions, \([p]\) and \([q]\), will be derived for one-dimensional and two-dimensional elements.

Using the discretization relations given by Eqs. (5.185) to (5.192), the weak form of the governing equations defined by Eqs. (5.182) to (5.184) are now written as follows:

\[\{\delta a\}^T \int [B]^T [D_j^f] ([B] \{ da_j \}) - \{ f_{,\sigma} \} [h] \{ d\Lambda_j^p \} - \{ g_{,\sigma} \} [h] \{ d\Lambda_j^d \} ) d\mathbf{V} \]
\[- \{\delta a\}^T \int [B]^T [D_j^f] ([Z_j] \{ f_{,x_j} \} [h] \{ d\Lambda_j^p \} + \{ g_{,x_j} \} [h] \{ d\Lambda_j^d \} ) d\mathbf{V} \]
\[= \{\delta a\}^T \left( \int [N]^T \{ b_j \} d\mathbf{V} + \int [N]^T \{ l_j \} d\Gamma - \int [B]^T \{ \sigma_j \} d\mathbf{V} \right) \]

\[\{\delta \Lambda^p\}^T \int [h]^T \left( -\{ f_{,\sigma} \} [D_j^f] [B] \{ da_j \} \right. \]
\[\left. + (h_{1p}^p [h] + \{ h_{2p}^p \} [p] + h_{3p}^p [q]) \{ d\Lambda_j^p \} + h_{4p}^d [h] \{ d\Lambda_j^d \} \right) d\mathbf{V} \]
\[= \{\delta \Lambda^p\}^T \int [h]^T f_j d\mathbf{V} \]

\[\{\delta \Lambda^d\}^T \int [h]^T \left( -\{ g_{,\sigma} \} [D_j^f] [B] \{ da_j \} \right. \]
\[\left. + h_{1d}^p [h] \{ d\Lambda_j^p \} + (h_{2d}^d [h] + \{ h_{3d}^d \} [p] + h_{4d}^d [q]) \{ d\Lambda_j^d \} \right) d\mathbf{V} \]
\[= \{\delta \Lambda^d\}^T \int [h]^T g_j d\mathbf{V} \]

As these governing equations must be admissible for any variation of \(\{\delta a\}\), \(\{\delta \Lambda^p\}\), and \(\{\delta \Lambda^d\}\), the governing equations can be written as the following set of algebraic equations:
\[
\begin{bmatrix}
[K_{aa}] & [K_{aa',p}] & [K_{aa',d}] \\
[K_{a'a}] & [K_{a'a',p}] & [K_{a'a',d}] \\
[K_{a'd,a}] & [K_{a'd',a}] & [K_{a'd',d}]
\end{bmatrix}
\begin{bmatrix}
\{da_j\}
\end{bmatrix}
= \begin{bmatrix}
[f_a] + [f_a'] + [f_b]
\end{bmatrix} \\
\begin{bmatrix}
[f_{A,p}]
\end{bmatrix}
\begin{bmatrix}
[f_{A,d}]
\end{bmatrix}
\]  
(5.196)

where the sub-matrices are defined as follows:

**Diagonal matrices**
\[
[K_{aa}] = \int_B \begin{bmatrix} B^T & D_j^c \end{bmatrix} [B] dV
\]  
(5.197)
\[
[K_{a'a',p}] = \int_B \begin{bmatrix} h_{1}^{pp} [h] + \{h_{2}^{pp}\} [p] + h_{3}^{pp} [q] \end{bmatrix} dV
\]  
(5.198)
\[
[K_{a'a',d}] = \int_B \begin{bmatrix} h_{1}^{dd} [h] + \{h_{2}^{dd}\} [p] + h_{3}^{dd} [q] \end{bmatrix} dV
\]  
(5.199)

**Off-diagonal matrices**
\[
[K_{aa',p}] = \int_B \begin{bmatrix} B^T & D_j^c \end{bmatrix} \left(- \{f_{,\sigma_j}\} - [Z_j]\{f_{,y_j}\} \right) [h] dV
\]  
(5.200)
\[
[K_{aa',d}] = \int_B \begin{bmatrix} B^T & D_j^c \end{bmatrix} \left(- \{g_{,\sigma_j}\} - [Z_j]\{g_{,y_j}\} \right) [h] dV
\]  
(5.201)
\[
[K_{a'a,d}] = \int_B \begin{bmatrix} h_{1}^T \end{bmatrix} \left(- \{f_{,\sigma_j}\} [D_j^c] \right) [B] dV
\]  
(5.202)
\[
[K_{a'a',d}] = \int_B \begin{bmatrix} h_{1}^T \end{bmatrix} h_{dd}^d [h] dV
\]  
(5.203)
\[
[K_{a'a,a}] = \int_B \begin{bmatrix} h_{1}^T \end{bmatrix} \left(- \{g_{,\sigma_j}\} ^T \{D_j^c\} \right) [B] dV
\]  
(5.204)
\[
[K_{a'a',a}] = \int_B \begin{bmatrix} h_{1}^T \end{bmatrix} h_{dp}^d [h] dV
\]  
(5.205)

**External force vector and body force vector**
\[
[f_a] = \int_{\Gamma} \{N\}^T \{i_j\} d\Gamma
\]  
(5.206)
\[
[f_b] = \int_{\Gamma} \{N\}^T \{b_j\} d\Gamma
\]  
(5.207)

**Vector of nodal forces (equivalent to internal stresses)**
\[
[f_a] = -\int_{\Gamma} \{N\}^T \{\sigma_j\} d\Gamma
\]  
(5.208)
Residual forces

\[ f_{N'} = \int_V [h]^T f_j dV \]  \hspace{1cm} (5.209)

\[ f_{N'}^* = \int_V [h]^T g_j dV \]  \hspace{1cm} (5.210)

Thus, the weak form of the governing equation has been written in terms of a stiffness matrix, a vector of degrees of freedom, and a vector of residuals in the standard form used by finite elements. These matrices and vectors can be computed for the elements which discretize a body and accumulated into global matrices and vectors for the entire body. A finite element procedure is then followed to solve the equations. The material behavior (damaged/undamaged, plastic/elastic) acting in a given domain is then determined by the solution of the plastic multiplier and damage multiplier degrees of freedom. Details of the solution of this type of mixed solution can be found in the works of de Borst and co-workers (de Borst & Mühlhaus, 1992; Pamin, 1994; de Borst et al., 1995; de Borst & Pamin, 1996; Pamin & de Borst, 1999).

The problem of a gradient enhanced model which includes Laplacians requires higher order shape functions in order to allow the Laplacian to be continuous across the element. Based on the selected degrees of freedom for the discretization of the plastic multiplier, a cubic function will be used to interpolate the plastic multiplier. This function is selected such that it satisfies prescribed conditions at the nodal points of the element. These nodal prescribed conditions are the element degrees of freedom.

As advocated in for example de Borst & Mühlhaus (1992) and Pamin (1994), \( C^1 \) cubic Hermitian polynomials are used to interpolate the multipliers since the field equations involve second order derivatives of multipliers. Though cubic polynomials can be derived as either \( C^0 \) or \( C^1 \) elements, \( C^1 \) shape functions allow the use of additional boundary conditions in terms of the gradients of the multipliers.

### 5.5.1 One-Dimensional Hermitian Bar Elements

One-dimensional bar elements as introduced by Pamin (1994) and de Borst et al. (1995) are used here such that \( C^0 \) shape functions are used for the interpolation of displacements and \( C^1 \) shape functions are used for the interpolation of the plastic multiplier and/or damage multiplier (Figure 5.1.1, a & b). In labeling these elements, the first letter ‘M’ indicates a multifield displacement/multiplier element, the second pair ‘1D’ indicates a one-dimensional bar element, and the final number indicates the number of nodes used to discretize the displacements.

This element basically behaves as two separate elements. The displacement discretization for this element uses standard \( C^0 \) shape functions from either a two-node linear interpolating element (Figure 3.7.1, a; Figure 5.1.1, a) or a three-node quadratic interpolating element (Figure 3.7.1, b; Figure 5.1.1, b). The displacement degrees of
freedom for these elements are defined by a single axial displacement, \( u_i \), at each node, \( i \), and Eq. (3.197) is used for the interpolation.

As the same shape functions will be used for the damage multiplier and for the plastic multiplier, a general multiplier defined by \( \lambda \) is used for the derivations of the shape functions. In order to discretize either the plastic multiplier or the damage multiplier, higher order shape functions are required in order to properly capture the Laplacians. Though the displacement field can be interpolated in order to properly capture the Laplacians, it will be shown that the multiplier field is discretized only using the vertex nodes (Figure 5.1.1, a & b).

In defining the element for the discretization of the displacements, isoparametric formulations are followed such that the same shape functions are used to interpolate the coordinates of the nodes and the displacements. As the multiplier is only discretized at the vertex nodes, a different set of shape functions are required for the formulation of the Hermitian shape functions to define the element geometry. To this end, the two-node linear bar element shape functions given by Eq. (3.206) are used for the interpolation of the coordinates. As the shape functions used for the interpolation of the coordinates are linear and the shape functions used for the interpolation of the multiplier are cubic, the formulations followed for the derivation of this element are sub-parametric. For this element, the interpolation of the nodal coordinates and the interpolation of the multiplier are given as follows:

\[
x = [N_{\text{linear}}] \{c\} \\
\lambda = [h] \{\Lambda\}
\]  
(5.211)  
(5.212)

The geometry for the multiplier part of the element can be represented by a vector containing the global coordinates for the Hermitian element as follows:

\[
\{c\} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T
\]  
(5.213)

In order to derive the Hermitian shape functions, \([h]\), in Eq. (5.212), a natural coordinate system is used as shown in Figure 5.1.2 such that the reference nodal coordinates for nodes 1 and 2 are located at \( \xi = -1 \) and \( \xi = +1 \), respectively. Thus, the reference nodal coordinates can be contained in the following vector:

\[
\{\hat{c}\} = \begin{bmatrix} -1 \\ +1 \end{bmatrix}^T
\]  
(5.214)

Degrees of freedom for this Hermitian element will need to be selected and will include gradients of the multiplier fields. In considering an individual element, the derivative degrees of freedom can be taken with respect to the natural coordinate system; however, if the derivatives are to be continuous between elements, the derivatives must be taken with respect to the global coordinate system as the reference coordinate system changes from element to element.
Figure 5.1.1: Elements presented in the global coordinate system with standard $C^0$ interpolation of displacement field (all nodes) and Hermitian cubic interpolation of plastic multiplier field and damage multiplier field (corner nodes).

Figure 5.1.2: Elements presented in the natural coordinate system.
This being the case, the degree of freedom derivatives used in this formulation are taken with respect to the global coordinate system. Shape functions are derived utilizing the reference coordinate system and a reference coordinate system set of degrees of freedom, \( \{ \tilde{\Lambda} \} \). A set of global shape functions to be used in Eq. (5.212) will then be obtained by transforming the reference degrees of freedom to the global degrees of freedom.

Thus, the multiplier related degrees of freedom at each vertex node, \( i \), are the multiplier and its first-order derivative with respect to \( x \). The interpolation relation of the multiplier in Eq. (5.212) utilizing these degrees of freedom is presented in Figure 5.2. For this element, vectors containing the element degrees of freedom and the set of shape functions are defined as follows:

\[
\{ \Lambda \} = \{ \lambda, \lambda_{x1}, \lambda_2, \lambda_{x2} \}^T
\]

\[
[h] = [h_1, h_{x1}, h_2, h_{x2}]
\]

(5.215)  
(5.216)

As the degrees of freedom for the discretization of the multiplier involves gradients with respect to \( x \) in the global coordinate system, a set of shape functions is defined in the reference coordinate system, and the geometry defined by Eq. (5.211) is used to transform the shape functions to the global coordinate system. Thus, the following interpolation must first be considered:

\[
\lambda = [h] \{ \tilde{\Lambda} \}
\]

(5.217)

where the set of degrees of freedom and the shape functions are defined in the reference coordinate system as follows:

**Figure 5.2**: Cubic interpolation of multiplier, \( \lambda \), denoting nodal degrees of freedom
To transform the shape functions to the global coordinate system, the reference configuration degrees of freedom, Eq. (5.218), can be written in terms of the global coordinate system degrees of freedom, Eq. (5.215), through the use of the chain rule such that:

$$\{\tilde{\lambda}\} = \left[\tilde{\lambda}_1 \quad \tilde{\lambda}_{x1} \quad \tilde{\lambda}_2 \quad \tilde{\lambda}_{x2}\right]^T$$

(5.218)

$$[\tilde{h}] = \begin{bmatrix} \tilde{h}_1 & \tilde{h}_{\xi 1} & \tilde{h}_2 & \tilde{h}_{\xi 2} \end{bmatrix}$$

(5.219)

where the term used for the transformation is found from the Jacobian of the two-node linear element given by Eq. (3.213) and is rewritten here as follows:

$$J = \frac{\partial x}{\partial \xi} = \frac{1}{2} (x_2 - x_1)$$

(5.220)

Using the reference degrees of freedom, Eq. (5.220), in the interpolation given by Eq. (5.217) and expanding, the global form of interpolation, Eq. (5.212), can be recovered by writing the matrix of shape functions in the global coordinate system as follows:

$$[h] = \begin{bmatrix} \tilde{h}_1 & \tilde{h}_{\xi 1} & \tilde{h}_2 & \tilde{h}_{\xi 2} \end{bmatrix}$$

(5.221)

Utilizing the natural coordinate system, a polynomial is assumed for the discretization of the multiplier field such that:

$$\{\hat{\lambda}\} = \{\hat{X}\}^T \{\hat{d}\}$$

(5.222)

where the vector $\{\hat{X}\}$ defines the order of the interpolation and the vector $\{\hat{d}\}$ contains coefficients acting as generalized degrees of freedom for this polynomial. For the Hermitian element, this polynomial is cubic in $\xi$ such that these vectors take the following forms:

$$\{\hat{X}\} = \{1 \quad \xi \quad \xi^2 \quad \xi^3\}^T$$

(5.223)

$$\{\hat{d}\} = \{\hat{a}_1 \quad \hat{a}_2 \quad \hat{a}_3 \quad \hat{a}_4\}^T$$

(5.224)
In order to write the generalized degrees of freedom in terms of the nodal degrees of freedom, \( \{\tilde{\Lambda}\} \), the following expression is used:

\[
\{\tilde{\Lambda}\} = \left[\begin{array}{c}
\tilde{A}
\end{array}\right] \{\tilde{d}\}
\]  (5.226)

where each row of this relation is found by evaluating Eq. (5.223) and its corresponding derivative with respect to \( \xi \) for the corresponding degree of freedom. Thus, the matrix \( \left[\begin{array}{c}
\tilde{A}
\end{array}\right] \) is defined as follows:

\[
\left[\begin{array}{cccc}
1 & -1 & 1 & -1 \\
0 & 1 & -2 & 3 \\
1 & 1 & 1 & 1 \\
0 & 1 & 2 & 3
\end{array}\right]
\]  (5.227)

The vector \( \{\tilde{d}\} \) can now be solved for in Eq. (5.226) and substituted into Eq. (5.223) such that the desired interpolation relation given by Eq. (5.217) is obtained. The set of interpolating functions in this relation are defined as follows:

\[
\left[\begin{array}{c}
\tilde{h}
\end{array}\right] = \{\tilde{X}\}^T \left[\begin{array}{c}
\tilde{A}
\end{array}\right]^{-1}
\]  (5.228)

The solution of this equation gives the components of the shape function matrices in terms of the reference coordinate system as follows:

\[
\tilde{h}_i = \frac{1}{4} \left[\xi_i (3\xi - \xi^3) + 2\right]
\]  (5.229)

\[
\tilde{h}_i = \frac{1}{4} \left(\xi^3 + \xi \xi^2 - \xi^2 - \xi\right)
\]  (5.230)

Plots of each of these component shape functions for each node is given in Figure 5.3. In these plots, it is seen that the shape functions given by Eq. (5.229) have a unit value at their corresponding nodes, a zero value at the opposite node, and a slope of zero at both nodes. Each of these curves can be obtained for the multiplier field by applying a unitary value to the multiplier degree of freedom at the node of interest and a zero value to the remaining degrees of freedom. Similarly, for the shape functions given by Eq. (5.230), the shape function has a unit slope at the respective node, a zero value at both nodes, and a zero slope at the opposite node. Again, the curves can be obtained for the multiplier field by applying a unitary value for the multiplier derivative nodal degree of freedom at the node of interest and a zero value to the remaining degrees of freedom.
In the same way that strains were determined in Section 3.6.1, the gradients and Laplacians of the multiplier field are computed in the element using shape functions with the multiplier field. For the one-dimensional bar case, the gradient and Laplacian reduce to derivatives of the multiplier with respect to the $x$ direction such that:

\[
\nabla \lambda = \lambda_x = \frac{\partial \lambda}{\partial x} = [p]\{\Lambda\} \tag{5.231}
\]

\[
\nabla^2 \lambda = \lambda_{xx} = \frac{\partial^2 \lambda}{\partial x^2} = [q]\{\Lambda\} \tag{5.232}
\]

These additional gradient and Laplacian shape functions are written in the following forms:

\[
[p] = \frac{\partial}{\partial x}[h] = \left[ \frac{\partial h_1}{\partial x}, \frac{\partial h_{s1}}{\partial x}, \frac{\partial h_2}{\partial x}, \frac{\partial h_{s2}}{\partial x} \right] = [p_1, p_{s1}, p_2, p_{s2}] \tag{5.233}
\]

\[
[q] = \frac{\partial^2}{\partial x^2}[h] = \left[ \frac{\partial^2 h_1}{\partial x^2}, \frac{\partial^2 h_{s1}}{\partial x^2}, \frac{\partial^2 h_2}{\partial x^2}, \frac{\partial^2 h_{s2}}{\partial x^2} \right] = [q_1, q_{s1}, q_2, q_{s2}] \tag{5.234}
\]

Using the chain rule, the global coordinate system gradient and Laplacian of the multiplier can be written in terms of the reference coordinate system gradient and Laplacian as follows:

![Figure 5.3: Plots of shape function components for the cubic Hermitian polynomial](image)

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\[ \nabla \lambda = \frac{\partial \lambda}{\partial \xi} \frac{\partial \xi}{\partial x} \]  
(5.235)

\[ \nabla^2 \lambda = \frac{\partial^2 \lambda}{\partial \xi^2} \left( \frac{\partial \xi}{\partial x} \right)^2 + \frac{\partial \lambda}{\partial \xi} \frac{\partial^2 \xi}{\partial \xi \partial x^2} \]  
(5.236)

where the term used for the transformations are found from the inverse of the Jacobian of the two-node linear element, Eq. (5.221). For the 1D linear shape functions used, the second derivative of the reference configuration coordinate, \( \xi \), with respect to the global configuration coordinate, \( x \), in Eq. (5.236) is zero.

Utilizing the interpolation given by Eq. (5.212), the gradient and Laplacian can be written as follows:

\[ \nabla \lambda = \frac{\partial \xi}{\partial x} \left[ h \right] \left[ \Lambda \right] \]  
(5.237)

\[ \nabla^2 \lambda = \left( \frac{\partial \xi}{\partial x} \right)^2 \left( \frac{\partial^2 \xi}{\partial \xi \partial x^2} \right) \left[ h \right] \left[ \Lambda \right] \]  
(5.238)

The following set of shape function derivatives are defined to be used in this transformation:

\[ \left[ \tilde{p} \right] = \frac{\partial}{\partial \xi} \left[ \hat{h} \right] = \left[ \tilde{p}_1 \quad \tilde{p}_{\xi 1} \quad \tilde{p}_2 \quad \tilde{p}_{\xi 2} \right] \]  
(5.239)

\[ \left[ \tilde{q} \right] = \frac{\partial^2}{\partial \xi^2} \left[ \hat{h} \right] = \left[ \tilde{q}_1 \quad \tilde{q}_{\xi 1} \quad \tilde{q}_2 \quad \tilde{q}_{\xi 2} \right] \]  
(5.240)

such that the global forms of interpolation, Eqs. (5.231) and (5.232), can be recovered from Eqs. (5.237) and (5.238), where the matrices of gradient and Laplacian shape functions in the global coordinate system are given as follows:

\[ \left[ p \right] = \frac{\partial \xi}{\partial x} \left[ \tilde{h} \right] = \left[ \tilde{p}_1 \quad \tilde{p}_{\xi 1} \quad \tilde{p}_2 \quad \tilde{p}_{\xi 2} \right] \]  
(5.241)

\[ \left[ q \right] = \left( \frac{\partial \xi}{\partial x} \right)^2 \left[ \tilde{h} \right] = \left[ \tilde{q}_1 \quad \tilde{q}_{\xi 1} \quad \tilde{q}_2 \quad \tilde{q}_{\xi 2} \right] \]  
(5.242)

By differentiating the Hermitian shape functions given by Eqs. (5.229) and (5.230), with respect to the reference coordinate, \( \xi \), the components of the gradient shape function matrix are given as follows:
\[
\tilde{p}_i = \frac{1}{4} \xi_i \left( 3 - 3 \xi_i^2 \right) 
\]

\[
\tilde{p}_{\xi_i} = \frac{1}{4} \left( 3 \xi_i^2 + 2 \xi_i \xi_{\xi_i} - 1 \right) 
\]

Similarly, the components of the Laplacian shape function matrix are given as follows:

\[
\tilde{q}_i = -\frac{3}{2} \xi_i \xi_{\xi_i} 
\]

\[
\tilde{q}_{\xi_i} = \frac{1}{2} \left( 3 \xi_i^2 + \xi_{\xi_i} \right) 
\]

These gradient and Laplacian shape function components defined in the reference coordinate system can now be substituted into the corresponding definitions of the global gradient and Laplacian shape function matrices, Eqs. (5.241) and (5.242), in order to properly define the interpolation of the gradient and Laplacian, Eqs. (5.231) and (5.232).

The introduction of additional degrees of freedom for this element requires additional boundary conditions. In the work of Pamin (1994), it was suggested that the following conditions on the model boundaries meet the requirements to avoid a singular stiffness matrix:

\[
\lambda_n = 0 
\]

where \( n \) denotes the normal to the model boundary. For the one-dimensional problem considered here, this “normal” coincides with the global \( x \) coordinate axis.

### 5.5.2 Two-Dimensional Hermitian Quadrilateral Elements

Two-dimensional quadrilateral elements as introduced by Pamin (1994) and de Borst et al. (1995) are used here such that \( C^0 \) shape functions are used for the interpolation of displacements and \( C^1 \) shape functions are used for the interpolation of the plastic multiplier and/or damage multiplier (Figure 5.1.1, c & d). In labeling these elements, the first letter ‘M’ indicates a multifield displacement/multiplier element, the second pair ‘PE’ indicates a plane-strain quadrilateral element, and the final number indicates the number of nodes used to discretize the displacements.

This element basically behaves as two separate elements. The displacement discretization for this element uses standard \( C^0 \) shape functions from either a four-node linear interpolating element (Figure 3.7.1, c; Figure 5.1.1, c) or an eight-node quadratic interpolating element (Figure 3.7.1, d; Figure 5.1.1, d). The displacement degrees of freedom for these elements are defined by a horizontal displacement, \( u_i \), and a vertical displacement, \( v_i \), at each node, \( i \), and Eq. (3.217) is used for the interpolation.
As the same shape functions will be used for the damage multiplier and for the plastic multiplier, a general multiplier defined by $\lambda$ is used for the derivations of the shape functions. In order to discretize either the plastic multiplier or the damage multiplier, higher order shape functions are required in order to properly capture the Laplacians. Though the displacement field can be interpolated using mid-side nodes, it will be shown that the multiplier field is discretized only using the vertex nodes (Figure 5.1.1, c & d).

In defining the element for the discretization of the displacements, isoparametric formulations are followed such that the same shape functions are used to interpolate the coordinates of the nodes and the displacements. As the multiplier is only discretized at the vertex nodes, a different set of shape functions are required for the formulation of the Hermitian shape functions to define the element geometry. To this end, the four-node linear bar element shape functions given by Eq. (3.245) are used for the interpolation of the coordinates. As the shape functions used for the interpolation of the coordinates are linear and the shape functions used for the interpolation of the multiplier are cubic, the formulations followed for the derivation of this element are sub-parametric. For this element, the interpolation of the nodal coordinates and the interpolation of the multiplier are given as follows:

$$x = [N_{\text{linear}}] \{c\} \quad (5.248)$$

$$\lambda = [h] \{\Lambda\} \quad (5.249)$$

The geometry for the multiplier part of the element can be represented by a vector containing the global coordinates for the Hermitian element as follows:

$$\{c\} = \{x_1, y_1, x_2, y_2, x_3, y_3, x_4, y_4\}^T \quad (5.250)$$

In order to derive the Hermitian shape functions, $[h]$, in Eq. (5.249), a natural coordinate system as shown in Figure 5.1.2 (c & d) is used. As the geometry is defined by only the vertex nodes, the vector of reference nodal coordinates can be defined for the $\xi$ coordinates and for the $\eta$ coordinates as follows:

$$\{\xi_{\xi}\} = \{-1, +1, +1, -1\}^T \quad (5.251)$$

$$\{\xi_{\eta}\} = \{-1, -1, +1, +1\}^T \quad (5.252)$$

Degrees of freedom for this Hermitian element will need to be selected and will include gradients of the multiplier fields. In considering an individual element, the derivative degrees of freedom can be taken with respect to the natural coordinate system; however, if the derivatives are to be continuous between elements, the derivatives must be taken with respect to the global coordinate system as the reference coordinate system changes from element to element. Shape functions are derived utilizing the reference
coordinate system and a reference coordinate system set of degrees of freedom, $\{\tilde{\Lambda}\}$. A set of global shape functions to be used in Eq. (5.212) will then be obtained by transforming the reference degrees of freedom to the global degrees of freedom.

In the derivation of the cubic polynomial, it will be required to use degrees of freedom which include a mixed derivative with respect to the reference coordinate system, $\lambda_{\xi\eta}$. Note here that the transformation of this mixed derivative term by the chain rule is given as follows:

$$
\tilde{\lambda}_{\xi\eta} = \lambda_{,xx} \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} + \lambda_{,xy} \left( \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \eta} + \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} \right) + \lambda_{,yy} \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} + \lambda_{,x} \frac{\partial^2 x}{\partial \xi^2 \partial \eta} + \lambda_{,y} \frac{\partial^2 y}{\partial \xi \partial \eta^2} \quad (5.253)
$$

Thus, this transformation leads to the necessity of having the second order derivatives of the multiplier with respect to $x$ and with respect to $y$ as additional degrees of freedom when used for non-rectangular elements. These higher order derivatives must be retained in the formulation if first-order continuity across element boundaries is required. If we assume that we can neglect these higher order derivatives as degrees of freedom in the global coordinate system, the gradients will be continuous at the nodes, but generally not across element boundaries. Alternately, in order to avoid introducing simplifications and additional degrees of freedom, the works of Petera & Pittman (1994) and Chen & Yuan (2002) is followed such that this mixed degree of freedom in the reference configuration is not transformed to the global coordinate system. Thus, the multiplier related degrees of freedom at each vertex node, $i$, are the multiplier, its first-order derivatives with respect to $x$ and with respect to $y$, and the mixed derivative with respect to both $\xi$ and $\eta$. The interpolation relation of the multiplier in Eq. (5.249) is now defined by the vector containing the element degrees of freedom and the set of shape functions as follows:

$$
\{\Lambda\} = \begin{bmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \\ \Lambda_4 \end{bmatrix}^T
$$

$$
[h] = \begin{bmatrix} H_1 \\ H_2 \\ H_3 \\ H_4 \end{bmatrix}
$$

(5.254)  (5.255)

where, at node $i$, the sub-vectors of degrees of freedom, $\{\Lambda_i\}$, and the sub-matrices of Hermitian shape functions, $[H_i]$, are written as follows:

$$
\{\Lambda_i\} = \begin{bmatrix} \lambda_i \\ \lambda_{,x1} \\ \lambda_{,y1} \\ \lambda_{,\xi\eta1} \end{bmatrix}
$$

$$
[H_i] = \begin{bmatrix} h_i \\ h_{x1} \\ h_{y1} \\ h_{\xi\eta1} \end{bmatrix}
$$

(5.256)  (5.257)

As the degrees of freedom for the discretization of the multiplier involves gradients with respect to the global coordinate system, a set of shape functions in the reference coordinate system is derived and the geometry defined by Eq. (5.248) is used to transform the shape functions to the global coordinate system. In deriving the Hermitian shape functions, the multiplier related degrees of freedom in the reference coordinate system...
system at each vertex node, \( i \), are the multiplier, its derivatives with respect to \( \xi \) and with respect to \( \eta \), and the mixed derivative with respect to both \( \xi \) and \( \eta \). Thus, the following interpolation must first be considered:

\[
\lambda = \begin{bmatrix} \tilde{h} \end{bmatrix} \{ \tilde{\Lambda} \} \quad (5.258)
\]

For the reference configuration, the matrix of Hermitian shape functions and the set of degrees of freedom are defined as follows:

\[
\begin{bmatrix} \tilde{h} \\ \tilde{\lambda} \end{bmatrix} = \begin{bmatrix} \tilde{H}_1 \\ \tilde{H}_2 \\ \tilde{H}_3 \\ \tilde{H}_4 \end{bmatrix} \quad (5.259)
\]

\[
\begin{bmatrix} \tilde{\lambda} \end{bmatrix} = \begin{bmatrix} \tilde{\lambda}_1 \\ \tilde{\lambda}_2 \\ \tilde{\lambda}_3 \\ \tilde{\lambda}_4 \end{bmatrix}^T \quad (5.260)
\]

where the sub-matrices \( \tilde{H}_i \) and the sub-vector \( \{ \tilde{\lambda}_i \} \) represent the reference configuration shape functions and degrees of freedom at node \( i \) and are written as follows:

\[
\begin{bmatrix} \tilde{H}_i \end{bmatrix} = \begin{bmatrix} \tilde{h}_i \\ \tilde{h}_{\xi i} \\ \tilde{h}_{\eta i} \\ \tilde{h}_{\xi \eta i} \end{bmatrix} \quad (5.261)
\]

\[
\{ \tilde{\lambda}_i \} = \{ \tilde{\lambda}_i, \tilde{\lambda}_{\xi i}, \tilde{\lambda}_{\eta i}, \tilde{\lambda}_{\xi \eta i} \} \quad (5.262)
\]

To transform the shape functions to the global coordinate system, we see that we can rewrite the reference configuration degrees of freedom, Eq. (5.260), in terms of the global coordinate system degrees of freedom, Eq. (5.254), through the use of the chain rule such that, for a given node \( i \), we have the following:

\[
\{ \tilde{\lambda}_i \} = [K] \{ \lambda_i \} \quad (5.263)
\]

where the transformation matrix \([K]\) is defined as follows:

\[
[K] = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & 0 \\
0 & \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \quad (5.264)
\]

The components of this transformation matrix are found from the Jacobian matrix of the bi-linear element given by Eq. (3.265) and rewritten here as follows:
Using the reference degrees of freedom, Eq. (5.263), in the interpolation given Eq. (5.258) and expanding, the global form of interpolation, Eq. (5.249), can be recovered by writing the matrix of shape functions in the global coordinate system as follows:

$$
[H_i] = [H_i][K]
$$

(5.266)

Utilizing the natural coordinate system, a polynomial is assumed for the discretization of the multiplier field such that:

$$
\lambda = \{\tilde{X}\}^T\{\tilde{d}\}
$$

(5.267)

where the vector $\{\tilde{X}\}$ defines the order of the interpolation and the vectors $\{\tilde{d}\}$ contain coefficients acting as generalized degrees of freedom for this polynomial. For the four-node Hermitian element, the interpolating polynomial is cubic in $\xi$ and in $\eta$ such that these vectors take the following forms:

$$
\{\tilde{X}\} = \{1 \quad \xi \quad \eta \quad \xi\eta \quad \xi^2 \quad \eta^2 \quad \xi^2\eta \quad \xi^2\eta^2 \quad \xi^3 \quad \eta^3 \quad \xi\eta^3 \quad \xi^2\eta^3 \quad \xi^3\eta \quad \xi^3\eta^3\}
$$

(5.268)

$$
\{\tilde{d}\} = \{\tilde{d}_1 \quad \tilde{d}_2 \quad \ldots \quad \tilde{d}_{16}\}^T
$$

(5.269)

In order to write the generalized degrees of freedom, $\{\tilde{d}\}$, in terms of the nodal degrees of freedom, $\{\tilde{\Lambda}\}$, the following expression is used:

$$
\{\tilde{\Lambda}\} = [\tilde{A}]\{\tilde{d}\}
$$

(5.270)

where each row of this relation is found by evaluating Eq. (5.267) and its derivatives with respect to $\xi$ and $\eta$ for the corresponding degree of freedom. Thus, the matrix $[\tilde{A}]$ is defined as follows:
The vector \( \{ \vec{d} \} \) can now be solved for in Eq. (5.270) and substituted into Eq. (5.267) such that the desired interpolation relation given by Eq. (5.258) is obtained. The set of interpolating functions in this relation are defined as follows:

\[
[h] = \{ \tilde{X} \}^T \begin{bmatrix} A \end{bmatrix}^{-1}
\]  

(5.272)

The solution of this equation gives the components of the shape function matrices in terms of the reference coordinate system as follows:

\[
\tilde{h}_i = f_{\tilde{s}_i} (\tilde{\xi}) f_{\tilde{\eta}_i} (\eta) 
\]  

(5.273)

\[
\tilde{h}_{\tilde{s}_i} = g_{\tilde{s}_i} (\tilde{\xi}) f_{\tilde{\eta}_i} (\eta) 
\]  

(5.274)

\[
\tilde{h}_{\tilde{\eta}_i} = f_{\tilde{s}_i} (\tilde{\xi}) g_{\tilde{\eta}_i} (\eta) 
\]  

(5.275)

\[
\tilde{h}_{\tilde{s}\tilde{\eta}} = g_{\tilde{s}_i} (\tilde{\xi}) g_{\tilde{\eta}_i} (\eta) 
\]  

(5.276)

where, by introducing a variable \( s \) as either \( \tilde{\xi} \) or \( \tilde{\eta} \), these shape functions are written in terms of the following first order Hermitian polynomials (Pamin & de Borst, 1992):

\[
f_{\tilde{s}_i} (s) = \frac{1}{4} \left[ s_i \left( 3s - s^3 \right) + 2 \right]
\]  

(5.277)
\[ g_s(s) = \frac{1}{4} \left( s^3 + s^2s - s - s' \right) \] (5.278)

In the same way that strains were determined in Section 3.6.1, the gradients and Laplacians of the multiplier field are computed in the element using shape functions with the multiplier field. For the two-dimensional bar case, the gradient and Laplacian reduce to derivatives of the multiplier with respect to the \( x \) direction and with respect to the \( y \) direction such that:

\[
\{ \nabla \lambda \} = \left\{ \begin{array}{l} \lambda_x \\ \lambda_y \end{array} \right\} = [p] \left\{ \Lambda \right\} \tag{5.279}
\]

\[
\nabla^2 \lambda = \lambda_{xx} + \lambda_{yy} = [q] \left\{ \Lambda \right\} \tag{5.280}
\]

These additional gradient and Laplacian shape functions are written in the following forms:

\[
[p] = \left[ \begin{array}{c} \frac{\partial}{\partial x}[h] \\ \frac{\partial}{\partial y}[h] \end{array} \right] = \begin{bmatrix} P_1 & P_2 & P_3 & P_4 \end{bmatrix} \tag{5.281}
\]

\[
[q] = \left[ \frac{\partial^2}{\partial x^2}[h] + \frac{\partial^2}{\partial y^2}[h] \right] = \begin{bmatrix} Q_1 & Q_2 & Q_3 & Q_4 \end{bmatrix} \tag{5.282}
\]

where the sub-matrices \([P_i]\) and \([Q_i]\) represent the gradient and Laplacian shape functions at node \( i \) and are written as follows:

\[
[P_i] = \left[ \begin{array}{c} \frac{\partial}{\partial x}[H_i] \\ \frac{\partial}{\partial y}[H_i] \end{array} \right] = \begin{bmatrix} p_i & p_{xi} & p_{yi} & p_{xsi} & p_{ysi} \end{bmatrix} \tag{5.283}
\]

\[
[Q_i] = \left[ \frac{\partial^2}{\partial x^2}[H_i] + \frac{\partial^2}{\partial y^2}[H_i] \right] = \begin{bmatrix} q_i & q_{xi} & q_{yi} & q_{xsi} & q_{ysi} \end{bmatrix} \tag{5.284}
\]

Using the chain rule, the global coordinate system gradient and Laplacian of the multiplier can be written in terms of the reference coordinate system gradient and Laplacian as follows:
\[
\{\nabla \lambda \} = \begin{bmatrix}
\lambda_x \frac{\partial \xi}{\partial x} + \lambda_{\eta} \frac{\partial \eta}{\partial x} \\
\lambda_x \frac{\partial \xi}{\partial y} + \lambda_{\eta} \frac{\partial \eta}{\partial y}
\end{bmatrix}
\]  
(5.285)

\[
\nabla^2 \lambda = \lambda_{\xi \xi} \left( \frac{\partial \xi}{\partial x} \right)^2 + 2 \lambda_{\xi \eta} \left( \frac{\partial \eta}{\partial x} \right) \left( \frac{\partial \xi}{\partial x} \right) + \lambda_{\eta \eta} \left( \frac{\partial \eta}{\partial x} \right)^2 \\
+ \lambda_{\xi \eta} \left( \frac{\partial \xi}{\partial y} \right)^2 + 2 \lambda_{\xi \eta} \left( \frac{\partial \eta}{\partial y} \right) \left( \frac{\partial \xi}{\partial y} \right) + \lambda_{\eta \eta} \left( \frac{\partial \eta}{\partial y} \right)^2
\]  
(5.286)

where the components used for the transformations are found from the inverse of the Jacobian matrix of the bi-linear element given by Eq. (3.256) which is rewritten here as follows:

\[
[G] = \begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\
\frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y}
\end{bmatrix}
\]  
(5.287)

Utilizing the interpolation given by Eq. (5.249), the gradient and the Laplacian can be written as follows:

\[
\{\nabla \lambda \} = [G] \begin{bmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta}
\end{bmatrix} \begin{bmatrix} h \end{bmatrix} \{\Lambda\}
\]  
(5.288)

\[
\nabla^2 \lambda = \begin{bmatrix}
\left( \frac{\partial \xi}{\partial x} \right)^2 + \left( \frac{\partial \xi}{\partial y} \right)^2 \\
\left( \frac{\partial \eta}{\partial x} \right)^2 + \left( \frac{\partial \eta}{\partial y} \right)^2 \\
2 \left( \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial y} \right)
\end{bmatrix} \begin{bmatrix}
\frac{\partial^2}{\partial \xi^2} \\
\frac{\partial^2}{\partial \eta^2} \\
\frac{\partial^2}{\partial \xi \partial \eta}
\end{bmatrix} \begin{bmatrix} h \end{bmatrix} \{\Lambda\}
\]  
(5.289)

The following set of shape function derivatives are defined to be used in this transformation:
\[
\begin{bmatrix}
\frac{\partial}{\partial \xi} \begin{bmatrix} \tilde{h} \end{bmatrix} \\
\frac{\partial}{\partial \eta} \begin{bmatrix} \tilde{h} \end{bmatrix}
\end{bmatrix} =
\begin{bmatrix}
\tilde{P}_1 & \tilde{P}_2 & \tilde{P}_3 & \tilde{P}_4
\end{bmatrix}
\]  \hspace{1cm} (5.290)

\[
\begin{bmatrix}
\frac{\partial^2}{\partial \xi^2} \begin{bmatrix} \tilde{h} \end{bmatrix} \\
\frac{\partial^2}{\partial \eta^2} \begin{bmatrix} \tilde{h} \end{bmatrix} \\
\frac{\partial^2}{\partial \xi \partial \eta} \begin{bmatrix} \tilde{h} \end{bmatrix}
\end{bmatrix} =
\begin{bmatrix}
\tilde{Q}_1 & \tilde{Q}_2 & \tilde{Q}_3 & \tilde{Q}_4
\end{bmatrix}
\]  \hspace{1cm} (5.291)

where the sub-matrices \([\tilde{P}_i]\) and \([\tilde{Q}_i]\) are defined at node \(i\) as follows:

\[
\begin{bmatrix}
\frac{\partial}{\partial \xi} \begin{bmatrix} \tilde{H}_i \end{bmatrix} \\
\frac{\partial}{\partial \eta} \begin{bmatrix} \tilde{H}_i \end{bmatrix}
\end{bmatrix} =
\begin{bmatrix}
\tilde{P}_i & \tilde{p}_{\xi i} & \tilde{p}_{\eta i} & \tilde{p}_{\xi \eta i}
\end{bmatrix}
\]  \hspace{1cm} (5.292)

\[
\begin{bmatrix}
\frac{\partial^2}{\partial \xi^2} \begin{bmatrix} \tilde{H}_i \end{bmatrix} \\
\frac{\partial^2}{\partial \eta^2} \begin{bmatrix} \tilde{H}_i \end{bmatrix} \\
\frac{\partial^2}{\partial \xi \partial \eta} \begin{bmatrix} \tilde{H}_i \end{bmatrix}
\end{bmatrix} =
\begin{bmatrix}
\tilde{Q}_i & \tilde{q}_{\xi i} & \tilde{q}_{\eta i} & \tilde{q}_{\xi \eta i}
\end{bmatrix}
\]  \hspace{1cm} (5.293)

By transforming the shape functions in Eqs. (5.288) and (5.289) according to Eq. (5.266), the global form of interpolation, Eqs. (5.279) and (5.280), can be recovered by defining the matrix of shape functions in the global coordinate system for each node \(i\) as follows:

\[
[P_i] =
\begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\
\frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y}
\end{bmatrix}
\begin{bmatrix}
\tilde{P}_i
\end{bmatrix}[K]
\]  \hspace{1cm} (5.294)
By taking the appropriate derivatives of the Hermitian shape functions, Eqs. (5.273) to (5.276), with respect to the reference coordinates, $\xi$ and $\eta$, the components of the reference coordinate system gradient shape function matrix corresponding to node $i$ are given as follows:

$$\tilde{p}_i = \left\{ f_{i,\xi} (\xi) f_{i,\eta} (\eta), f_{i,\xi} (\xi) f_{i,n,\eta} (\eta) \right\}$$

(5.296)

$$\tilde{q}_i = \left\{ g_{i,\xi} (\xi) f_{i,\eta} (\eta), g_{i,\xi} (\xi) f_{i,n,\eta} (\eta) \right\}$$

(5.297)

$$\tilde{p}_{\xi i} = \left\{ f_{i,\xi} (\xi) g_{i,\eta} (\eta), f_{i,\xi} (\xi) g_{i,n,\eta} (\eta) \right\}$$

(5.298)

$$\tilde{p}_{\eta i} = \left\{ g_{i,\xi} (\xi) g_{i,\eta} (\eta), g_{i,\xi} (\xi) g_{i,n,\eta} (\eta) \right\}$$

(5.299)

Similarly, the components of the reference coordinate system Laplacian shape function matrix corresponding to node $i$ are given as follows:

$$\tilde{q}_i = \left\{ f_{i,\xi} (\xi) f_{i,\eta} (\eta), f_{i,\xi} (\xi) f_{i,n,\eta} (\eta) \right\}$$

(5.300)

$$\tilde{q}_{\xi i} = \left\{ g_{i,\xi} (\xi) f_{i,\eta} (\eta), g_{i,\xi} (\xi) f_{i,n,\eta} (\eta) \right\}$$

(5.301)

$$\tilde{q}_{\eta i} = \left\{ f_{i,\xi} (\xi) g_{i,\eta} (\eta), f_{i,\xi} (\xi) g_{i,n,\eta} (\eta) \right\}$$

(5.302)
where the gradient and Laplacian shape functions are written in terms of the following functions:

\[
\tilde{q}_{\xi\eta} = \begin{pmatrix}
g_{\xi,\xi} (\xi) g_{\eta,\eta} (\eta) 
g_{\xi,\eta} (\xi) g_{\eta,\eta} (\eta) 
g_{\xi,\eta} (\xi) g_{\eta,\eta} (\eta)
\end{pmatrix}
\] (5.303)

These gradient and Laplacian shape function components defined in the reference coordinate system can now be substituted into the corresponding definitions of the global gradient and Laplacian shape function matrices, Eqs. (5.292) and (5.293), in order to properly define the interpolation of the gradient and Laplacian, Eqs. (5.279) and (5.280).

The introduction of additional degrees of freedom for this element requires additional boundary conditions. In the work of Pamin (1994), it was suggested that the following conditions on the model boundaries meet the requirements to avoid a singular stiffness matrix:

\[
\lambda_{n} = 0 \\
\lambda_{nm} = 0
\] (5.308) (5.309)

where \(n\) and \(m\) denote the normal and tangential directions to the model boundary. These boundary conditions can easily be applied in either the global coordinate system or the reference coordinate system when the surface normal is directed along either of the global coordinate system axes. Along this surface, the normal and tangential directions coincide with both the global coordinate system and the reference coordinate system. As an example, consider the model presented in Figure 5.4. For the horizontal and vertical surfaces shown, the following boundary conditions can be applied:
**Horizontal Boundary**
\[
\begin{align*}
\lambda_x &= \lambda_\eta = 0 \\
\lambda_{xy} &= \lambda_{\xi\eta} = 0 
\end{align*}
\]

**Vertical Boundary**
\[
\begin{align*}
\lambda_x &= \lambda_\eta = 0 \\
\lambda_{xy} &= \lambda_{\xi\eta} = 0 
\end{align*}
\]

When considering a surface at an angle to the global coordinate system, the boundary conditions in Eqs. (5.308) and (5.309) have to be decomposed using the angle that the surface makes with the global coordinate system. Petera & Pittman (1994) suggested the following decomposition of normal boundary conditions along a surface into components in the global coordinate system, and the mixed derivative boundary conditions can be presented in a similar fashion:

**Angled Boundary**
\[
\begin{align*}
\lambda_n &= \lambda_{x,n} + \lambda_{y,n} = 0 \\
\lambda_{,nn} &= \lambda_{xx,n,n} + \lambda_{xy,n,y} + \lambda_{,yy,n,n} = 0 
\end{align*}
\]

For the boundary condition given by Eq. (5.315) to hold for any given element geometry, the derivatives with respect to both the \(x\) and \(y\) directions must be zero, such

---

**Figure 5.4**: Example mesh of a non-perpencicular boundary and coordinate systems corresponding to elements near this boundary.
that the following boundary conditions satisfy Eq. (5.314):

**Angled Boundary (normal boundary conditions)**

\[ \lambda_x = 0 \]  
\[ \lambda_y = 0 \]

(5.316) (5.317)

Transformation of the mixed derivative boundary condition to the global coordinate system, Eq. (5.315), requires the introduction of additional second-order derivative degrees of freedom. Alternatively, it is noted that the reference coordinate system and the surface normal directions coincide such that, for the angled surface in the model of Figure 5.4, the following boundary conditions satisfy Eq. (5.315):

**Angled Boundary (mixed derivative boundary condition)**

\[ \lambda_{\xi\eta} = 0 \]

(5.318)

The application of this mixed derivative boundary condition is another justification for keeping the mixed derivative degree of freedom in the reference configuration as a degree of freedom in the global coordinate system.

### 5.6 Conclusions

In this chapter, the framework for the gradient enhanced plasticity model coupled with gradient enhanced damage was derived through thermodynamically consistent theoretical formulations. The numerical implementation for this coupled model was also given. Following standard thermodynamics and using nonlocal state variables, a complete set of constitutive equations were derived where a gradient enhanced yield surface was used to determine the occurrence of plasticity and a gradient enhanced damage surface was used to determine the occurrence of damage. Hardening conjugate forces (stress like terms) for both plasticity and damage were defined as general functions of their corresponding hardening state variables (strain like terms), and the gradients and Laplacians of these conjugate forces were defined in terms of the derivatives of these functions and the gradients of the hardening state variables. An integration shame was developed and a set of governing equations were derived to be solved in a Newton-Raphson solution procedure. In order to solve for the plastic and damage multiplier in addition to the strains, the governing equations included the plasticity and damage consistency conditions in addition to the equilibrium equation. The next chapter discusses the implementation of this gradient theory model accounting for isotropic hardening plasticity into the commercial finite element code ABAQUS (2003), and analytical and numerical examples of localization will be given to demonstrate the effectiveness of the gradient model in removing the mesh sensitivity problem.
CHAPTER 6: RESULTS AND DISCUSSIONS

6.1 INTRODUCTION

In this work, the effectiveness of the gradient model is evaluated by studying the mesh-dependence issue in localization problems through numerical examples. The implementation of the gradient model into the finite element code ABAQUS (2003) is also discussed. The numerical solutions of strain localization problems will demonstrate the effectiveness of the gradient theory as a localization limiter and will demonstrate how the gradient theory removes the mesh-dependency found in classical continuum models. Numerical results from this work are qualitatively compared with numerical simulations by other authors for different formulations. The problems considered here will be focused on ill-posed initial boundary value problems which behave in a strain softening manner due to material instabilities and due to structural instabilities.

6.2 FINITE ELEMENT IMPLEMENTATION

In CHAPTER 5, the gradient enhanced model was presented in which gradient enhancements were introduced into the yield condition and into the damage condition, and a finite element framework was developed to be solved by a Newton-Raphson solution scheme. The solution of this model required the creation of new finite elements which were developed both in the commercial finite element code ABAQUS (2003) and in the C++ research code Tahoe developed at Sandia National Laboratories. The discussion given here is focused on the implementation in which ABAQUS/Standard is used with the material subroutine UEL. In using this subroutine, ABAQUS is essentially used as a solver for our system of equations.

For each element defined as a user-defined element, ABAQUS calls the UEL subroutine when the element stiffness matrix (AMATRX) and the element residuals (RHS) of the governing equations are required (Figure 6.1). ABAQUS provides the incremental degrees of freedom for the element (DU) as well as various properties defined in the input file. An array (SVARS) is also available to store state dependent variables for the entire element.

In the UEL subroutine, it is required to define the Gaussian integration rules, the element displacement and multiplier shape functions, and the model integration scheme. Based on the incremental degrees of freedom and the state variables, the stiffness matrices and the residual vectors presented in Section 5.5 must be assembled into AMATRX and RHS.

As the state variables are assembled into an array for the entire element, ABAQUS is unable to create spatial contour plots from the variables. In order to view the results, a
A fictitious mesh with matching nodes and matching elements is laid on top of the model mesh. The material of the elements in this mesh is defined as a user material, and the UMAT user subroutine is used to define the material behavior.

ABAQUS provides the subroutine UMAT with the incremental strains at the integration point, and the subroutine is required to compute the stresses and the tangent modulus at the integration point based on the material model (Figure 6.1). In order to not have an effect on the results of the boundary value problem, the material of the fictitious mesh must not resist any strains. To obtain this behavior, the material is defined as elastic.

Figure 6.1: ABAQUS and its relationships to the user subroutines UEL and UMAT.
with a tangent modulus equal to almost zero ($10^{-15}$). An array (STATEV) is available in the user subroutine UMAT in order to store state dependent variables for the integration point. As visualization is supported for the UMAT subroutines, the state dependent variables computed by the UEL subroutine must be transferred from the UEL subroutine array SVARS to the UMAT subroutine array STATEV.

With the two meshes defined using the same nodes, the solution of the boundary value problem is obtained for both meshes simultaneously. As each of the UEL elements is solved for, the state variables are stored in the UEL array SVARS. The state variables are also stored using a common statement. Then, when the UMAT subroutine is called for a given integration point in the fictitious mesh, the state variables are extracted from the common statement and stored in the UMAT array STATEV. As the UMAT subroutine does support visualization, the contour plots can now be obtained.

### 6.3 PATCH TEST

In order to check the elements created using Hermitian shape functions to discretize the plastic multipliers, a simple patch test is analyzed here. The patch considered here consists of a mesh with at least one internal element and a non-rectangular geometry. The geometry for the initial mesh of the body consists of five elements with nodal coordinates

![Figure 6.2: Storage of state variables by the user subroutines UEL and UMAT.](image)
given in Figure 6.3 \((B = 60\ mm)\). The refined meshes to be analyzed are created by repeatedly bisecting the sides the quadrilateral elements, thus creating four elements from each original element. The material from Pamin (1994) is used here such that the elastic shear modulus \(\mu^e = 4000\ N/m^2\) and the Poisson’s ratio \(\nu = 0.49\), corresponding to a Young’s modulus \(E = 2\mu^e(1+\nu) = 11920\ N/m^2\). The linear softening material used in Pamin (1994) corresponds to the use of a linear isotropic hardening law, Eq. (3.29), with a hardening coefficient \(H_R = \frac{1}{2}(-0.1\mu^e) = -600\ N/m^2\) and a yield stress \(\sigma_{yp} = 100\ N/m^2\). All boundary nodes are displaced by a prescribed linear field such that (Belytschko et al., 2000):

\[
u(x, y) = \alpha_x x + \alpha_y y
\]

To satisfy the patch test, the total strains should be constant across the element and should be given by the following relations:

\[
\varepsilon_x = u_x = \alpha_x
\]

\[
\varepsilon_y = v_y = \alpha_y
\]

\[
2\varepsilon_{xy} = u_y + v_x = \alpha_x + \alpha_y
\]

For this example, the coefficients in the prescribed linear displacement field at time \(t\) are given as follows:

\[
\{\alpha_{x1}\} = \{0.0\ 0.25\ mm\ 0.75\ mm\}tB^{-1}
\]

\[
\{\alpha_{y1}\} = \{0.0\ 0.75\ mm\ 0.25\ mm\}tB^{-1}
\]

where the simulation is run from \(t = 0.0\) to \(t = 1.0\). For these coefficients, in order for the elements to pass this patch test, the strains across the body should be as follows:

\[
\varepsilon_x = 4.167 \times 10^{-03} = \frac{\alpha_x}{B}
\]

\[
\varepsilon_y = 4.167 \times 10^{-03} = \frac{\alpha_y}{B}
\]

\[
2\varepsilon_{xy} = 2.500 \times 10^{-02} = \frac{\alpha_x + \alpha_y}{B}
\]

The patch test is passed for the various elements discussed in this work (C.PE.4, C.PE.8, M.PE.4, M.PE.8) as the results obtained from ABAQUS give a constant stress across the body. These stresses are given here as follows:
Figure 6.3: Patch test with all boundary displacements prescribed.
\[
\begin{align*}
\sigma_x &= 1662.0 \text{ N/mm}^2 \\
\sigma_y &= 1662.0 \text{ N/mm}^2 \\
\sigma_{xy} &= 54.4 \text{ N/mm}^2
\end{align*}
\] (6.11)
(6.12)
(6.13)

The strains obtained also correspond with the correct strains computed directly from the applied linear field as given by Eqs. (6.8) to (6.10).

### 6.4 1D Tensile Bar Localization: Linear Softening

Localization in a 1D bar with linear isotropic plasticity softening is presented here. The bar of length \(L\) is assumed to be discretized into \(n\) elements (Figure 6.4). In order to trigger localization, it can be assumed that an imperfection in the material is introduced into the model. This imperfection is introduced in the form of a reduced yield stress in the middle element of the discretized bar.

The bar considered here is a 120 \(mm\) rod discretized by \(n\) elements. The material of the rod is assumed to be elasto-plastic with linear isotropic softening. The material has an initial yield stress, \(\sigma_{yp}\), of 100 \(N/mm^2\), a Poisson’s ratio, \(\nu\), of 0.49, a Young’s modulus, \(E\), of 11920 \(N/mm^2\), and an isotropic softening coefficient, \(H_s\), of –600 \(N/mm^2\). Numerical results are only given for isotropic softening; however, the analytical solution also includes kinematic hardening for generality.

#### 6.4.1 Local Analytical Solution

Following the work of Pamin (2004), an analytical solution of the localization problem for a 1D bar in uniaxial tension is presented here. Once softening occurs in this local model, the solution becomes unstable and plasticity will concentrate into the weakened middle element. All plastic strains will localize in this element, and all other elements will unload elastically. Thus, plasticity will occur in a “shear band” at the

![Figure 6.4: 1D bar in uniaxial tension discretized into \(n\) elements.](image)
middle of the bar with a width of \( w \) equal to \( L/n \). For the uniaxial tension problem, the sign of the stress is always positive. Thus, the evolution equations for the internal state variables can be simplified as follows:

\[
\dot{\varepsilon}_{11}^p = \sqrt{\frac{2}{3}} \dot{\lambda}^p \tag{6.14}
\]

\[
\dot{\varepsilon} = \sqrt{\frac{2}{3}} \dot{\lambda}^p = \dot{\varepsilon}_{11}^p \tag{6.15}
\]

\[
\dot{\alpha}_{11} = \sqrt{\frac{2}{3}} \dot{\lambda}^p = \frac{1}{2} \dot{\varepsilon}_{11}^p \tag{6.16}
\]

Assuming linear softening both for the isotropic and kinematic hardening state laws, the yield condition is written in the following form:

\[
f = \sqrt{\frac{2}{3}} \left[ \left( \sigma_{11} - \frac{3}{4} H_r \varepsilon_{11}^p \right) - \left( \sigma_{11} + H_r \varepsilon_{11}^p \varepsilon_{11}^p \right) \right] \leq 0 \tag{6.17}
\]

In the plastic regime, the Kuhn-Tucker loading conditions enforce that the yield condition, \( f \), is equal to zero. Thus, from the previous equation, the plastic strain can be solved in terms of the stress:

\[
\varepsilon_{11}^p = \frac{\sigma_{11} - \sigma_{11}^p}{H_r + \frac{3}{4} H_a} \tag{6.18}
\]

The total axial strain at a given point along the bar is defined as the sum of the axial elastic strain and of the axial plastic strain, where the axial elastic strain for a 1D bar is given as follows:

\[
\varepsilon_{11}^e = \frac{\sigma_{11}}{E} \tag{6.19}
\]

Thus, the total strain at a given point in the localized zone of the bar is the sum of Eqs. (6.18) and (6.19) and is given as follows:

\[
\varepsilon_{11} = \frac{\sigma_{11}}{E} + \frac{\sigma_{11} - \sigma_{11}^p}{H_r + \frac{3}{4} H_a} \tag{6.20}
\]

When the bar is loaded in tension up to the reduced yield stress, the material only experiences elastic strains. After reaching a state of stress equal to the reduced yield stress, additional deformation for the case of a linear softening material causes the entire weakened portion of the bar to enter the plastic regime; however, the remainder of the bar remains in the elastic regime. Thus, the middle portion of the beam accumulates plastic strains, whereas the outer portion strains only elastically. And from the previous equation, these plastic strains in the middle portion are uniform across the domain since, for equilibrium, the stress is uniform along the bar. Thus, the portion of the bar outside of the
weakened zone will never reach a stress level above its yield stress, and all of the plastic strains will localize in a shear band of constant magnitude.

The average strain in the bar is the total displacement applied to the end of the bar, \( \bar{u}_{i1} \), divided by the length of the bar. The total displacement at the end of the bar is found by integrating the strains over the domain. Now for the case of a softening material, the plastic strains are zero outside of the boundary of the shear band \( (\varepsilon_{i1}^p = 0 \text{ at } |x| \geq \frac{1}{2} w) \). As mentioned previously, the width of the shear band is equal to the width of the middle element \( (w = L/n) \). Thus, the total displacement is obtained as an integration of the elastic strains over the entire body and of the plastic strains over the weakened zone such that:

\[
\bar{u}_{i1} = \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \varepsilon_{i1}^e \, dx + \int_{-\frac{1}{2}w}^{\frac{1}{2}w} \varepsilon_{i1}^p \, dx \tag{6.21}
\]

From the use of the 1D Hookean stress-strain relationship and Eq. (6.18), the relation between the average strain and the stress is given as follows:

\[
\bar{u}_{i1} = L \frac{\sigma_{i1}}{E} + L \frac{\sigma_{i1} - \sigma_{yp}}{n(H_r + \frac{q}{4} H_a)} \tag{6.22}
\]

Dividing this equation by the bar length and solving for the stress, the post-peak relationship between the stress and the average strain is given as follows:

\[
\sigma_{i1} = \frac{E(\varepsilon_{i1} n(H_r + \frac{q}{4} H_a) + \sigma_{yp})}{n(H_r + \frac{q}{4} H_a) + E} \tag{6.23}
\]

where the slope of the curve from this relationship can be obtained as follows:

\[
\frac{d\sigma_{i1}}{d\varepsilon_{i1}} = \frac{nE(H_r + \frac{q}{4} H_a)}{n(H_r + \frac{q}{4} H_a) + E} \tag{6.24}
\]

For this bar, the plastic strain along the bar, Eq. (6.18), and the stress-average strain relationship, Eq. (6.23), are given in Figure 6.5. As all plasticity occurs in the weakened element, the reduced yield stress of the weakened element is used. This reduced yield stress is taken as 90% of the yield stress for the unweakened material. As shown, refinement of the mesh causes the width of the shear band to decrease, the maximum plastic strain in the shear band to increase, and the slope of the post peak stress-strain curve to increase. This is not a physical behavior, and it will be shown that the gradient model gives a solution which is not dependent on the mesh size.
Figure 6.5: Analytical solution of mesh effects on local model with linear isotropic softening: (a) axial plastic strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
6.4.2 Gradient-Enhanced Analytical Solution

Once softening occurs in the gradient model, stability is maintained and plasticity will concentrate into a localized zone of width $w$. For the uniaxial tension problem, the sign of the stress is always positive. Thus, the evolution equations for the internal state variables can be simplified as follows:

$$\dot{\varepsilon}_{11}^p = \sqrt{\frac{1}{3}} \dot{\lambda}^p$$  \hspace{1cm} (6.25)
$$\dot{\varepsilon}_{11} = \sqrt{\frac{1}{3}} \dot{\lambda}^p = \frac{1}{2} \dot{\varepsilon}_{11}^p$$  \hspace{1cm} (6.26)
$$\dot{\alpha}_{11} = \sqrt{\frac{1}{3}} \dot{\lambda}^p = \frac{1}{2} \dot{\varepsilon}_{11}^p$$  \hspace{1cm} (6.27)

Assuming linear softening both for the isotropic hardening state law and for the kinematic hardening state laws, the state laws and Laplacians of the state laws can be written as follows:

$$R = H_r r = H_r \varepsilon_{11}^p$$  \hspace{1cm} (6.28)
$$\nabla^2 R = H_r \nabla^2 r = H_r \nabla^2 \varepsilon_{11}^p$$  \hspace{1cm} (6.29)

$$X_{11} = H_a \alpha_{11} = \frac{1}{2} H_a \varepsilon_{11}^p$$  \hspace{1cm} (6.30)
$$\nabla^2 X_{11} = H_a \nabla^2 \alpha_{11} = \frac{1}{2} H_a \nabla^2 \varepsilon_{11}^p$$  \hspace{1cm} (6.31)

The yield condition can now be written in the following form:

$$f = \left[ \sigma_{11} - \frac{2}{3} H_a \left( \varepsilon_{11}^p + c_x \nabla^2 \varepsilon_{11}^p \right) \right] - \left[ \sigma_{yy} + H_r \left( \varepsilon_{11}^p + c_x \nabla^2 \varepsilon_{11}^p \right) \right] \leq 0$$  \hspace{1cm} (6.32)

Thus, the yield condition is now an inhomogeneous second order differential equation. In the plastic regime, the Kuhn-Tucker loading conditions enforce that the yield condition, $f$, is equal to zero. Thus, from the previous equation, the plastic strain terms are separated from the stress term such that the following differential equation is obtained:

$$\left( H_r c_R + \frac{2}{3} H_a c_X \right) \nabla^2 \varepsilon_{11}^p + \left( H_r + \frac{2}{3} H_a \right) \varepsilon_{11}^p = \left( \sigma_{11} - \sigma_{yy} \right)$$  \hspace{1cm} (6.33)

A combination of the homogeneous and inhomogeneous solutions for this differential equation can be given in the following form:

$$\varepsilon_{11}^p = \frac{\sigma_{11} - \sigma_{yy}}{H_r + \frac{2}{3} H_a} + C_1 \cos \left( x \sqrt{\frac{H_r + \frac{2}{3} H_a}{H_r c_R + \frac{2}{3} H_a c_X}} \right) + C_2 \sin \left( x \sqrt{\frac{H_r + \frac{2}{3} H_a}{H_r c_R + \frac{2}{3} H_a c_X}} \right)$$  \hspace{1cm} (6.34)
For the case of a softening material, the plastic strains are zero outside the boundary of the shear band \( \varepsilon_{11}^p = 0 \) at \( |x| \geq \frac{1}{2} w \). Substitution of these boundary conditions into Eq. (6.34) gives the following relations:

\[
0 = \frac{\sigma_{11} - \sigma_{3p}}{H_r + \frac{9}{4} H_a} + C_1 \cos \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right) + C_2 \sin \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right) \quad (6.35)
\]

\[
0 = \frac{\sigma_{11} - \sigma_{3p}}{H_r + \frac{9}{4} H_a} + C_1 \cos \left( -\frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right) + C_2 \sin \left( -\frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right) \quad (6.36)
\]

This set of equations can be used to solve for the two coefficients in the differential equation solution such that:

\[
C_1 = \frac{\frac{\sigma_{11} - \sigma_{3p}}{H_r + \frac{9}{4} H_a}}{\cos \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right)} \quad (6.37)
\]

\[
C_2 = 0 \quad (6.38)
\]

Using these coefficients in the differential equation solution, Eq. (6.34), the plastic strain can be written in terms of the stress as follows:

\[
\varepsilon_{11}^p = \left( \frac{\sigma_{11} - \sigma_{3p}}{H_r + \frac{9}{4} H_a} \right) \left\{ 1 - \frac{\cos \left( x \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right)}{\cos \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right)} \right\} \quad (6.39)
\]

The total axial strain at a given point along the bar is defined as the sum of the axial elastic strain and of the axial plastic strain. Thus, the total strain at a given point in the localized zone of the bar is the sum of Eqs. (6.19) and (6.39) and is given as follows:

\[
\varepsilon_{11} = \frac{\sigma_{11}}{E} + \left( \frac{\sigma_{11} - \sigma_{3p}}{H_r + \frac{9}{4} H_a} \right) \left\{ 1 - \frac{\cos \left( x \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right)}{\cos \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right)} \right\} \quad (6.40)
\]

When the bar is loaded in tension up to the reduced yield stress, the material only experiences elastic strains. After reaching a state of stress equal to the reduced yield stress, additional deformation for the case of a linear softening material causes a shear
band to develop in which the entire portion of the bar in the shear band enters the plastic regime; however, the remainder of the bar remains in the elastic regime. Thus, the middle portion of the beam in the shear band accumulates plastic strains, whereas the outer portion strains only elastically. Note that this middle portion is not necessarily the weakened zone. It will be shown that the width of the shear band can be computed, and Eq. (6.40) allows the plastic strains and the total strains along the bar to vary across the shear band domain.

The average strain in the bar is the total displacement applied to the end of the bar, \( \bar{u}_{11} \), divided by the length of the bar. The total displacement at the end of the bar is found by integrating the strains over the domain. As mentioned previously for the case of a softening material, the plastic strains are zero outside of the boundary of the shear band \( (\varepsilon_{11}^p = 0 \text{ at } |x| \geq \frac{1}{2} w) \). Thus, the total displacement is obtained as an integration of the elastic strains over the entire body and of the plastic strains over the shear band such that:

\[
\bar{u}_{11} = \frac{1}{L} \int_{-\frac{1}{2} L}^{\frac{1}{2} L} \varepsilon_{11}^e dx + \int_{-\frac{1}{2} w}^{\frac{1}{2} w} \varepsilon_{11}^p dx
\]

From the use of the 1D Hookean stress-strain relationship and Eq. (6.39), the relation between the total displacement and the stress is given as follows:

\[
\bar{u}_{11} = L \frac{\sigma_{11}}{E} + \left( \frac{\sigma_{11} - \sigma_{sp}}{H_r + \frac{9}{2} H_a} \right) \left( w - \frac{2}{L} \sqrt{\frac{H_c R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} \tan \left( \frac{1}{2} w \sqrt{\frac{H_c R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} \right) \right)
\]

Dividing by the bar length gives the post-peak relationship between the stress and the average strain as follows:

\[
\bar{\varepsilon}_{11} = \frac{\sigma_{11}}{E} + \frac{1}{L} \left( \frac{\sigma_{11} - \sigma_{sp}}{H_r + \frac{9}{2} H_a} \right) \left( w - \frac{2}{L} \sqrt{\frac{H_c R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} \tan \left( \frac{1}{2} w \sqrt{\frac{H_c R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} \right) \right)
\]

In determining the width of the shear band, the critical solution of this equation is given as follows (Pamin, 1994):

\[
\frac{d \bar{\varepsilon}_{11}}{dw} = \frac{1}{L} \left( \frac{\sigma_{11} - \sigma_{sp}}{H_r + \frac{9}{2} H_a} \right) \left( 1 - \sec^2 \left( \frac{1}{2} w \sqrt{\frac{H_c R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a c_X}} \right) \right) = 0
\]

From this condition, the following relationship is obtained:

\[
\cos^3 \left( \frac{1}{2} w \sqrt{\frac{H_r + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a c_X}} \right) = 1
\]
Multiple solutions of this equation exist; however, the shear band width is taken as the smallest nontrivial solution and is given as follows:

$$w = 2\pi \sqrt{\frac{H_r c_R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}}$$  

(6.46)

Using this definition of the shear band in Eqs. (6.39) and (6.43), the following relationships for the plastic strain and the average strains are now given in terms of material parameters and stress as follows:

$$
\varepsilon_{11}^p = \left( \frac{\sigma_{11} - \sigma_{yy}}{H_r + \frac{9}{4} H_a} \right) \left( 1 + \cos \left( x \sqrt{\frac{H_r + \frac{2}{3} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} \right) \right) 
$$  

(6.47)

$$
\overline{\varepsilon}_{11} = \frac{\sigma_{11}}{E} + \frac{2\pi}{L} \left( \frac{\sigma_{11} - \sigma_{yy}}{H_r + \frac{9}{4} H_a} \right) \sqrt{\frac{H_r c_R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} 
$$  

(6.48)

This last equation can be solved for the stress to obtain the following stress-average strain relationship:

$$
\sigma_{11} = \frac{E \left( \overline{\varepsilon}_{11} \frac{L}{2\pi} + \frac{\sigma_{yy}}{H_r + \frac{9}{4} H_a} \sqrt{\frac{H_r c_R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} \right)}{L + \frac{E}{2\pi} \frac{H_r + \frac{9}{4} H_a}{H_r c_R + \frac{9}{4} H_a c_X}} 
$$  

(6.49)

where the slope of the curve from this relationship can be given as follows:

$$
\frac{d\sigma_{11}}{d\overline{\varepsilon}_{11}} = \frac{L}{2\pi} \frac{E}{H_r + \frac{9}{4} H_a} \sqrt{\frac{H_r c_R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a}} 
$$  

(6.50)

Note that, in defining the material parameters to be used in this model, the following constraint must be enforced:

$$\frac{H_r c_R + \frac{9}{4} H_a c_X}{H_r + \frac{9}{4} H_a} > 0$$  

(6.51)

As the state laws for both the isotropic hardening and the kinematic hardening have been assumed to behave in a linearly softening fashion, i.e. $H_r < 0$ and $H_a < 0$, this condition is satisfied.
For this 1D bar utilizing the gradient enhanced model, the plastic strain along the bar, Eq. (6.47), and the stress-average strain relationship, Eq. (6.49), are given in Figure 6.6. As the majority of plasticity occurs in the weakened element, the reduced yield stress of the weakened element is used. This reduced yield stress is taken as 90% of the parent material yield stress. In this example, the width of the shear band is independent of the mesh size, and various length scales are used in the plots to show the dependence of the results on this material parameter.

6.4.3 Local Tahoe Solution

The 1D bar elements introduced in CHAPTER 3 were implemented into the finite element program Tahoe and were used for the problem of localization of a 1D bar. Once softening occurs in this local model, the solution becomes unstable and plasticity concentrates into the middle element. All plastic strains localize in this element, and all other elements unload elastically. Thus, plasticity occurs in a “shear band” at the middle of the bar with a width of \( w \) and a constant magnitude of plastic strains.

In order to control the localization for this 1D bar problem, a weakened region is introduced into the model in the form of a 10% reduced yield stress. The width of this weakened region, \( \tilde{w} \), is defined as the length of the bar \( (L = 120 \text{ mm}) \) divided by an integer, \( n \). Thus, for each weakened region defined by \( n \), the solution corresponds to the analytical solution for the bar discretized by \( n \) elements. This is because the localization of plastic strains occurs in the entire weakened region for this problem, which corresponds to a single element in the analytical solution.

For this 1D bar utilizing the local model, the plastic strain along the bar and the stress-average strain relationship are given in Figure 6.7 for various meshes of C.1D.3 elements. As with the analytical solution, as the mesh is refined, the width of the shear band decreases, the maximum plastic strain in the shear band increases, and the slope of the post peak stress-strain curve increases. This is not a physical behavior, and it will be shown that the gradient model gives a solution which is independent of the mesh size.
Figure 6.6: Analytical solution of length scale effects on gradient model with linear isotropic softening: (a) axial plastic strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
Figure 6.7: Tahoe solution of mesh effects on local model with linear isotropic softening using C.1D.3 elements: (a) total axial strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
6.4.4 Gradient Enhanced Tahoe Solution

The 1D bar elements introduced in CHAPTER 5 were implemented into the finite element program Tahoe. Using this code, the problems of softening discussed in this section were analyzed using various meshes. Once softening occurs in the gradient model, stability is maintained and plasticity will concentrate into a localized zone of width $w$. All plastic strains localize in this zone, and the material outside of this shear band will unload elastically.

In order to control the localization for this 1D bar problem, a weakened region is introduced into the model in the form of a 10% reduced yield stress. The width of this weakened region, $\tilde{w}$, is defined as the length of the bar ($L = 120 \, mm$) divided by an integer, $n$. Thus, for each weakened region defined by $n$, the solution corresponds to the analytical solution for the bar discretized by $n$ elements. Though the overall behavior of the boundary value problem is expected to be somewhat affected by the change in the material parameters of this weakened zone, this effect should be small. The reduction in the yield stress serves only to induce an inhomogeneous state of deformation which will trigger localization.

For this 1D bar utilizing the gradient model, the plastic strain along the bar and the stress-average strain relationship are given in Figure 6.8 for various weakened zones with an isotropic hardening length scale, $c_R$, of $25 \, mm^2$. The discretization consists of 90 M.1D.3 elements. In these plots, the shear band tends to a constant width based on the material length scale given. Note that a problem does arise when using a weak zone corresponding to $n = 3$ ($\tilde{w} = 40 \, mm$). The problem arises because the length scale used defines a shear band for this problem of approximately $20 \, mm$ as can be seen by the solutions corresponding to $n = 5$ ($\tilde{w} = 24 \, mm$) and $n = 9$ ($\tilde{w} = 13.3 \, mm$). As this width of the shear band is much smaller than the width of the weakened zone, a second shear band forms outside of the actual shear band and within the weakened zone. Though this may have a small effect on the problem corresponding to $n = 5$ due to the comparable size of the weakened zone and of the shear band, it can be seen in Figure 6.8 that the solution for $n = 5$ ($\tilde{w} = 24 \, mm$) and $n = 9$ are almost identical. Thus, the effectiveness of the gradients in obtaining mesh independent results can be seen in these figures. As the mesh is refined, the width of the shear band remains independent of the mesh size, and the stress-strain behavior becomes independent of the discretization.
Figure 6.8: Tahoe solution of mesh effects on gradient model with linear isotropic softening using M.1D.3 elements: (a) total axial strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
The simulations for the 1D bar are repeated using M.1D.2 elements, and the plots of the plastic strain along the bar and the stress-average strain relationships are given in Figure 6.9. The results exhibit a mesh independence on the shear band width, though as before a second shear band forms for the case corresponding to \( n = 3 \). The solution using the M.1D.2 element diverges early in the simulation. A possible cause for this divergence is due to a stress fluctuation occurring along the bar in the M.1D.2 elements (Figure 6.10) due to the inconsistency between the orders of the discretization of the displacement and of the plastic multiplier in the equilibrium equation (Pamin, 2004).

Plots of the plastic strain along the bar and the stress-average strain relationship are given in Figure 6.11 for a mesh of 90 M.1D.3 elements with a weakened zone corresponding to \( n = 9 \). In these plots, various length scales are used to demonstrate the dependence of the width of the shear band on the length scales. Thus, the width of the shear band is dependent on a material parameter, not on the mesh.

### 6.5 1D TENSILE BAR LOCALIZATION: EXPONENTIAL SOFTENING

Localization in a 1D bar with exponential isotropic plasticity softening is presented here in order to demonstrate the ability of this work to model nonlinear material behavior. As in the previous section, the bar of length \( L \) is assumed to be discretized into \( n \) elements (Figure 6.4). In order to control the localization for this 1D bar problem, a weakened region is introduced into the model in the form of a 10% reduced yield stress. The width of this weakened region, \( \tilde{w} \), is defined as the length of the bar \( (L = 120 \text{ mm}) \) divided by an integer, \( n \). Though the overall behavior of the boundary value problem is expected to be somewhat affected by the change in the material parameters of this weakened zone, this effect should be small. The reduction in the yield stress serves only to induce an inhomogeneous state of deformation which will trigger localization.

The bar considered here is a 120 mm rod discretized by \( m \) elements. The material of the rod is assumed to be elasto-plastic with exponential isotropic softening. The material has an initial yield stress, \( \sigma_{yp} \), of 100 \( N/\text{mm}^2 \), a Poisson’s ratio, \( \nu \), of 0.49, and a Young’s modulus, \( E \), of 11920 \( N/\text{mm}^2 \). The Chaboche isotropic softening model is used with \( R_\infty = -100 \text{ N/mm}^2 \) and \( \gamma_r = 10.0 \).

Plots of the plastic strain along the bar and the stress-average strain relationship are given in Figure 6.12 for a mesh of 90 M.1D.3 elements with a weakened zone corresponding to \( n = 9 \). In these plots, various length scales are used to demonstrate the dependence of the width of the shear band on the length scales. Thus, the width of the shear band is dependent on a material parameter, not on the mesh.
Figure 6.9: Tahoe solution of mesh effects on gradient model with linear isotropic softening using M.1D.2 elements: (a) total axial strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
Figure 6.10: Stress variation along bar in gradient model Tahoe solution using (a) M.1D.2 elements and (b) M.1D.3 elements.
Figure 6.11: Tahoe solution of length scale effects on gradient model with linear isotropic softening using M.1D.3 elements: (a) total axial strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
Figure 6.12: Tahoe solution of length scale effects on gradient model with exponential isotropic softening using M.1D.3 elements: (a) total axial strain along bar with a total applied end displacement of 1.2 mm; (b) axial stress-average axial strain for tensile bar.
6.6 Biaxial Compression

A plane strain specimen under a biaxial state of loading (Figure 6.13) is considered here to demonstrate the capability of the gradient model for a 2D localization problem. This problem has been investigated by numerous authors for the linear softening case of plasticity and is investigated here to verify the model behavior. The specimen is considered to be on a smooth rigid surface such that all vertical displacements are zero on the bottom edge. Horizontal displacement is also constrained at the middle node of the bottom boundary to avoid rigid body displacement. A 1 mm vertical displacement is applied to the upper edge of the specimen through a rigid, frictionless plate such that there are no rotations along the upper edge.

The dimensions of the specimen are $B = 60 \text{ mm}$ and $H = 120 \text{ mm}$. The refined meshes to be analyzed are created by repeatedly bisecting the sides the quadrilateral elements, thus creating four elements from each original element. The discretizations to be considered include meshes of 6x12, 12x24, and 24x48 elements. Solutions will be obtained using elements with 8-node discretization of the displacement field, and integration will be carried out with 2x2 integration points. To create an inhomogeneous loading state such that a shear band is initiated, a 10 mm by 10 mm area in the bottom left-hand corner of the sample is assigned a yield strength which is reduced by 10%. The imperfect area is the same for each mesh.

6.6.1 Linear Isotropic Softening Law

The material from Pamin (1994) is used here such that the material is assumed to be elasto-plastic with linear isotropic softening. The material has an elastic shear modulus, $\mu^e$, of $4000 \text{ N/mm}^2$, and a Poisson’s ratio, $\nu$, of 0.49, corresponding to a Young’s modulus, $E$, of $2\mu^e(1+\nu)=11920 \text{ N/mm}^2$. The linear softening material used in Pamin (1994) corresponds to the use of a linear isotropic softening law, Eq. (3.29), with a softening coefficient, $H_R$, or $\frac{1}{2}(0.1\mu^e) = -600 \text{ N/mm}^2$, a length scale, $c_R$, of $(3.0 \text{ mm})^2$, and an initial yield stress, $\sigma_{yp}$, of $100 \text{ N/mm}^2$.

In order to demonstrate the mesh dependency of a local model, the length scale in the gradient model is set to zero ($c_R = 0.0 \text{ mm}^2$). Figure 6.14 shows the solution of this
problem where the shear band tends to localize along a row of elements. As the mesh is refined, the width of the shear band reduces such that the width of the shear band tends to zero. Also, as the width of the shear band decreases, the magnitude of the equivalent plastic strains at the center of the shear band increases and tends to infinity. Note that the solution for the 24x48 mesh cannot be obtained at the total 1 mm displacement, as the intensity of the isotropic softening along the shear band increases to such an extent that points in the body are unable to provide any additional stress resistance and the simulation diverges.

Setting the length scale to $c_R = 9.0 \text{mm}^2$, the solution of this problem using the gradient enhanced model demonstrates the effectiveness of the gradients in obtaining mesh independent results (Figure 6.15). The shear band width becomes independent of the mesh used and dependent on the material length scale as shown in Figure 6.16. As the mesh is refined, the width of the shear band remains independent of the mesh size, and the stress-strain behavior becomes independent of the discretization (Figure 6.17).

![Figure 6.14](image)

**Figure 6.14**: Mesh dependence of the equivalent plastic strain and the displacements for a local linear softening model using C.PE.8 elements. Meshes consist of (a) 6x12, (b) 12x24, and (c) 24x48 elements.
Figure 6.15: Mesh independence of the equivalent plastic strain and displacements for the gradient linear softening model using M.PE.8 elements. Meshes consist of (a) 6x12, (b) 12x24, and (c) 24x48 elements.

Figure 6.16: Length scale effects on the equivalent plastic strain and displacements for the gradient linear softening model using M.PE.8 elements and meshes of 24x48 elements. Length scales used are (a) 9 mm$^2$, (b) 25 mm$^2$, and (c) 100 mm$^2$. 

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Figure 6.17: ABAQUS solution of length scale effects on Von Mises stress-average axial strain for the gradient model with linear isotropic softening using M.PE.8 elements.

Axial Stress ($N/mm^2$) vs. Average Axial Strain
6.6.2 Exponential Isotropic Softening Law

Localization for the biaxial compression example is presented here for a material experiencing exponential isotropic plasticity softening in order to demonstrate the ability of this work to model nonlinear material behavior. The material is assumed to be elasto-plastic with an initial yield stress, $\sigma_{yp}$, of 100 $N/mm^2$, a Poisson’s ratio, $\nu$, of 0.49, and a Young’s modulus, $E$, of 11920 $N/mm^2$. The Chaboche isotropic softening model is used with $R_\sigma = -100N/mm^2$ and $\gamma_r = 10.0$.

Setting the length scale to $c_g = 9.0 mm^2$, the solution of this problem using the gradient enhanced model demonstrates the effectiveness of the gradients in obtaining mesh independent results (Figure 6.18) for a nonlinear material softening model. The shear band width becomes independent of the mesh used and dependent on the material length scale as shown in Figure 6.19. As the mesh is refined, the width of the shear band remains independent of the mesh size, and the stress-strain behavior becomes independent of the discretization (Figure 6.20).

**Figure 6.18**: Mesh independence of the equivalent plastic strain and displacements for the gradient exponential softening model using M.PE.8 elements. Meshes consist of (a) 6x12, (b) 12x24, and (c) 24x48 elements.
Figure 6.19: Length scale effects on the equivalent plastic strain and displacements for the gradient exponential softening model using M.PE.8 elements and meshes of 24x48 elements. Length scales used are (a) 9 mm$^2$, (b) 25 mm$^2$, and (c) 100 mm$^2$.

Figure 6.20: ABAQUS solution of length scale effects on Von Mises stress-average axial strain for the gradient model with exponential isotropic softening using M.PE.8 elements.
6.7 TENSILE SPECIMEN

In the previous example, the evolution of the shear band in a plane strain specimen under a biaxial state of loading plane was investigated and the capability of the gradient theory in providing the mesh objective results was demonstrated. The localization in the biaxial test was initiated by a material defect in the corner of the bar which initiated an inhomogeneous state of loading leading to localization. In this example, localization in the tensile specimen is induced by a structural inhomogeneity, namely the shape of the specimen. By increasing the width of the bar at the top by a small amount, the state of deformation becomes inhomogeneous, and localization will occur.

The specimen is considered to be on a smooth rigid surface such that all vertical displacements are zero on the bottom edge. Horizontal displacement is also constrained at the middle node of the bottom boundary to avoid rigid body displacement. A 0.9 mm vertical displacement is applied to the upper edge of the specimen through a rigid, frictionless plate such that there are no rotations along the upper edge.

The dimensions of the specimen are $B = 60 \text{ mm}$, $H = 120 \text{ mm}$, and $\tilde{w} = 1 \text{ mm}$. The refined meshes to be analyzed are created by repeatedly bisecting the sides the quadrilateral elements, thus creating four elements from each original element. The discretizations to be considered include meshes of 6x12, 12x24, and 24x48 elements. Solutions will be obtained using elements with 8-node discretization of the displacement field, and integration will be carried out with 2x2 integration points.

The linear isotropic softening material parameters of Section 6.6.1 and the exponential isotropic softening material parameters of Section 6.6.2 are used here to analyze this tensile specimen. To demonstrate the mesh dependency of a local model, the linear isotropic softening model is used with the length scale in the gradient model set to zero ($c_R = 0.0 \text{ mm}^2$). Figure 6.22 shows the solution of this problem where the shear band tends to localize along a row of elements. As the mesh is refined, the width of the shear band reduces such that the width of the shear band tends to zero. Also, as the width of the shear band decreases, the magnitude of the equivalent plastic strains at the center of the shear band increases and tends to infinity.
Setting the length scale to $c_R = 9.0 \text{mm}^2$ for the linear and exponential softening materials, the solution of this problem using the gradient enhanced model demonstrates the effectiveness of the gradients in obtaining mesh independent results (Figure 6.23, Figure 6.24) such that the shear band width becomes independent of the mesh used and dependent on the material length scale.

6.8 CONCLUSIONS

Utilizing the gradient model presented in CHAPTER 5, this chapter discussed the implementation of the model accounting for isotropic softening plasticity into the commercial finite element code ABAQUS (2003), and analytical and numerical examples of localization were used to demonstrate the effectiveness of the gradient model in removing the mesh sensitivity problem. The numerical solutions of strain localization problems demonstrated the effectiveness of the gradient theory as a localization limiter and demonstrated how the gradient theory removes the mesh-dependency found in classical continuum models. Problems due to both a material instability and due to a structural instability were used to investigate the use of the gradient theory in an ill-posed initial boundary value problem.

Figure 6.22: Mesh dependence of the equivalent plastic strain and the displacements for a local linear softening model using C.PE.8 elements. Meshes consist of (a) 12x24 and (b) 24x48 elements.
Figure 6.23: Mesh independence of the equivalent plastic strain and displacements for the gradient linear softening model using M.PE.8 elements. Meshes consist of (a) 12x24 and (b) 24x48 elements.

Figure 6.24: Mesh independence of the equivalent plastic strain and displacements for the gradient exponential softening model using M.PE.8 elements. Meshes consist of (a) 12x24 and (b) 24x48 elements.
CHAPTER 7 : MATERIAL LENGTH SCALES

7.1 INTRODUCTION

In the previous chapter, localization problems were presented and were solved utilizing the gradient theory in order to demonstrate the effectiveness of the gradient theory in removing mesh sensitivity. For the problems investigated, typical values of material length scales were used in order to obtain a basic understanding of the effect of the length scales on the model. In this chapter, the length scale introduced through gradient enhanced plasticity is examined and defined in terms of microstructure in an attempt to bridge the length scales. A discussion is given for size effect problems in which the length scale is defined in terms of dislocation densities, and a discussion is also given for localization problems in which the length scale is defined in terms of grain sizes. In order to simplify the problem of determining the length scale, the model of CHAPTER 5 will be simplified to the case of gradient enhanced plasticity with isotropic hardening.

7.2 SIZE EFFECT PROBLEMS

It has been shown that materials display strong size effects when investigating problems at a scale on the order of the length scale of the microstructure. Specifically, it has been shown through numerous experimental investigations that materials exhibit a strong size effect when the characteristic length scale associated with the plastic deformation is on the order of micrometers. Investigators (Nix, 1989; De Guzman et al., 1993; Stelmashenko et al., 1993; Ma & Clarke, 1995; Poole et al., 1996; McElhaney et al., 1998) have demonstrated through micro-indentation tests that the measured indentation hardness increases by a factor of two as the depth of indentation decreases from 10 µm to 1 µm. Fleck et al. (1993) demonstrated through micro-torsion of thin copper wires that the normalized shear strength of the wire increased by a factor of 3 as the wire diameter decreased from 170 µm to 12 µm, and Stolken & Evans (1998) demonstrated for micro-bending a significant increase in the normalized bending strength as the beam thickness decreased from 100 µm to 12.5 µm.

For these type of problems, standard continuum plasticity cannot capture the size effect as it does not contain an internal length scale. It has been shown (Bammann & Aifantis, 1982; Fleck & Hutchinson, 1993; Gao et al., 1999; Menzel & Steinmann, 2000; Gao & Huang, 2001) that strain-gradient theories can be connected to dislocation mechanics in order to bridge the length scales from the dislocation scale (<0.1 µm) to the continuum scale. To this end, the influence of dislocation tensors on material hardening is discussed here in order to introduce a micromechanical justification for the use of the gradient terms in size effect problems.
7.2.1 Dislocation Mechanics

The theory of dislocations was independently introduced in 1934 by Orowan, Taylor, and Polanyi in order to describe a mechanism which would account for the discrepancy between theoretical values for the yield strength compared to relatively low experimental values for the yield strength. This mechanism allows the material to deform without requiring the slip of entire planes which would require simultaneously breaking all the bonds connecting the planes.

The introduction of permanent plastic deformation through dislocations can be described by the movement of a caterpillar (Figure 7.1, a). As the caterpillar tries to move, a resistance occurs between the caterpillar and the ground which can be thought of as many bonds between the caterpillar and the ground. In a metal, this would be described as many atomic bonds across the slip plane. If the caterpillar attempted to slide its entire body at once, the effort necessary to move the caterpillar would have to overcome the friction between the entire caterpillar and the substrate, or in other words, the caterpillar would have to overcome all of the so called interatomic bonds simultaneously. This would require a large effort on the caterpillar’s part. However, if the caterpillar creates a hump at its tail end, and passes this hump (which can be described as a dislocation) from the tail to its head, the caterpillar moves a net displacement once the hump (dislocation) passes entirely through its body. The distance that the caterpillar moves is based on the size of the hump. This process involves much less effort as the breaking of atomic bonds occurs consecutively which requires much less effort than moving the entire caterpillar at once.

A similar example is that of the movement of a carpet (Figure 7.1 b). In the same manner as for a caterpillar, the hump (described as a dislocation) is pushed through the rug from one end to the other. If you tried to slide the rug all at once, the effort necessary to move the rug would have to overcome the friction between the entire rug and the floor.

![Figure 7.1: Dislocation motion described by the movement of (a) a caterpillar and (b) a rug.](image-url)
The resistance between the carpet and the floor can be thought of as the atomic bond across the slip plane. If you push the dislocation through the rug, the effort to move the “dislocation” does not have to take into account the friction stresses of the entire rug. In other words, the breaking of atomic bonds occurs consecutively which requires much less effort than moving the entire rug at once. By the time the “dislocation” passes all the way through the rug, the carpet has moved a net distance equal to the size of the hump.

For a crystal lattice, dislocations are typically described as either an edge or screw dislocation. The deformed lattice due to the introduction of a dislocation is shown in Figure 7.2. The edge dislocation denoted by the symbol $\perp$ is described by a line with an extra half-plane of atoms on one side of it. As with the previous examples, as the dislocation moves in the direction of the Burgers vector, $\mathbf{b}$, a resistance occurs between the atoms across the slip plane. As the extra half plane of atoms moves, the bond of atoms in the neighboring plane of atoms and across the slip plane is broken. The extra half plane of atoms joins with the separated atoms across the slip plane, and the dislocation line has translated in the direction of the Burgers vector by one Burgers-vector magnitude, $b = \|\mathbf{b}\|$.

Although dislocations exist in all materials, this movement is insignificant until the yield point occurs. At this point, loading causes dislocations to be generated, moved, and stored. The ease with which dislocations are able to move determines the hardness of the material. With an increase in the dislocation density, there begins to be more dislocation-dislocation interactions such that movement becomes more difficult and the stress required to produce additional plastic deformation increases, i.e. the material hardens.

![Figure 7.2: Slip in an idealized cubic crystal by means of an edge dislocation](image-url)
Storage of dislocations occurs either from an accumulation due to trapping of each other in a random way or due to a requirement for compatible deformation between various parts of the material. Statistically stored dislocations (SSD) are dislocations stored by trapping each other in a random way (Ashby, 1970) and geometrically necessary dislocations (GND) are dislocations that relieve deformation incompatibilities. Though the motion of both forms of dislocations results in plastic deformation, Fleck & Hutchinson (1993) also proposed that the equivalent plastic strain can be used as a scalar measure for the SSD density. It has also been shown that the density of the GND’s, $\rho_G$, is directly proportional to the gradient of the effective plastic strain (Nye, 1953; Cottrell, 1964; Ashby, 1970) such that:

$$\rho_G = \frac{\overline{r}\eta}{b}$$  \hspace{1cm} (7.1)

where $\eta$ is an effective strain gradient. For the case of the effective strain gradient being in terms of first order gradient of the equivalent plastic strain, $\overline{r}$ is the Nye factor (Arsenlis & Park, 1999) which accounts for the ratio of average density of geometrically necessary dislocations to that for the most efficient dislocation configurations considered by Gao et al. (1999). As presented in Arsenlis & Parks (1999), this Nye factor takes the value of 1.85 for bending of FCC polycrystals and 1.93 for torsion of FCC polycrystals. In this work, the effective strain gradient will be defined in terms of the first order gradient of plastic strain and in terms of the Laplacian of the plastic strain. Based on the definition of the effective strain gradient, the factor $\overline{r}$ must be defined such that the dislocation density has units of per length squared.

In order to determine how the length scales are incorporated into the material behavior, Taylor’s hardening law is used and is assumed to apply to both the SSD density and to the GND density such that the following relationships hold:

$$\tau_S = \mu^e a b \rho_S^{1/2}$$  \hspace{1cm} (7.2)

$$\tau_G = \mu^e a b \rho_G^{1/2}$$  \hspace{1cm} (7.3)

where $\tau_S$ is a shear flow stress due to the SSD’s, $\tau_G$ is a shear flow stress due to the GND’s, $\mu^e$ is the shear modulus as defined by Eq. (3.20), $\alpha$ is an empirical constant usually on the order of 1 (e.g., Nix & Gibeling, 1985), and $b$ is the Burgers vector. Both $\tau_S$ and $\tau_G$ are assumed to be components of the total shear flow stress, and a functional form for the critical shear stress, or the flow shear stress, is used here as follows (Columbus & Grujicic, 2002):

$$\tau_f = \left[ \tau_S^\beta + \tau_G^\beta \right]^{1/\beta}$$  \hspace{1cm} (7.4)
where $\beta$ defines the method for coupling the SSD’s and the GND’s. Thus, the critical shear stress can be written in terms of the components of the dislocations as follows:

$$\tau_f = \mu \alpha b \left[ \rho_S^{\beta_2/2} + \rho_G^{\beta_2/2} \right]^{1/\beta} \quad (7.5)$$

Thus, for the case of $\beta = 1$, the shear flow stress corresponds to the superposition of the contributions of the SSD’s and GND’s to the flow stress such that (Columbus & Grujicic, 2002):

$$\tau_f = \mu \alpha b \left[ \rho_S^{1/2} + \rho_G^{1/2} \right] \quad (7.6)$$

For the case of $\beta = 2$, the shear flow stress corresponds to a superposition of the densities of the SSD’s and the GND’s such that (Nix & Gao, 1998):

$$\tau_f = \mu \alpha b \left[ \rho_S + \rho_G \right]^{1/2} \quad (7.7)$$

Following the work of Voyiadjis & Abu Al-Rub (2005), a more general form of the shear flow stress can be defined in terms of a set of interaction coefficients $\beta_1 = \beta / 2$, $\beta_2 = \beta / 2$, and $\beta_3 = \beta$ as follows:

$$\tau_f = \mu \alpha b \left[ \left( \alpha^2 b^2 \rho_S \right)^{\beta_1} + \left( \alpha^2 b^2 \rho_G \right)^{\beta_2} \right]^{1/\beta_3} \quad (7.8)$$

The Taylor factor, $Z$, is defined as the ratio of the tensile flow stress to the shear flow stress as follows (Taylor, 1938):

$$Z = \frac{\sigma_f}{\tau_f} \quad (7.9)$$

This Taylor factor takes the value of 3.06 for FCC polycrystals (Taylor, 1938) and the value of $\sqrt{3}$ for isotropic solids (Nix & Gao, 1998). Using this relationship, the flow stress can now be defined in terms of the dislocation densities as follows:

$$\sigma_f = Z \mu \alpha b \left[ \left( \alpha^2 b^2 \rho_S \right)^{\beta_1} + \left( \alpha^2 b^2 \rho_G \right)^{\beta_2} \right]^{1/\beta_3} \quad (7.10)$$

This flow stress is the current yield stress including hardening of the material due to dislocations and will be related to the flow stress derived by the gradient theory in order to define the length scale.
7.2.2 Gradient Model Length Scale

The isotropic hardening variable in macro-plasticity (denoted here by \( r \)) is a scalar quantity. Removing damage, the evolution of \( r \) is expressed in terms of the evolution of the equivalent plastic strain, \( \dot{\varepsilon}_{eq}^p \), through Eq. (5.98). Assuming a proportional, monotonic loading, this isotropic hardening variable can alternatively be written as equal to the total equivalent plastic strain, \( \varepsilon_{eq}^p \), such that:

\[
\dot{\varepsilon}_{eq}^p = \sqrt{\frac{2}{3}} \varepsilon_{eq}^p : \varepsilon_{eq}^p = r 
\]  

(7.11)

The gradient enhanced yield condition, (5.89), is rewritten here without damage and with isotropic hardening as follows:

\[
f' = ||\varepsilon|| - \sqrt{\frac{2}{3}} \sigma_f \leq 0 \] 

(7.12)

The flow stress used in this equation has been defined as follows:

\[
\sigma_f = \sigma_{yp} + R + c_R \nabla^2 R 
\] 

(7.13)

where:

\[
R = R(\varepsilon_{eq}^p) 
\] 

(7.14)

\[
\nabla^2 R = \frac{\partial^2 R}{\partial \varepsilon_{eq}^p} \nabla \varepsilon_{eq}^p \cdot \nabla \varepsilon_{eq}^p + \frac{\partial R}{\partial \varepsilon_{eq}^p} \nabla^2 \varepsilon_{eq}^p 
\] 

(7.15)

For the case of uniform uniaxial tension where no gradients of strain occur, the uniaxial flow stress is written in terms of the SSD density from Eq. (7.10) and in terms of the isotropic hardening conjugate force from Eq. (7.13) as follows:

\[
\sigma_f = Z \mu' \left( \alpha^2 b^2 \rho_S \right)^{\beta_i/\beta_h} = \sigma_{yp} + R 
\] 

(7.16)

Thus, the SSD can be defined in terms of the continuum model isotropic hardening conjugate force as follows:

\[
\rho_S = \frac{1}{\alpha^2 b^2} \left( \frac{\sigma_{yp} + R}{Z \mu'} \right)^{\beta_i/\beta_h} 
\] 

(7.17)

The GND density has now been written in terms of a continuum effective plastic strain gradient, \( \eta \), by Eq. (7.1) and the SSD density has been written in terms of the continuum isotropic hardening conjugate force by Eq. (7.17), where the isotropic
hardening conjugate force is a function of the equivalent plastic strain. Substitution of the
definitions for the dislocation densities into Eq. (7.10) gives the following relationship:

$$\sigma_f = \sigma_{yp} \left[ \left( 1 + \frac{R}{\sigma_{yp}} \right)^{\beta_1} + \left( \frac{Z \mu^e}{\sigma_{yp}} \right)^{\beta_1} \left( \alpha^2 b \overline{\varphi} \eta \right)^{\beta_2} \right]^{1/\beta_1}$$

(7.18)

Writing this equation in terms of the original interaction coefficient, $\beta$, gives the
following relationship:

$$\sigma_f = \sigma_{yp} \left[ \left( 1 + \frac{R}{\sigma_{yp}} \right)^{\beta} + \left( \frac{Z \mu^e}{\sigma_{yp}} \right)^{\beta} \left( \alpha^2 b \overline{\varphi} \eta \right)^{\beta/2} \right]^{1/\beta}$$

(7.19)

In order for the dislocation based definiti on of the flow stress to correspond to the
flow stress defined through gradient enhanced continuum plasticity, the interaction
coefficient, $\beta$, must be as 1 such that:

$$\sigma_f = \sigma_{yp} + R + \left[ Z \left( \frac{\mu^e}{\sigma_{yp}} \right) \left( \alpha^2 b \overline{\varphi} \right)^{1/2} \right] \sigma_{yp}^{1/2}$$

(7.20)

Thus, comparing this equation with Eq. (7.13), the gradient coefficient, $c_r$, and the
effective gradient of plastic strain, $\eta$, are defined from the dislocation based flow stress
as follows:

$$c_r = l^2 = Z \left( \frac{\mu^e}{\sigma_{yp}} \right) \left( \alpha^2 b \overline{\varphi} \right)^{1/2}$$

(7.21)

$$\eta = \left( \frac{\nabla^2 R}{\sigma_{yp}} \right)^2$$

(7.22)

From the units of the Laplacian of the isotropic hardening (force per length to the
power four) and the yield stress (force per length squared), the units of the effective strain
gradient term, $\eta$, are defined to be per length to the power four. Thus, in order to
maintain consistency of units in Eq. (7.1), the factor $\overline{\varphi}$ is defined as a coefficient with
units of length to the power of three which gives the correct units for the length scale in
Eq. (7.21).

Expanding the Laplacian of the isotropic hardening conjugate force in terms of the
equivalent plastic strain and its gradients, the tensile flow stress is written in terms of first
order gradients of the equivalent plastic strain and in terms of the Laplacian of the
equivalent plastic strain as follows:
\[ \sigma_f = \sigma_{yp} + R + c_1 \nabla \varepsilon_e^p \cdot \nabla \varepsilon_e^p + c_2 \nabla^2 \varepsilon_e^p \]  
(7.23)

where:

\[ c_1 = c_r \frac{\partial^2 R}{\partial \varepsilon_e^p} \]  
(7.24)

\[ c_2 = c_r \frac{\partial R}{\partial \varepsilon_e^p} \]  
(7.25)

Note that these coefficients are not constant and are in fact functions of the equivalent plastic strain based on the state law defined for the isotropic hardening conjugate force, Eq. (7.14).

In order to obtain the enhanced Nye factor used in Eq. (7.21), consider polycrystal copper such that the following parameters are used: \( \alpha = 1 \), \( b = 9.04 \times 10^{-11} \text{m} \), \( Z = 3.06 \), \( \mu^e = 45 \times 10^9 \text{N/m}^2 \), and \( \sigma_{yp} = 226 \times 10^6 \text{N/m}^2 \). From this data, the length scale, \( l \), is defined from Eq. (7.21) as follows:

\[ l = \left( 7.61 \times 10^{-2} \text{m}^{1/4} \right) \left( \frac{r}{\text{m}} \right)^{1/4} \]  
(7.26)

From the micro-torsion experimental results (Fleck et al., 1994) and micro-bending experimental results (Stolken & Evans, 1998), the length parameter has been defined as 4 \( \mu \text{m} \) for copper. Thus, the enhanced Nye factor is defined for copper to be 7.63 \( \mu \text{m}^3 \). Further research needs to be performed in order to define this enhanced Nye factor for a range of materials; however, this is beyond the focus of this study.

7.3 LOCALIZATION PROBLEMS

Though softening behavior typically occurs when the shape of the body and the boundary conditions induce an inhomogeneous state of deformation, material microstructure also gives rise to an inhomogeneous state of deformation. Shear bands occurring from material inhomogeneities can occur in a number of materials such as metals, polymers, and granular materials and are typically originated due to a material heterogeneity or defect in the material, such as micro-cracks, micro-voids, or dislocations. This localization can be attributed to a coupling of inelastic mechanisms such as micro-crack and micro-void growth with plastic flow and fracture.

The width, point of emergence, and angle of inclination of the shear bands can depend on material factors including the grain diameter (either soil or metal crystal); the distribution and density of fibers in a metal-matrix composite; and the angle of internal
friction and density and can depend on structural factors including the geometry of the body and the loading boundary conditions.

From the analytical solution of the 1D localization example in Section 6.4.2, the shear band width defined by Eq. (6.46) is written for plasticity with isotropic hardening in terms of a length scale as follows:

\[ w = 2\pi \sqrt{c_R} = 2\pi l \]  

(7.27)

In the previous section, the length scale of the gradient theory was defined in terms of material parameters from dislocation mechanics to be used in problems of size effect and was defined to be on the order of a few micro-meters; however, for problems of localization, the characteristic length being the shear band width is typically on the order of a few millimeters. Thus, a different length scale must be defined for localization problems in terms of larger scale microstructure such as larger scale dislocation structures or grain sizes.

To this end, the Hall-Petch relation gives the flow stress as a decreasing function of the grain size as follows (Hall, 1951; Petch, 1953):

\[ \sigma_f = \sigma_0 + \frac{k}{d^{1/2}} \]  

(7.28)

where \( \sigma_0 \) is a frictional stress required to moved dislocations, \( k \) is a temperature-dependent material constant with units of force/length\(^{3/2} \), and \( d \) is the grain diameter. Thus, from this relation, the larger the grain size of a crystalline material, the weaker it is. In his work, Hall also showed that the length of slip bands correspond to grain sizes and thus a relationship could be established between the two. In the work of Smyshlyaev & Fleck (1996), the grain size effect was proposed to be due to the presence of spatial gradients of strain in each single grain, and these gradients were associated with the plastic inhomogeneity of slip.

In the work of Li (1963), experimental observations suggested that the dislocation density is proportional to the inverse of the grain diameter. Utilizing this and the fact that the grain size effect is due to the spatial gradients of strain, a relationship similar to Eq. (7.1) is proposed such that:

\[ \frac{1}{d} = \frac{\bar{r}\eta}{b} \]  

(7.29)

where \( b \) is the Burgers vector, \( \eta \) is an effective gradient of the equivalent plastic strain, and \( \bar{r} \) is an enhanced Nye factor similar to that used in Eq. (7.1) which is used to adjust the units of the problem. Eq. (7.22) will be used for the relationship between the
Laplacian of the isotropic hardening conjugate force, such that the enhanced Nye factor used here has units of length to the power four.

For the case of uniform uniaxial tension where no gradients of strain occur, the uniaxial flow stress is written in terms of the frictional stress, $\sigma_0$, from Eq. (7.28), and in terms of the isotropic hardening conjugate force from Eq. (7.13) as follows:

$$\sigma_f = \sigma_0 = \sigma_{yp} + R$$  \hspace{1cm} (7.30)

such that the frictional stress is defined in terms of the continuum model isotropic hardening conjugate force. Substitution of the definitions for the grain size and for the frictional stress into Eq. (7.28) gives the following relationship:

$$\frac{\sigma_f}{\rho} = R + k \left( \frac{\bar{\rho}}{b} \right)^{1/2} \eta^{1/2}$$  \hspace{1cm} (7.31)

Utilizing the relationship between the effective strain gradient term, $\eta$, and the Laplacian of the isotropic hardening conjugate force as given by Eq. (7.22) and comparing Eq. (7.31) with Eq. (7.13), the gradient coefficient, $c_r$, is defined from the grain size based flow stress as follows:

$$c_r = l^2 = \left( \frac{k}{\sigma_{yp}} \right) \left( \frac{\bar{\rho}}{b} \right)^{1/2}$$  \hspace{1cm} (7.32)

In order to obtain the enhanced Nye factor used in this equation, consider polycrystal copper such that the following parameters are used: $b = 9.04 \times 10^{-11} \text{m}$, $\sigma_{yp} = 226 \times 10^6 \text{N/m}^2$, and $k = 0.11 \times 10^6 \text{N/m}^{3/2}$. The coefficient $k$ is obtained from Meyers & Chawla (1984) for a total strain of 0.005. From this data, the length scale, $l$, is defined from Eq. (7.32) as follows:

$$l = 7.15 \bar{\rho}^{1/4}$$  \hspace{1cm} (7.33)

The width of shear bands are typically on the order of a few millimeters. Assuming that the shear band width for copper is 4 mm, the enhanced Nye factor is defined for copper to be $\bar{\rho} = 9.77 \times 10^{-2} \text{mm}^4$. Further research needs to be performed in order to define this enhanced Nye factor for a range of materials; however, this is beyond the focus of this study.
7.4 Variable Length Scales

The length scales defined in Eqs. (7.21) and (7.32) are functions of material constants. For the size effect problem, the length scale was defined in terms of dislocation mechanics parameters; for the localization problem, the length scale was defined in terms of grain size mechanics. It has been discussed in the literature (Gracio, 1994; Begley & Hutchinson, 1998; Abu Al-Rub & Voyiadjis, 2004; Voyiadjis & Abu Al-Rub, 2005) that the length scale is not a constant but is explicitly dependent on such variables as the equivalent plastic strain, the grain size, the macroscopic specimen size, etc. For example, a length scale was defined in Voyiadjis & Abu Al-Rub (2005) as follows:

\[
l = \frac{hDd}{D + d^r/m}
\]

(7.34)

where \(d\) is the grain diameter, \(D\) is a macroscopic characteristic size of the microstructure being investigated (beam thickness in micro-bending, wire diameter in micro-torsion, etc.), and \(m\) is an exponent used to define a power law between the isotropic hardening conjugate force \(R\) and the isotropic hardening flux variable, \(r\). The term \(h\) is a function of dislocation theory coefficients. This relation allows for the length scale parameter to decrease with strain, to increase with grain size, to increase with \(D\), and to decrease with \(m\), such that an evolving length scale can be used in the gradient model. An extensive discussion on this topic can be found in Voyiadjis & Abu Al-Rub (2005).

7.5 Conclusions

Utilizing the gradient model presented in CHAPTER 5, this chapter discussed the definition of the length scale introduced through the gradient measure of isotropic hardening. For problems of size effect, a flow stress defined through dislocation mechanics was compared with the flow stress defined through gradient plasticity such that the length scale was defined in terms of dislocation mechanics. For problems of localization, a flow stress defined through the grain size was compared with the flow stress defined through gradient plasticity such that the length scale was defined in terms of grain size coefficients. Further experimental work is required to define the enhanced Nye factors for use in general models.
CHAPTER 8: SUMMARY AND CONCLUSIONS

8.1 SUMMARY

In this work, an extensive mathematical formulation of a rigorous, thermodynamically consistent gradient enhanced approach to coupled plasticity-damage has been presented. The enhanced continuum model used in this work provides a strong coupling between gradient-enhanced plasticity and gradient-enhanced damage and introduces a material length scale into the model. By the introduction of gradients and the corresponding material length scales, the proposed model can properly simulate localization problems without mesh dependency in the numerical solutions.

By following a mathematically consistent formulation in the expansion of the Laplacians of the hardening variables, first order gradients as well as the Laplacians of several variables are incorporated into the model. As opposed to previous theories in the literature with linear hardening, the gradient model proposed here consistently expands the Laplacian evolution equations to allow different nonlinear material models.

8.2 CONCLUDING REMARKS

Typically, researchers make use of the Laplacian to help in the regularization of numerical problems involving patterning, i.e. shear bands, and of the first order gradient for size effects when investigating micro-bending and micro-torsion. In order to account for both of these effects, first-order gradients should be incorporated into the model. Higher order gradients may also be required to capture other behaviors. In order to capture first-order gradients, second-order gradients, and higher-order gradients, previous researchers have had to make a definition for the gradient measure. The proposed model is unique in that (a) a Laplacian based measure is directly derived from the Taylor’s series approximation of a nonlocal measure and (b) the model incorporates first-order up to fourth-order gradients including odd-ordered gradients. Thus, the proposed capability of this model is increased to account for not just shape patterning such as localization problems, but also to simulate properly size dependent behavior of the materials.

A computational method for the implementation of this gradient model into a finite element framework has been introduced, and the framework is laid for full implementation for a number of localization problems. In order to solve the boundary value problem, a multifield approach has been adopted such that the plastic and damage multipliers are discretized in addition to the displacement field. Since the degrees of freedom are increased, two additional governing equations (i.e. the weak forms of the consistency conditions) are used to obtain a solution.
The governing equations involve both the first order gradient and the Laplacian of the plastic and damage multipliers; however, the governing equations only involve first order derivatives of the displacement field (i.e. strains). Thus, the discretization procedure for the plastic and damage multipliers uses \( C^1 \) continuous interpolation functions such as the Hermitian shape functions while the discretization procedure for the displacement field uses \( C^0 \) continuous interpolation functions. This type of discretization is a mixed finite element solution whereby different interpolation functions are used for different discretized fields.

Utilizing the gradient model, analytical and numerical examples of localization were used to demonstrate the effectiveness of the gradient model in removing the mesh sensitivity problem. The numerical solutions of strain localization problems demonstrated the effectiveness of the gradient theory as a localization limiter and demonstrated how the gradient theory removes the mesh-dependency found in classical continuum models. Problems due to both a material instability and due to a structural instability were used to investigate the use of the gradient theory in an ill-posed initial boundary value problem.
BIBLIOGRAPHY

PART I: BY THE AUTHOR


PART II: BY OTHER AUTHORS


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APPENDIX A : NOTATION

For convenience in developing the constitutive model and the finite element algorithm, tensorial notation will be used. In tensor notation, boldface terms indicate tensors of order one or greater, while italicized terms indicate scalars. In order to introduce the tensor notation used here, assume that we have a space of dimension \( n \), in a Cartesian coordinate system, and that this space contains a scalar denoted by \( c \), vectors denoted by \( \mathbf{a} \) and \( \mathbf{b} \), second order tensors denoted by \( \mathbf{A} \) and \( \mathbf{B} \), and a fourth order tensor denoted by \( \mathbf{C} \). In tensorial notation, the symbol \( \otimes \) denotes the dyadic product, and the components of this tensorial product are given as follows:

\[
C_{ijkl} = (\mathbf{A} \otimes \mathbf{B})_{ijkl} = A_{ij}B_{kl}
\]  

(E.1)

Einstein’s summation convention is used unless otherwise indicated. In this convention, whenever an index is repeated once, it is a dummy index indicating a summation with the index running through the integral numbers 1, 2, ..., \( n \), where \( n \) denotes the number of dimensions in the coordinate system. The following are examples of using this convention in an \( n \)-dimensional coordinate system to denote summations:

\[
tr(A_y) = \sum_{i=1}^{n} A_{yi} = A_{i1} + A_{i2} + \cdots + A_{in}
\]  

(E.2)

\[
\sum_{i=1}^{n} a_i b_i = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n
\]  

(E.3)

Note that the indicial notation is used in these examples demonstrating summations. In tensorial notation, dots and colons are used to indicate the products of vectors and tensors. The use of a single dot represents a contraction of the inner indices, whereas the use of a colon represents a double contraction of the inner indices:

\[
\mathbf{a} \cdot \mathbf{b} = a_i b_i
\]  

(E.4)

\[
(\mathbf{A} \cdot \mathbf{b})_i = A_y b_j
\]  

(E.5)

\[
(\mathbf{A} \cdot \mathbf{B})_{ij} = A_{im}B_{mj}
\]  

(E.6)

\[
\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}
\]  

(E.7)

\[
(\mathbf{C} : \mathbf{B})_{ij} = C_{ijkl}B_{kl}
\]  

(E.8)

Inverses of second-order and fourth-order tensors can be obtained using the following relations:
where the second-order and fourth-order identity tensors are defined here as $\mathbf{1}$ and $\mathbf{I}$, respectively. The components of these identity tensors are defined in terms of the Kronecker delta $\delta_{ij}$ (equal to 1 if $i = j$ and zero otherwise) as follows:

\[
I_{ij} = \delta_{ij}
\]

\[
I_{ijkl} = \frac{1}{2} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
\]

Use will be made of the $J_2$ plasticity flow theory in this work. We therefore define the following relationship for the second principal invariant of a tensor:

\[
J_2(A) = (A^D : A^D)^{\frac{1}{2}} = \left\| A^D \right\|
\]

where $\left\| \cdot \right\|$ is the norm of a tensor and $A^D$ is the deviatoric part of $A$. Using the deviatoric part of the fourth-order identity tensor which is defined as $I^D = \mathbf{I} - \frac{1}{4} \mathbf{1} \otimes \mathbf{1}$, the deviatoric part of $A$ can also be written as $A^D = I^D : A$.

Terms with a subscript preceded by a comma denote partial derivatives, i.e. $A_{,x} = \partial A / \partial x$. Terms with an over-dot denote derivatives with respect to time, i.e. $\dot{A} = \partial A / \partial t$.

Orthogonal tensors are used for transformation of the damage matrix from the principal directions to the global directions. A tensor $\mathbf{Q}$ is orthogonal if it preserves inner products:

\[
(\mathbf{Q} \cdot \mathbf{u}) \cdot (\mathbf{Q} \cdot \mathbf{v}) = \mathbf{u} \cdot \mathbf{v}
\]

for all vectors $\mathbf{u}$ and $\mathbf{v}$. If a tensor is orthogonal, then the following relationships are also true:

\[
\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{Q} \cdot \mathbf{Q}^T = \mathbf{I}
\]

\[
\mathbf{Q}^T = \mathbf{Q}^{-1}
\]
APPENDIX B: ADDITIONAL EQUATIONS

To avoid adding additional complexity to the main body of this document, a number of the more complex equations are given here. Indicial notation is used in order to better demonstrate how the various matrices interact.

B.1 EQUATIONS FOR CHAPTER 4

This section lists complex equations that are modified from the local plasticity theory to incorporate damage.

**Damage tensor and related derivatives**

\[
\hat{\varphi}_{ab} = Q_{ca} \hat{\varphi}_{ca} Q_{db} 
\]

\[
\frac{\partial \hat{\varphi}_{ab}}{\partial \hat{\varphi}_{cd}} = Q_{ca} Q_{db} = \frac{\partial \hat{\varphi}_{cd}}{\partial \hat{\varphi}_{ab}} 
\]

**Damage measure and related derivatives**

\[
M_{abcd} = \frac{Q_{ea} \hat{\varphi}_{fb} \hat{M}_{efgh} Q_{gc} Q_{hd}}{Q_{ca}} 
\]

\[
M_{abcd}^{-1} = \frac{Q_{ea} \hat{\varphi}_{fb} \hat{M}_{efgh}^{-1} Q_{gc} Q_{hd}}{Q_{ca}} 
\]

\[
\frac{\partial M_{abcd}}{\partial \hat{\varphi}_{wx}} = Q_{ea} \frac{\hat{\varphi}_{fb} \hat{M}_{efgh}}{\hat{\varphi}_{wx} \hat{M}_{efgh}} Q_{gc} Q_{hd} 
\]

\[
\frac{\partial M_{abcd}^{-1}}{\partial \hat{\varphi}_{ab}} = Q_{ea} \frac{\hat{\varphi}_{fb} \hat{M}_{efgh}^{-1}}{\hat{\varphi}_{ab} \hat{M}_{efgh}} Q_{gc} Q_{hd} 
\]

\[
\frac{\partial^2 M_{abcd}}{\partial \hat{\varphi}_{wx} \partial \hat{\varphi}_{yz}} = Q_{ea} \frac{\hat{\varphi}_{fb} \hat{M}_{efgh} \hat{\varphi}_{yz} Q_{gc} Q_{hd}}{\hat{\varphi}_{wx} \hat{\varphi}_{yz}} 
\]

**Principle damage measure related derivatives**

\[
\frac{\partial \hat{M}_{efgh}}{\partial \hat{\varphi}_{wx}} = \frac{\hat{\varphi}_{c} \hat{M}_{efgh}}{\hat{\varphi}_{wx} \hat{\varphi}_{wx}} 
\]

\[
\frac{\partial \hat{M}_{efgh}^{-1}}{\partial \hat{\varphi}_{wx}} = \frac{\hat{\varphi}_{c} \hat{M}_{efgh}^{-1}}{\hat{\varphi}_{wx} \hat{\varphi}_{wx}} 
\]

\[
\frac{\partial^2 \hat{M}_{efgh}}{\partial \hat{\varphi}_{wx} \partial \hat{\varphi}_{yz}} = \frac{\hat{\varphi}_{c} \hat{M}_{efgh} \hat{\varphi}_{yz} \hat{\varphi}_{yz} \hat{\varphi}_{yz}}{\hat{\varphi}_{wx} \hat{\varphi}_{yz}} 
\]

\[
\frac{\partial^2 \hat{M}_{efgh}^{-1}}{\partial \hat{\varphi}_{wx} \partial \hat{\varphi}_{yz}} = 0 
\]
Deviatoric damage measure and related derivatives

\[ N_{abcd} = M_{abcd} - \frac{1}{3} \delta_{ab} \delta_{cd} M_{p fades} = \left( \delta_{ac} \delta_{bf} - \frac{1}{3} \delta_{ab} \delta_{ef} \right) M_{efcd} \]  
(B.12)

\[ \frac{\partial N_{abcd}}{\partial \phi_{yz}} = \left( \delta_{av} \delta_{bx} - \frac{1}{3} \delta_{ab} \delta_{xz} \right) \delta_{cy} \delta_{dz} \]  
(B.13)

\[ \frac{\partial N_{abcd}}{\partial \phi_{yz}} = \left( \delta_{ac} \delta_{bf} - \frac{1}{3} \delta_{ab} \delta_{ef} \right) \frac{\partial M_{efcd}}{\partial \phi_{yz}} \]  
(B.14)

\[ \frac{\partial^2 N_{abcd}}{\partial \phi_{xs} \partial \phi_{yz}} = \left( \delta_{ac} \delta_{bf} - \frac{1}{3} \delta_{ab} \delta_{ef} \right) \frac{\partial^2 M_{efcd}}{\partial \phi_{xs} \partial \phi_{yz}} \]  
(B.15)

\[ \frac{N_{abcd}}{\partial Y_{yz}} = \frac{N_{abcd}}{\partial \phi_{ef} \left( \frac{\partial Y_{yz}}{\partial \phi_{ef}} \right)^{-1}} \]  
(B.16)

Damage conjugate force and related derivatives

\[ Y_{ab} = \frac{1}{2} \varepsilon_{cd} \frac{\partial C_{cdef}^e}{\partial \phi_{ab}} \varepsilon_{ef} = \frac{1}{2} \sigma_{cd} \frac{\partial C_{cdef}^{-e}}{\partial \phi_{ab}} \sigma_{ef} \]  
(B.17)

\[ \frac{\partial Y_{ab}}{\partial \sigma_{yz}} = \sigma_{cd} \frac{\partial C_{cdef}^{-e}}{\partial \phi_{ab}} \]  
(B.18)

\[ \frac{\partial^2 Y_{ab}}{\partial \sigma_{xc} \partial \sigma_{yz}} = \frac{\partial C_{cdef}^{-e}}{\partial \phi_{ab}} \]  
(B.19)

\[ \frac{\partial Y_{ab}}{\partial \phi_{yz}} = \frac{\partial \phi_{ab}}{\partial Y_{yz}} \left( \frac{\partial Y_{yz}}{\partial \phi_{ef}} \right)^{-1} = \frac{1}{2} \varepsilon_{cd} \frac{\partial^2 C_{cdef}^e}{\partial \phi_{ab} \partial \phi_{yz}} \varepsilon_{ef} \]  
(B.20)

Elasticity modulus and related derivatives

\[ C_{abcd}^e = M_{abcd}^{-1} \tilde{C}_{cdef}^e \tilde{M}_{cdgh}^{-1} \]  
(B.21)

\[ \frac{\partial C_{abcd}^e}{\partial \phi_{yz}} = 2 \tilde{M}_{abcd}^{-1} \tilde{C}_{cdef}^e \frac{\partial M_{cdgh}^{-1}}{\partial \phi_{yz}} = 2 C_{abcd}^e M_{ghcd} \frac{\partial M_{cdgh}^{-1}}{\partial \phi_{yz}} \]  
(B.22)

\[ \frac{\partial^2 C_{abcd}^e}{\partial \phi_{xs} \partial \phi_{yz}} = 2 \frac{\partial M_{abcd}^{-1}}{\partial \phi_{wx}} \tilde{C}_{cdef}^e \frac{\partial M_{cdgh}^{-1}}{\partial \phi_{yz}} \]  
(B.23)

Inverse elasticity modulus and related derivatives

\[ C_{abcd}^{-e} = M_{efab} \tilde{C}_{efgh}^{-e} M_{ghcd} \]  
(B.24)

\[ \frac{\partial C_{abcd}^{-e}}{\partial \phi_{yz}} = 2 M_{efab} \tilde{C}_{efgh}^{-e} \frac{\partial M_{ghcd}}{\partial \phi_{yz}} \]  
(B.25)

\[ \frac{\partial^2 C_{abcd}^{-e}}{\partial \phi_{xs} \partial \phi_{yz}} = 2 \frac{\partial M_{efab}}{\partial \phi_{wx}} \tilde{C}_{efgh}^{-e} \frac{\partial M_{ghcd}}{\partial \phi_{yz}} + 2 M_{efab} \tilde{C}_{efgh}^{-e} \frac{\partial^2 M_{ghcd}}{\partial \phi_{wx} \partial \phi_{yz}} \]  
(B.26)
Yield condition and damage condition

\[ F = f = \sqrt{N_{abcd} (\sigma_{cd} - X_{cd}) N_{abef} (\sigma_{ef} - X_{ef})} - \sqrt{\frac{2}{3}} \left[ \sigma_{y} + \frac{R}{1 - \sqrt{\phi_{ab} \phi}} \right] \leq 0 \]  \hspace{1cm} (B.27)

\[ G = g = \sqrt{Y_{y} Y_{g}} - \sqrt{\frac{2}{3}} [\sigma_{yd} + K] \equiv 0 \]  \hspace{1cm} (B.28)

Yield condition derivatives

\[ \frac{\partial F}{\partial \sigma_{yz}} = f_{,\sigma_{yz}} = \frac{N_{abef} N_{abcd} (\sigma_{ef} - X_{ef})}{\| \mathbf{N} : (\mathbf{\sigma} - \mathbf{X}) \|} \]  \hspace{1cm} (B.29)

\[ \frac{\partial F}{\partial \Delta \lambda^{p}} = f_{,\Delta \lambda^{p}} = -f_{,\sigma_{yz}} \frac{\partial R}{\partial r} - f_{,\sigma_{yz}} \frac{\partial X_{cd}}{\partial \alpha_{cd}} f_{,\sigma_{cd}} - f_{,\phi_{ab}} f_{,\gamma_{ab}} \]  \hspace{1cm} (B.30)

\[ \frac{\partial F}{\partial \Delta \lambda^{d}} = f_{,\Delta \lambda^{d}} = -f_{,\phi_{ab}} g_{,\gamma_{ab}} \]  \hspace{1cm} (B.31)

\[ \frac{\partial F}{\partial R} = f_{,R} = -\sqrt{\frac{2}{3}} \]  \hspace{1cm} (B.32)

\[ \frac{\partial F}{\partial X_{yz}} = f_{,X_{yz}} = -f_{,\sigma_{yz}} \]  \hspace{1cm} (B.33)

\[ \frac{\partial F}{\partial \phi_{ab}} = f_{,\phi_{ab}} = \frac{\partial N_{ghcd} (\sigma_{cd} - X_{cd}) N_{abef} (\sigma_{ef} - X_{ef})}{\| \mathbf{N} : (\mathbf{\sigma} - \mathbf{X}) \|} - \sqrt{\frac{2}{3}} \frac{R \phi_{ab}}{\| \phi \| (1 - \| \phi \|)^{2}} \]  \hspace{1cm} (B.34)

\[ \frac{\partial F}{\partial Y_{yz}} = f_{,Y_{yz}} = f_{,\phi_{ab}} \left( \frac{\partial Y_{yz}}{\partial \phi_{ab}} \right)^{-1} \]  \hspace{1cm} (B.35)

Damage condition derivatives

\[ \frac{\partial G}{\partial \sigma_{yz}} = g_{,\sigma_{yz}} = g_{,Y_{yz}} \frac{\partial Y_{yz}}{\partial \sigma_{yz}} \]  \hspace{1cm} (B.36)

\[ \frac{\partial G}{\partial \Delta \lambda^{p}} = g_{,\Delta \lambda^{p}} = -g_{,\phi_{ab}} f_{,\gamma_{ab}} \]  \hspace{1cm} (B.37)

\[ \frac{\partial G}{\partial \Delta \lambda^{d}} = g_{,\Delta \lambda^{d}} = -g_{,\phi_{ab}} g_{,\gamma_{ab}} \]  \hspace{1cm} (B.38)

\[ \frac{\partial G}{\partial K} = g_{,K} = -\sqrt{\frac{2}{3}} \]  \hspace{1cm} (B.39)

\[ \frac{\partial G}{\partial \phi_{yz}} = g_{,\phi_{yz}} = g_{,Y_{yz}} \frac{\partial Y_{yz}}{\partial \phi_{yz}} \]  \hspace{1cm} (B.40)

\[ \frac{\partial G}{\partial Y_{yz}} = g_{,Y_{yz}} = Y_{yz} \]  \hspace{1cm} (B.41)
Yield condition second-derivatives

\[
\frac{\partial^2 F}{\partial \sigma_{xz} \partial \sigma_{yz}} = f_{,\sigma_{xz}\sigma_{yz}} = \frac{N_{ab} N_{e} f_{,\sigma_{xz} f_{,\sigma_{yz}}} - f_{,\sigma_{xz} f_{,\sigma_{yz}}}}{\|N : (\sigma - X)\|} \\
\frac{\partial^2 F}{\partial \sigma_{xz} \partial \Delta \lambda^p} = f_{,\sigma_{xz}\Delta \lambda^p} = -f_{,\sigma_{xz}\sigma_{ab}} \frac{\partial X_{ab}}{\partial \alpha_{cd}} f_{,\sigma_{cd}} - f_{,\sigma_{xz} N_{abcd}} \frac{\partial N_{abcd}}{\partial \varphi_{ef}} f_{,\gamma_{ef}} \\
\frac{\partial^2 F}{\partial \sigma_{xz} \partial \Delta \lambda^d} = f_{,\sigma_{xz}\Delta \lambda^d} = -f_{,\sigma_{xz} N_{abcd}} \frac{\partial N_{abcd}}{\partial \varphi_{ef}} g_{,y_{ef}} \\
\frac{\partial^2 F}{\partial Y_{wx} \partial \sigma_{yz}} = f_{,\gamma_{wz}\sigma_{yz}} = f_{,\sigma_{yz} N_{abcd}} \frac{\partial N_{abcd}}{\partial Y_{wx}} \\
\frac{\partial^2 F}{\partial Y_{wx} \partial \Delta \lambda^p} = f_{,\gamma_{wz}\Delta \lambda^p} = -2 f_{,\gamma_{wz}\sigma_{ab}} \frac{\partial X_{ab}}{\partial \alpha_{cd}} f_{,\sigma_{cd}} - f_{,\gamma_{wz} \sigma_{ab} f_{,\sigma_{ab}}} f_{,\gamma_{wz} \sigma_{ab}} \\
\frac{\partial^2 F}{\partial Y_{yz} \partial \Delta \lambda^d} = f_{,\gamma_{wz}\Delta \lambda^d} = -f_{,\gamma_{wz} \sigma_{ab} g_{,y_{ab}}} - f_{,\gamma_{wz} \sigma_{ab} g_{,y_{ab}} Y_{ab}} \\
\frac{\partial^2 F}{\partial Y_{wx} \partial Y_{yz}} = f_{,\gamma_{wz} Y_{yz}} = f_{,\gamma_{wz} \varphi_{yz}} \left( \frac{\partial Y_{ab}}{\partial \varphi_{yz}} \right)^{-1} \\
\frac{\partial^2 F}{\partial Y_{yz} \partial Y_{yz}} = f_{,\gamma_{wz} Y_{yz}} = f_{,\gamma_{wz} \varphi_{yz}} \left( \frac{\partial Y_{ab}}{\partial \varphi_{yz}} \right)^{-1} \\
\frac{\partial^2 F}{\partial \varphi_{ab} \partial \varphi_{yz}} = f_{,\gamma_{wz} \varphi_{yz}} \\
\frac{\partial^2 F}{\partial \varphi_{ab} \partial \varphi_{yz}} = f_{,\gamma_{wz} \varphi_{yz}} \\
= \left( \sigma_{cd} - X_{cd} \right) \left( \frac{\partial^2 N_{ghcd}}{\partial \varphi_{ab} \partial \varphi_{yz}} N_{gh} f_{,\sigma_{ef} - X_{ef}} \right) \\
\frac{\partial^2 F}{\partial \varphi_{ab} \partial \varphi_{yz}} = \left( \sigma_{cd} - X_{cd} \right) N_{gh} f_{,\sigma_{ef} - X_{ef}} \frac{\partial N_{ijkl}}{\partial \varphi_{yz}} \left( \sigma_{kl} - X_{kl} \right) N_{ijmn} \left( \sigma_{mn} - X_{mn} \right) \\
- \frac{\partial N_{ghcd}}{\partial \varphi_{ab}} \left( \sigma_{cd} - X_{cd} \right) N_{gh} f_{,\sigma_{ef} - X_{ef}} \frac{\partial N_{ijkl}}{\partial \varphi_{yz}} \left( \sigma_{kl} - X_{kl} \right) N_{ijmn} \left( \sigma_{mn} - X_{mn} \right) \\
- \frac{\partial^2 F}{\partial \sigma_{yz} \partial N_{kln}} = f_{,\sigma_{yz} N_{kln}} \\
\frac{\partial^2 F}{\partial \sigma_{yz} \partial N_{kln}} = f_{,\sigma_{yz} N_{kln}} \\
= N_{kln} \left( \sigma_{mn} - X_{mn} \right) + \delta_{jm} \delta_{ze} N_{kij} \left( \sigma_{j} - X_{j} \right) \\
\frac{\partial^2 F}{\partial \sigma_{yz} \partial N_{kln}} = f_{,\sigma_{yz} N_{kln}} \\
N_{kln} \left( \sigma_{mn} - X_{mn} \right) + \delta_{jm} \delta_{ze} N_{kij} \left( \sigma_{j} - X_{j} \right) \\
= f_{,\sigma_{yz} N_{kln}} \\
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Damage condition second-derivatives

\[
\frac{\partial^2 G}{\partial \sigma_{aw} \partial \sigma_{yz}} = g_{\sigma_{aw} \sigma_{yz}} = g_{\sigma_{aw} \sigma_{yz}} \frac{\partial Y_{ab}}{\partial \sigma_{yz}} + g_{\sigma_{yz} \sigma_{yz}} \frac{\partial^2 Y_{ab}}{\partial \sigma_{yz}^2} \quad (B.52)
\]

\[
\frac{\partial^2 G}{\partial \sigma_{aw} \partial \Delta \lambda^p} = g_{\sigma_{aw} \Delta \lambda^p} = -g_{\sigma_{aw} \Delta \lambda^p} f_{\lambda_{ab}} \quad (B.53)
\]

\[
\frac{\partial^2 G}{\partial \sigma_{aw} \partial \Delta \lambda^d} = g_{\sigma_{aw} \Delta \lambda^d} = -g_{\sigma_{aw} \Delta \lambda^d} g_{\lambda_{ab}} - g_{\sigma_{ab} \sigma_{ab}} g_{\lambda_{ab}} \quad (B.54)
\]

\[
\frac{\partial^2 G}{\partial \sigma_{aw} \partial \phi_{yz}} = g_{\sigma_{aw} \phi_{yz}} = g_{\sigma_{aw} \phi_{yz}} \frac{\partial Y_{ab}}{\partial \phi_{yz}} \quad (B.55)
\]

\[
\frac{\partial^2 G}{\partial Y_{wa} \partial \sigma_{yz}} = g_{Y_{wa} \sigma_{yz}} = g_{Y_{wa} \sigma_{yz}} \frac{\partial Y_{ab}}{\partial \sigma_{yz}} \quad (B.56)
\]

\[
\frac{\partial^2 G}{\partial Y_{za} \partial \lambda_{ab}} = g_{Y_{za} \lambda_{ab}} = -g_{Y_{za} \lambda_{ab}} \frac{\partial Y_{ab}}{\partial \lambda_{cd}} f_{\lambda_{cd}} \quad (B.57)
\]

\[
\frac{\partial^2 G}{\partial Y_{za} \partial \lambda_{cd}} = g_{Y_{za} \lambda_{cd}} = -g_{Y_{za} \lambda_{cd}} \frac{\partial Y_{ab}}{\partial \lambda_{cd}} g_{\lambda_{cd}} \quad (B.58)
\]

\[
\frac{\partial^2 G}{\partial Y_{wa} \partial \phi_{yz}} = g_{Y_{wa} \phi_{yz}} = g_{Y_{wa} \phi_{yz}} \frac{\partial Y_{ab}}{\partial \phi_{yz}} \quad (B.59)
\]

\[
\frac{\partial^2 G}{\partial Y_{za} \partial \phi_{yz}} = g_{Y_{za} \phi_{yz}} = \delta_{yz} \frac{Y_{ab}}{\partial \phi_{yz}} - g_{Y_{za} \phi_{yz}} \quad (B.60)
\]

\[
\frac{\partial^2 G}{\partial \phi_{ab} \partial \phi_{yz}} = g_{\phi_{ab} \phi_{yz}} = g_{\phi_{ab} \phi_{yz}} \frac{\partial Y_{ab}}{\partial \phi_{yz}} \quad (B.61)
\]

B.2 EQUATIONS FOR CHAPTER 5

This section lists complex equations that are modified by the gradient enhancements, and are therefore different from the equations in the local damage-plasticity model of CHAPTER 4. If a given equation from APPENDIX B.1 is not given here in a gradient enhanced form, it can be assumed that the equation is either valid for CHAPTER 5 or it is not required for CHAPTER 5.

Yield condition and damage condition

\[
F = f = \sqrt{N_{abcd} \left( \sigma_{cd} - \bar{X}_{cd} \right)} N_{abef} \left( \sigma_{ef} - \bar{X}_{ef} \right) - \sqrt{\frac{\bar{R}}{3 \sqrt{3} \left( \sigma_{yp} + \frac{\bar{R}}{1 - \sqrt{3} \bar{R}} \phi_{ab} \phi_{ab} \right)}} \leq 0 \quad (B.62)
\]

\[
G = g = \sqrt{Y_{qg} Y_{qg}} - \sqrt{\frac{\bar{R}}{3 \sqrt{3} \left( \sigma_{yd} + K \right)}} \equiv 0 \quad (B.63)
\]
Yield condition derivatives

\[
\frac{\partial F}{\partial \sigma_{yz}} = f_{\sigma_{yz}} = \frac{N_{abyz}N_{abef}(\sigma_{ef} - \bar{X}_{ef})}{\|N : (\sigma - \bar{X})\|}
\]  
\[
\frac{\partial F}{\partial \nabla^2 R} = f_{\nabla^2 R} = c_B f_R
\]  
\[
\frac{\partial F}{\partial \nabla^2 X_{yz}} = f_{\nabla^2 X_{yz}} = -c_X f_{\sigma_{yz}}
\]  
\[
\frac{\partial F}{\partial \phi_{ab}} = f_{\phi_{ab}} = \frac{\partial N_{ghcd}(\sigma_{cd} - \bar{X}_{cd})N_{ghef}(\sigma_{ef} - \bar{X}_{ef})}{\partial \phi_{ab}} \left[\sqrt{\frac{2}{3}} \frac{\bar{R} \phi_{ab}}{\|\phi\|(1 - \|\phi\|)^2}\right]
\]  

Damage condition derivatives

\[
\frac{\partial G}{\partial \nabla^2 K} = g_{\nabla^2 K} = c_K g_{\nabla^2 K}
\]  

Yield condition second-derivatives

\[
\frac{\partial^2 F}{\partial \sigma_{wx} \partial \sigma_{yz}} = f_{\sigma_{wx},\sigma_{yz}} = \frac{N_{ahwx}N_{abyz} - f_{\sigma_{wx}} f_{\sigma_{yz}}}{\|N : (\sigma - \bar{X})\|}
\]  
\[
\frac{\partial^2 F}{\partial \sigma_{yz} \partial N_{klimn}} = f_{\sigma_{yz},N_{klimn}}
\]

\[
= \frac{N_{klyz}(\sigma_{mn} - \bar{X}_{mn}) + \delta_{ym} \delta_{zn} N_{klij}(\sigma_{ij} - \bar{X}_{ij})}{\|N : (\sigma - \bar{X})\|}
\]

\[
- f_{\sigma_{yz}} \left[\frac{(\sigma_{mn} - \bar{X}_{mn})N_{klcd}(\sigma_{cd} - \bar{X}_{cd})}{\|N : (\sigma - \bar{X})\|^2}\right]
\]
VITA

Robert Jason Dorgan was born the third child of Robert and Susan Dorgan on the 11th of August, 1977, in Mobile, Alabama. He attended the Alabama School of Mathematics and Science during his junior year of high school, and he graduated from McGill Toolen High School in 1995. Following high school, he began his college education at Louisiana State University (LSU) where he was awarded the LSU Tuition Exemption Academic Scholarship for his first four years of undergraduate education and the Gulf South Compression Academic Scholarship for his final year. During the summers at LSU, he worked structural engineering internships at Martin Marietta Aggregates in New Orleans and Lyle Stover Engineering in Mobile.

In December of 1999, he received his Bachelor of Science in Civil Engineering Degree with a structural engineering emphasis. After attending a course taught by Boyd Professor George Z. Voyiadjis during his last semester of undergraduate studies, Dr. Voyiadjis encouraged Mr. Dorgan to remain at LSU in order to perform his graduate studies under his guidance. Following their discussion, Mr. Dorgan enrolled in the graduate program at LSU and began his doctoral program in January of 2000 with Dr. Voyiadjis as his graduate advisor and committee chair. His research work has been accumulated into this document which will be nominated for the LSU Doctoral Dissertation Award. He will earn the degree of Doctor of Philosophy in the Department of Civil & Environmental Engineering with a focus in mathematics at the Spring 2006 Commencement.

Together, Mr. Dorgan and Dr. Voyiadjis have developed theoretical and computational aspects of a gradient–based thermodynamically consistent constitutive model. Generally, Mr. Dorgan’s research has been involved in several areas of mechanics, including structural mechanics, computational mechanics, mechanics of solids and structures, structural dynamics, mechanics of materials, fracture and damage mechanics, mechanics of fiber-reinforced composites. During his doctoral program, he has developed and implemented a number of numerical algorithms and integration schemes into numerical codes.

The work of Mr. Dorgan and Dr. Voyiadjis has been published in several journal articles and presented in numerous conferences, including several excellent presentations by Mr. Dorgan at national and international conferences. Most notable of these presentations was his presentation in the 41st Annual 2004 Society of Engineering Science Conference at the University of Nebraska-Lincoln, where he won first prize in the Student Paper Competition for his presentation. The technical presentations in this competition were judged by a panel of engineering scientists for their content, presentation format and style, and oral delivery.

During his time at LSU, Mr. Dorgan has also received other awards and recognitions that have contributed significantly to his funding at LSU. Upon beginning his studies, Mr.
Dorgan was awarded the Louisiana Board of Regents Fellowship which provided funding during his first four years of graduate studies. In the Spring of 2005, Mr. Dorgan became one of five graduate students in the College of Engineering to be awarded the LSU College of Engineering Inaugural Donald W. Clayton Excellence in Engineering Award, providing him with an enhancement to his research assistant stipend for his final year of graduate school. This award is bestowed upon a student who has demonstrated exemplary character, scholarly accomplishment, leadership, and has served as a role model and ambassador for the College of Engineering at LSU.

During four summers of his graduate studies, Mr. Dorgan was one of a handful of graduate students from universities around the country selected to intern in the Engineering Sciences Summer Institute at Sandia National Laboratories, Livermore. The program is specific to applied mechanics graduate students and is offered by the Science-based Materials Modeling Department of Sandia. At Sandia, he worked under the supervision of Sandia mentors and in collaboration with a number of researchers on projects in different areas as well as projects directly related to his Doctoral studies. He also had the opportunity to attend a series of expository seminars in applied mechanics presented in a tutorial manner by Sandia staff.

Mr. Dorgan was also instrumental during the planning of the 2005 Joint ASME/ASCE/SES Conference on Mechanics and Materials (McMat2005) hosted in Baton Rouge, Louisiana, where Mr. Dorgan took the initiative to become an integral member of the organizing committee. He made himself responsible for being involved in every detail of the organizing of this conference including coordinating services such as accommodations and catering, and he had email contact with almost all of the several hundred participants of this conference to assist them with their problems and special needs. He was responsible for gathering the conference abstracts and obtaining their reviews, and he compiled these abstracts onto the conference CD-ROM proceedings of which he and Professor Voyiadjis were co-editors. He initiated the promotion of the department by coordinating with professors to have tours of the department’s facilities, and he worked on numerous requests to obtain financial sponsors and equipment donations, from which a significant amount of the equipment was donated for use by the conference.