Implementation of Solid Shell Element for Modelling of Paperboard

Master's Dissertation by

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Abstract

This paper is trying to combine a complex anisotropic constitutive model for paperboard developed by Borgqvist et. al. [5] with a special purpose solid shell element. The element considered for this task is the eight-node solid shell element proposed by Schwarze and Reese in [17]. In this thesis the explicit version of the solid shell element is implemented within the commercial software ABAQUS as a user written subroutine. The element in the explicit context was previously studied by Pagani et. al. [15] in which they reduced the computational effort by introducing an explicit update of the enhanced degree of freedom present in the element. The costly part for this method is the need to calculate an algorithmic tangent matrix. A further relaxation of the explicit update is proposed in this thesis in which no algorithmic tangent is needed. Reduced integration is also present in the element and hourglass stabilization is applied based on a number of Taylor expansions. In this process a complex tangent present in the hourglass stabilization part is replaced by an adaptive isotropic matrix. The work done in this thesis is showing that this approach is failing with the highly anisotropic paperboard model. A new anisotropic matrix specially tailored to this model is proposed and it is able to remove hourglass modes for the examples tried in this paper.
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8.1 Appendix A
Chapter 1

Introduction

Paperboard is one of the most frequently used materials for packaging food and beverages. The process of converting paperboard into a functional container includes a number of operations such as creasing to reduce resistance to bending and folding in which the material is subject to large bending. Being able to analyse converting processes of this kind using computer simulation as oppose to experiments can be very beneficial for design and optimization. A mathematical constitutive model for paperboard which showed promising results were developed by Borgqvist et. al. in [5]. This model has a high degree of complexity mainly because of the large degree of anisotropy in the in-plane and out-of-plane properties of paperboard. The model also includes plasticity with distorting hardening to accurately model the non-recoverable strains observed in the laboratory.

One of the most powerful methods to solve the equilibrium equations in solid mechanics for an arbitrary geometry is the finite element method. For many finite element simulations involving paperboard the thickness dimension in the geometry is much smaller than the characteristic length for the in-plane directions. This would suggest the use of special purpose shell elements. The paperboard model has previously been implemented in the commercial software Abaqus [7] as a user subroutine. But because of the complexity in the model, use of shell elements in Abaqus standard library did not work to a satisfactory degree.

The aim in this master thesis was to implement a promising shell element from the research community and try to combine it with the paperboard model in Abaqus. The element chosen was the solid shell element developed by Schwarze and Reese in [17] which showed promising results when compared with competing elements in the community. One promising feature of this element is that it belongs to the 'solid' branch of shell theory, this implies that no alteration in terms of degeneration of the constitutive model need to be addressed which is the case for classical shell elements.
Chapter 2

Solid Shell Element

2.1 Introduction to Solid Shell Elements

For a long time classical shell elements has been the element of choice when modelling thin structural problems undergoing dominate modes of bending. Elements belonging to this family is derived by imposing kinematic constraints. One outcome is that new rotational degrees of freedoms are introduced in the element. This allows the element to deform in a more complex manner and naturally this is a key ingredient when modelling structures subject to large bending. Classical shell elements usually also impose plane stress conditions and therefore continuum based 3D material models need to be modified to fit this framework. The theoretical body of work within classical shell elements is huge, largely because the subject is quite old and still vibrant within the research community to this date. An introduction to the theory of classical shells can be found in the series by Zienkiewicz at al at [20],[19] and a more extensive review of the subject is presented in [8].

This thesis is focusing on an element belonging to another branch of shell theory called solid shell theory or sometimes continuum shell theory. In contrast to the classical theory, solid shell elements contains only displacement degrees of freedoms. Combining this with the fully three dimensional nodal representation of the element implies that the implementation of a constitutive model is straight forward which is not the case for classical shell elements. In some sense solid shell elements are more like solid 3D continuum elements from a geometrical point of view. They are given the name shell elements because they are able to compete with classical shell elements when modelling shell like structures. Broadly speaking, classical shell elements are better at representing bending modes due to the rotational degrees of freedoms embedded in the formulation while solid shells are easier to use in combination with other continuum elements and consequently they can be more compatible in contact problems.

The solid shell element chosen to be implemented in this thesis is the explicit version of the 8-node hexahedron element developed by Schwarze and Reese in [17]. Transferring the element to the explicit finite element formulation was done by Pagani et. al in [15]. This element is quite new (2011) and it seems to be able to compete with classical shell elements even in problems subject to large modes of bending. The formulation for the solid shell is derived within the framework of finite deformation theory and the element is based on reduced integration together with the concepts of assumed natural strains (ANS), enhanced
assumed stains (EAS) and Taylor expansions in combination with hourglass stabilization. The following chapters is introducing the necessary background and thoroughly explains the element formulation and the concepts it is based on.

2.2 Basic Concepts in Continuum Mechanics

The solid shell element of interest is constructed within finite deformation theory using the Green Lagrangian strain tensor $E$ as the strain measurement. This section is describing the necessary background in continuum mechanics and the important principle of virtual work is introduced which is the basis for the finite element formulation. The presentation of this elementary theory is to a large extent inspired by [10].

The first task is to describe the new configuration of a body undergoing an arbitrary deformation with respect to a fixed Cartesian basis. Before deformation occurs the body is described by the initial configuration denoted $\beta_0$ and the material coordinates for a material particle referring to this configuration is defined as $X$. After deformation, current body is denoted $\beta_t$ with spatial coordinates $x$ referring to same material particle. The motion is then described by $\mathcal{X}$, and given as

$$x = \mathcal{X}(X, t) = X + U(t)$$

with $U$ being the displacement vector relating the two configurations throughout time, $t$. All vector quantities are given as components of a fixed Cartesian system denoted $(e_1, e_2, e_3)$ and the motion described by $\mathcal{X}$ is schematically illustrated in figure 2.1. Use of differenti-
strain and give zero strain contribution when rigid deformations occurs. A strain tensor fulfilling this criteria can be identified using the definition of the axial Green strain $\epsilon_G = \frac{ds^2 - ds_0^2}{2ds_0^2}$ with $ds$ and $ds_0$ being the length of the infinitesimal vectors in the deformed and undeformed configuration, respectively. Using the relation for the infinitesimal vectors (2.2) in the definition of the axial Green strain results in the following,

$$
\epsilon_G = \frac{ds^2 - ds_0^2}{2ds_0^2} = \frac{dx^T dx - dx_0^T dx_0}{2ds_0^2}
$$

$$
= \frac{1}{2s_0} \left( F^T F - I \right) dx_0
$$

$$
= \frac{1}{ds_0} E dx_0
$$

with $E$ being the Green Lagrangian strain tensor. It is possible to show that this tensor fulfills the necessary requirements to be used as a strain measurement, more details can be found in [10]. The Green Lagrangian strain tensor have the following form in matrix and index notation,

$$
E = E_{ij} e_i \otimes e_j = \frac{1}{2} \left( F^T F - I \right) = \frac{1}{2} \left( \frac{\partial U}{\partial X} + \frac{\partial U^T}{\partial X} + \frac{\partial U}{\partial X} \frac{\partial U}{\partial X} \right)
$$

$$
E_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} + \frac{\partial U_k}{\partial X_j} \frac{\partial U_k}{\partial X_i} \right)
$$

(2.3)

To be able to use the principle of virtual work it is necessary to establish an expression for the virtual components of the Green Lagrangian strain tensor denoted $\delta E$. This is obtained by taking the variation of (2.3),

$$
\delta E = \delta \left( \frac{1}{2} (F^T F - I) \right)
$$

$$
= \frac{1}{2} \left( \delta F^T F + F \delta F^T \right)
$$

$$
= \frac{1}{2} \left( \frac{\partial (\delta U^T)}{\partial X} F + F^T \frac{\partial (\delta U)}{\partial X} \right)
$$
When written in a direct format with a corresponding index notation the following expression is obtained,

\[
\delta E = \delta E_{ij} e_i \otimes e_j
\]

\[
\delta E_{ij} = \frac{1}{2} \left( \frac{\partial (\delta U_k)}{\partial X_j} \frac{\partial x_k}{\partial X_i} + \frac{\partial (\delta U_k)}{\partial X_i} \frac{\partial x_k}{\partial X_j} \right)
\]

(2.4)

It should be noted that the Green Lagrangian strain tensor \( E \) is symmetric according to (2.3) and therefore the same is also true for the virtual tensor \( \delta E \) given by expression (2.4). The next task is to establish the corresponding stress measure with the characteristics of being energy conjugate to the Green Lagrangian strain. This is done by the principle of virtual work which is also the basis for the finite element formulation. In the initial configuration \( \beta_0 \) the principle of virtual work states the following,

\[
g = g_{int} - g_{ext} = 0
\]

\[
g_{int} = \int_{\beta_0} S_{ij} \delta E_{ij} dV
\]

\[
g_{ext} = \int_{\beta_0} \delta U_i p_i dV + \int_{\partial \beta_0} \delta U_i t_i dS
\]

(2.5)

with \( g_{ext} \) being the external work achieved when applying the external forces to an arbitrary virtual displacement field \( \delta U_i \). There are two types of external forces present in the formulation. One is the traction force per unit area \( t_i \) applied at the boundary \( \partial \beta_0 \) of the initial configuration. The second one is the body force per unit volume present within the interior \( \beta_0 \) of the geometry. The internal force is denoted \( g_{int} \) and it is the result of combining the virtual Green Lagrangian strain \( \delta E_{ij} \), which is a function of an arbitrary virtual displacement field \( \delta U_i \), with the corresponding energy conjugate stress quantity \( S_{ij} \). The quantity \( S_{ij} \) is termed the second Piola Kirchhoff stress and the next goal is to identify the characteristics of this quantity. The Green Lagrangian strain is a symmetric tensor, this implies that the product \( S_{ij} \delta E_{ij} \) will only give contribution from the symmetric part of \( S_{ij} \). The second Piola Kirchhoff tensor can therefore also be introduced as a symmetric tensor. Rewriting the virtual work (2.5) by using expression (2.4) followed by splitting the volume integral using the theorem of Green Gauss and exploiting the arbitrary state of the virtual displacements the following is obtained,

\[
t_i = \left( \frac{\partial x_i}{\partial X_j} S_{jk} \right) n_k \quad \Rightarrow \quad t = t_i e_i = S_{jk} n_k \frac{\partial (x_i e_i)}{\partial X_j}
\]

with \( n_k \) being the Cartesian components of the normal vector to the surface \( \beta_0 \). The above relation indicates that the second Piola Kirchhoff stress has the physical property of representing the traction vector along the set of non-orthogonal deformed base vectors. This property has limited use in practice, the main reason for using the second Piola Kirchhoff stress is the symmetry of \( S_{ij} \) and the direct connection to the principle of virtual work.
2.3 Isoparametric Mapping and Interpolation

The principle of virtual work (2.5) is the basis for the finite element formulation. This is partly the case due to the additive nature of integrals and the main idea is to divide the body into smaller sub-domains which are simpler to analyse. The solution for the whole domain is then obtained by an assembling process for all sub-domains. A sub-domain in this context is called an element and the discretization, defining the geometry, into elements is denoted the mesh.

The element considered here is the isoparametric eight-node hexahedral element illustrated in figure 2.3 with the corresponding convention of how to order nodal points. Isoparametric elements make use of a mapping, here denoted $\Phi$, between an isoparametric domain represented by the points $\xi = (\xi_1, \xi_2, \xi_3)^T = (\xi, \eta, \zeta)^T$ and the real more complicated domain corresponding to the points $X = (X_1, X_2, X_3)^T$ for the material configuration and $x = (x_1, x_2, x_3)^T$ for the spatial configuration. The mapping between the isoparametric and the material configuration is also illustrated in figure 2.3. In order to get a convenient representation of the mapping $\Phi$ an approximation is made using tri-linear shape functions,

$$X_i = \sum_{I=1}^{8} N_I(\xi, \eta, \zeta) X_{i_I}, \quad i = 1, 2, 3$$

$$N_I = \frac{1}{8}(1 + \xi_I \xi)(1 + \eta_I \eta)(1 + \zeta_I \zeta)$$

with $(\bullet)_I$ referring to the value of the given quantity at nodal point $I$. Using the nodal convention established in figure 2.3 the following isoparametric coordinates are identified,

$$\begin{bmatrix} \xi_1 & \ldots & \xi_8 \\ \eta_1 & \ldots & \eta_8 \\ \zeta_1 & \ldots & \zeta_8 \end{bmatrix} = \begin{bmatrix} -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The shape functions $N_I$ has the desired property of being one at nodal point $I$ and zero at all other nodes. Using the above relation the mapping can be introduced in the following
compact form,
\[ \mathbf{X}(\xi) = \mathbf{X}_{\text{node}} \mathbf{N}(\xi) \]  \hspace{1cm} (2.6)
with \( \mathbf{X}_{\text{node}} \) being a matrix containing the coordinates for the material configuration at the nodal points,
\[ \mathbf{X}_{\text{node}} = [\mathbf{X}_{1e}, \mathbf{X}_{2e}, \mathbf{X}_{3e}]^T \quad , \quad \mathbf{X}_{ie} = [X_{i1}, ..., X_{i8}] \]
and \( \mathbf{N} \) being the shapefunctions \( N_i \) stored in a column vector according to,
\[ \mathbf{N}(\xi) = [N_1, ..., N_8]^T \]
\[ = \mathbf{r} + \xi \mathbf{g}_1 + \eta \mathbf{g}_2 + \zeta \mathbf{g}_3 + \xi \eta \mathbf{h}_1 + \xi \zeta \mathbf{h}_2 + \eta \zeta \mathbf{h}_3 + \xi \eta \zeta \mathbf{h}_4 \]  \hspace{1cm} (2.7)
It is straightforward to calculate the polynomial coefficients \( \mathbf{r}, \mathbf{g}_i, \mathbf{h}_i \) and for the sake of completeness they are tabulated in appendix A, expression (A1). The idea behind the isoparametric format is to use the same interpolation for the unknown displacements,
\[ \mathbf{U}(\xi) = \mathbf{U}_{\text{node}} \mathbf{N}(\xi) \]  \hspace{1cm} (2.8)
with \( \mathbf{U}_{\text{node}} \) containing values for displacement at the nodal points,
\[ \mathbf{U}_{\text{node}} = [U_{1e}, U_{2e}, U_{3e}]^T \quad , \quad \mathbf{U}_{ie} = [U_{i1}, ..., U_{i8}] \]
In order to establish the principle of virtual work the corresponding virtual displacements needs to be constructed. This is done by using the approach of Galerkin which implies using the same interpolation when approximating the virtual quantity,
\[ \delta \mathbf{U}(\xi) = \delta \mathbf{U}_{\text{node}} \mathbf{N}(\xi) \]  \hspace{1cm} (2.9)
with \( \delta \mathbf{U}_{\text{node}} \) containing the nodal values for the virtual displacements. For the solid shell element used in this thesis it turns out to be convenient to describe strain quantities with a certain non-orthogonal set of base vectors. In order to identify this favourable set it is necessary to establish a relation between infinitesimal vectors in the isoparametric domain and the real domain. One such relation is achieved by differentiating the map \( \Phi \) with respect to the natural coordinates \( \xi \). When the real domain is given by the material coordinates \( \mathbf{X} \) this differentiation results in,
\[ d\mathbf{X} = \frac{\partial \mathbf{X}}{\partial \xi} d\xi \]
\[ \mathbf{J} = \frac{\partial \mathbf{X}}{\partial \xi} = [\mathbf{J}_1, \mathbf{J}_2, \mathbf{J}_3] = \left[ \frac{\partial \mathbf{X}}{\partial \xi}, \frac{\partial \mathbf{X}}{\partial \eta}, \frac{\partial \mathbf{X}}{\partial \zeta} \right] \]  \hspace{1cm} (2.10)
\[ \mathbf{J}_i = \mathbf{J}_{ij} \mathbf{e}_j \quad , \quad \mathbf{J}_{ij} = \frac{\partial X_j}{\partial \xi_i} \]
with \( \mathbf{J} \) being the Jacobian matrix with the property of transforming vectors from the isoparametric configuration to the material configuration. A similar relation is achieved when the real domain is given by the spatial configuration \( \mathbf{x} \), for later use it is tabulated here as the following,
\[ dx = \frac{\partial \mathbf{x}}{\partial \xi} d\xi \]
\[ \tilde{\mathbf{J}} = \frac{\partial \mathbf{x}}{\partial \xi} = [\tilde{\mathbf{J}}_1, \tilde{\mathbf{J}}_2, \tilde{\mathbf{J}}_3] = \left[ \frac{\partial \mathbf{x}}{\partial \xi}, \frac{\partial \mathbf{x}}{\partial \eta}, \frac{\partial \mathbf{x}}{\partial \zeta} \right] \]  \hspace{1cm} (2.11)
\[ \tilde{\mathbf{J}}_i = \tilde{\mathbf{J}}_{ij} \mathbf{e}_j \quad , \quad \tilde{\mathbf{J}}_{ij} = \frac{\partial x_j}{\partial \xi_i} \]
with $\mathbf{J}$ being the Jacobian of the current configuration. Given a point in the isoparametric domain $\xi = \xi^*$ the columns of the Jacobian matrix with respect to this point $\mathbf{J}(\xi^*)$ represent a covariant non-orthogonal set of base vectors, this is schematically illustrated for the a two-dimensional case in figure 2.4. The set of base vectors which turn out to be advantageous to work with is the set of contravariant non-orthogonal base vectors $\mathbf{H}_i$ with the property of begin orthogonal to the covariant set $\mathbf{J}_i$, this property is schematically illustrated for a two dimensional case in figure 2.5. Vectors $\mathbf{H}_i$ with this property turn out to be components of the inverse Jacobian according to,

$$\mathbf{H}_i = j_{ij} \mathbf{e}_j, \quad j_{ij} = \frac{\partial \xi_i}{\partial X_j} \quad (2.12)$$

which can be proven using expression (2.10) and (2.12) with the definition of orthogonality,

$$\mathbf{J}_i \cdot \mathbf{H}_j = \frac{\partial X_k}{\partial \xi_i} \mathbf{e}_k \cdot \frac{\partial \xi_j}{\partial X_n} \mathbf{e}_n = \frac{\partial \xi_i}{\partial X_j} \frac{\partial X_k}{\partial X_n} \mathbf{e}_k \cdot \mathbf{e}_n = \delta_{ij} \delta_{kn} \mathbf{e}_k \cdot \mathbf{e}_n = \delta_{ij}$$

The set of base vectors $\mathbf{H}_i$ in (2.12) has the property of representing the set of isoparametric base vectors in the real domain. This is very convenient when doing modifications to the Green Lagrangian strain. If $\mathbf{E}$ is represented by the base vectors $\mathbf{H}_i$ such modifications can be formulated using simple coordinates from the isoparametric domain $(\xi, \eta, \zeta)$ and then $\mathbf{E}$ can be transformed back to the Cartesian system. Representation of the Green Lagrangian strain for the two different configurations can be written as,

$$\mathbf{E} = E_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = \bar{E}_{ij} \mathbf{H}_i \otimes \mathbf{H}_j \quad (2.13)$$
with \( E_{ij} \) being components in the Cartesian system and \( \bar{E}_{ij} \) components to the non-orthogonal system. The components of the non-orthogonal system \( \bar{E}_{ij} \) is the coordinates expressed with the isoparametric set of base vectors, therefore the following convention is adopted,

\[
\bar{E}_{ij} = \bar{E}_{\xi_i \xi_j} \quad \text{with} \quad \xi_1 = \xi, \quad \xi_2 = \eta \quad \text{and} \quad \xi_3 = \zeta
\]

In order to conveniently deal with products between the Green Lagrangian strain and the second Piola Kirchhoff stress, Voigt matrix format is introduced as the following,

\[
\hat{E} = \begin{bmatrix} E_{11} & E_{22} & E_{33} & 2E_{12} & 2E_{23} & 2E_{13} \end{bmatrix}^T
\]

\[
\delta\hat{E} = \begin{bmatrix} \delta E_{11} & \delta E_{22} & \delta E_{33} & 2\delta E_{12} & 2\delta E_{23} & 2\delta E_{13} \end{bmatrix}^T
\] \quad (2.14)

for the strain tensors. The hat notation (\( \hat{\bullet} \)) is adopted to indicate Voigt matrix format. The corresponding Voigt matrix format for the stress tensor is defined as,

\[
\hat{S} = \begin{bmatrix} S_{11} & S_{22} & S_{33} & S_{12} & S_{23} & S_{13} \end{bmatrix}^T
\] \quad (2.15)

With this convention the internal work \( g_{int} \) in principle of virtual work (2.5) can be expressed as,

\[
g_{int} = \int_{\gamma_0} \hat{S}^T \delta\hat{E} \, dV
\]

Later on the strain quantities in (2.14) will be described by the non-orthogonal set \( H_i \). It is therefore necessary to find a relation between this set and the orthogonal Cartesian system. This is done by identifying the \( 6 \times 6 \) transformation matrix \( T \) in the following expression,

\[
\hat{E} = T \hat{\bar{E}}
\] \quad (2.16)

with \( \hat{E} \) being the components of the non-orthogonal set in Voigt matrix format. The transformation matrix is derived by first using the definition of \( H_i \) from (2.12) in expression (2.13),

\[
E_{ij} \, e_i \otimes e_j = \bar{E}_{ij} \, H_i \otimes H_j = j_{ik} \, j_{jn} \, \bar{E}_{ij} \, e_k \otimes e_n
\]

and then expanding the sum followed by matching the dyad products. For instance multiplying with \( e_1 \) from left and right provides,

\[
E_{11} = j_{11}^2 \bar{E}_{11} + j_{21}^2 \bar{E}_{22} + j_{31}^2 \bar{E}_{33} + 2 j_{11} j_{21} \bar{E}_{12} + 2 j_{21} j_{31} \bar{E}_{23} + 2 j_{11} j_{31} \bar{E}_{13}
\]

Using this procedure to compare all dyad products in the above relation results in the following transformation matrix,

\[
T = \begin{bmatrix}
j_{11}^2 & j_{21}^2 & j_{31}^2 & j_{11} j_{21} & j_{21} j_{31} & j_{11} j_{31} \\
j_{12}^2 & j_{22}^2 & j_{32}^2 & j_{12} j_{22} & j_{22} j_{32} & j_{12} j_{32} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
2 j_{11} j_{21} & 2 j_{21} j_{12} & 2 j_{31} j_{32} & j_{11} j_{21} + j_{11} j_{22} & j_{22} j_{31} + j_{21} j_{32} & j_{11} j_{31} + j_{11} j_{32} \\
2 j_{12} j_{13} & 2 j_{22} j_{23} & 2 j_{32} j_{33} & j_{13} j_{22} + j_{12} j_{23} & j_{23} j_{32} + j_{22} j_{33} & j_{13} j_{32} + j_{12} j_{33} \\
2 j_{11} j_{13} & 2 j_{21} j_{23} & 2 j_{31} j_{33} & j_{13} j_{21} + j_{11} j_{23} & j_{23} j_{31} + j_{21} j_{33} & j_{13} j_{31} + j_{11} j_{33}
\end{bmatrix}
\] \quad (2.17)

The transformation in (2.16) is illustrated using the Green Lagrangian strain tensor \( E \) but the exact same relation is achieved for the corresponding virtual strains \( \delta E \).
2.4 Kinematics in Isoparametric Framework

The goal of this section is to identify the contravariant components of the basis \( H_i \) for the Green Lagrangian stain and its corresponding virtual quantity. When \( \bar{E}_{ij} \) and \( \delta \bar{E}_{ij} \) are established, use of (2.14) to transfer the quantity's to Voigt matrix format can be utilized due to the symmetry of the tensors. Finally the transformation (2.16) will give the components corresponding to the Cartesian system. When investigating the quantity \( \delta \bar{E}_{ij} \) it will also be necessary to identify the corresponding \( \bar{B}_{ij} \) matrix with the property of separating the dependence upon the virtual displacement, this is crucial in the last steps of deriving the numerical scheme when the virtual components need to be removed from the formulation.

When transferring the Green Lagrangian quantities in (2.3) and (2.4) to an isoparametric framework it is convenient to define the following quantity,

\[
D_{ij} = \frac{\partial U_i}{\partial \xi_j} , \quad D = [D_1, D_2, D_3] , \quad D_j = D_{ij} e_i = \frac{\partial U}{\partial \xi_j} \quad (2.18)
\]

The first goal is to identify the Green Lagrangian strain components in the contravariant basis \( H_i \) given in (2.12). Using the chain rule of the last term in (2.3) results in the following,

\[
\frac{\partial U_n}{\partial X_i} \frac{\partial U_n}{\partial X_j} = \frac{\partial U_n}{\partial \xi_k} \frac{\partial U_n}{\partial \xi_m} = D_{nk} D_{nm} \delta_{ki} \delta_{mj}
\]

where notations from (2.10),(2.12) and (2.18) has been utilized. Using the above result in (2.3) leads to,

\[
E = E_{ij} e_i \otimes e_j = \frac{1}{2} \left( \frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} + \frac{\partial U_n}{\partial X_i} \frac{\partial U_n}{\partial X_j} \right) e_i \otimes e_j
\]

\[
= \frac{1}{2} \left( J_{nk} D_{nm} + J_{nm} D_{nk} + D_{nk} D_{nm} \right) j_{ki} j_{mj} e_j
\]

\[
= \frac{1}{2} \left( J_{k}^{T} D_{m} + J_{m}^{T} D_{k} + D_{k}^{T} D_{m} \right) H_{k} \otimes H_{m}
\]

where use have been made of (2.10),(2.18) and the transformation of Cartesian base vectors according to (2.12). The above expression is used to identify the contravariant components of the Green Lagrangian strain tensor,

\[
\bar{E}_{ij} = \frac{1}{2} \left( J_{i}^{T} D_{j} + J_{j}^{T} D_{i} + D_{i}^{T} D_{j} \right) \quad (2.19)
\]

The next task is to do the same for the virtual Green Lagrangian strains and also identify the corresponding \( \bar{B}_{ij} \) matrix which separates the dependence on the virtual displacements. In order to achieve this some modifications of the corresponding virtual quantity in (2.18) need to be addressed,

\[
\delta D_{ij} = \frac{\partial (\delta U_i)}{\partial \xi_j} , \quad \delta D_j = \delta D_{ij} e_i = \frac{\partial (\delta U)}{\partial \xi_j} \quad (2.20)
\]
This is done by using the interpolation in (2.9) and rearranging the matrix multiplication in the following manner,

\[
\delta U = \begin{bmatrix}
N_1 & 0 & 0 & \ldots & N_I & 0 & 0 & \ldots & N_8 & 0 & 0 \\
0 & N_1 & 0 & \ldots & 0 & N_I & 0 & \ldots & 0 & N_8 & 0 \\
0 & 0 & N_1 & \ldots & 0 & 0 & N_I & \ldots & 0 & 0 & N_8 \\
\end{bmatrix}
\]

Using this format in the above expression for \( \delta D \) results in,

\[
\delta D = L_i \delta U_e
\]

(2.21)

where the following notations have been introduced,

\[
\delta U_e = \begin{bmatrix}
\delta U_{11} & \delta U_{21} & \delta U_{31} & \ldots & \delta U_{1I} & \delta U_{2I} & \delta U_{3I} & \ldots & \delta U_{18} & \delta U_{28} & \delta U_{38}
\end{bmatrix}^T
\]

(2.22)

here \( I \) is the 3 × 3 identity matrix. Finally the virtual Green Lagrangian strain can be transferred into the contravariant basis and the corresponding contravariant \( \bar{B}_{ij} \) matrix can be identified,

\[
\delta E_{ij} e_i \otimes e_j = \{(2.4)\} = \frac{1}{2} \left( \frac{\partial (\delta U_k)}{\partial X_j} \frac{\partial x_k}{\partial X_i} + \frac{\partial (\delta U_k)}{\partial X_i} \frac{\partial x_k}{\partial X_j} \right) e_i \otimes e_j
\]

(2.12),(2.11),(2.20)

\[
= \left( \tilde{J}_m^T \delta D_n + \tilde{J}_n^T \delta D_m \right) H_m \otimes H_n
\]

(2.21)

\[
= \{(2.21)\} = \left( \left( \tilde{J}_m^T L_n + \tilde{J}_n^T L_m \right) \delta U_e \right) H_m \otimes H_n
\]

Using the above expression the following is identified,

\[
\delta \tilde{E}_{ij} = \bar{B}_{ij} \delta U_e , \quad \bar{B}_{ij} = \left( \tilde{J}_i^T L_j + \tilde{J}_j^T L_i \right)
\]

(2.23)

2.5 Assumed Natural Strain Concept

In order for the solid shell element to perform well for shell-like structures, a Taylor approximation of the second Piola Kirchhoff stress along the out-of-plane direction is performed in combination with reduced integration for the in-plane direction. When this expansion is done it turns out to be advantageous to also do a Taylor expansion of the Green Lagrangian strain around the center of the element. To prepare for this procedure the Green Lagrangian...
strain tensor is enhanced by the assumed natural strain concept (ANS), which will be explained in this section.

The assumed natural strain concept (ANS) is initially introduced to cure traversal shear locking and curvature thickness locking. Later on the enhanced assumed strain method (EAS) will be included to the element formation. The combination of the ANS and EAS concept will also cure both Poissons thickness locking and volumetric locking.

Shear locking is a phenomena present for thin structures undergoing pure bending. The state of deformation after pure bending around the \( \eta \)-axis using a single eight node isoparametric element with linear shapefunctions is illustrated in figure 2.6. If the structure is thin the real solution to this problem reveals that the shear term \( \bar{E}_{13} \) will approach zero. This is not the case for the isotropic element in which the shear term is only zero in the mid-plane \( \xi = 0 \). The non-zero shear \( \bar{E}_{13} \) is called a parasitic term and it can potentially carry the whole bending load thereby locking the element from deforming in an analytically correct manner. A more in depth discussion about shear locking in the context of isoparametric elements can be found in [12].

![Image](image.png)

**Figure 2.6:** State of deformation for the isoparametric element after pure bending around the \( \eta \)-axis

The idea behind the ANS concept is to directly modify the parasitic strain terms and this is done by interpolation between some sampling points in the element. For the bending situation in figure 2.6 it can be shown that \( \bar{E}_{13} \) is zero for the element in the midplane \( \xi = 0 \). This term is therefore modified using the sampling points \( J, K, L \) and \( M \) corresponding to the plane \( \xi = 0 \) in figure 2.7 and the new strain term reads,

\[
\tilde{E}_{13}^{\text{ANS}} = \tilde{N}_J \tilde{E}_{13}^J + \tilde{N}_K \tilde{E}_{13}^K + \tilde{N}_L \tilde{E}_{13}^L + \tilde{N}_M \tilde{E}_{13}^M = \sum_{K=J}^M \tilde{N}_K \tilde{E}_{13}^K
\]  

(2.24)

with the upper case letter referring to the evaluation of the strain at the given sampling point, this is done by using expression (2.19). The interpolation in the mid plane \( \xi = 0 \) is established by using the following bilinear shapefunctions,

\[
\tilde{N}_K = \frac{1}{4} (1 + \eta_K \eta) (1 + \zeta_K \zeta) \quad \text{for } K = J, ..., M
\]

(2.25)

\[
\begin{bmatrix}
\eta_K \\
\zeta_K
\end{bmatrix} = \begin{bmatrix}
-1 & 1 & 1 & -1 \\
-1 & -1 & 1 & 1
\end{bmatrix}
\]
Because of the in-plane symmetry for the element there exist a similar parasitic shear term given by $\bar{E}_{23}$. In a completely analogous manner this term is interpolated as,

$$E^{\text{ANS}}_{23} = \bar{N}_E \bar{E}^A_{23} + \bar{N}_F \bar{E}^B_{23} + \bar{N}_G \bar{E}^C_{23} + \bar{N}_H \bar{E}^D_{23} = \sum_{K=E}^{H} \bar{N}_K \bar{E}^K_{23}$$ (2.26)

with E, F, G and H being the sampling points corresponding to the plane $\eta = 0$ in figure 2.7. Furthermore the bilinear shapefunctions for this term reads,

$$\bar{N}_K = \frac{1}{4}(1 + \xi_K \xi)(1 + \zeta_K \zeta) \quad \text{for} \quad K = E, \ldots, H$$ (2.27)

Curvature thickness locking is a phenomena which can occur for the element when the initial configuration is strongly curved. When an isoparametric element with such initial configuration is deformed using pure bending, the thickness stretch $\bar{E}_{33}$ is only zero in the outer points of the midplane. This scenario is schematically illustrated in figure 2.8 using a two dimensional setting. The analytical solution is that no such out-of-plane stretch $\bar{E}_{33}$ should exist, this artificial strain can therefore carry the load during deformation and potentially lock the element from correct deformation. A more detailed discussion regarding curvature thickness locking is found in [3].
Figure 2.8: Bending situation for initially curved isoparametric element in two dimensional setting. Only the outer points $B$ and $A$ has zero out-of-plane stretch $\bar{E}_{33}$ after deformation.

To cure curvature thickness locking the parasitic term $E_{33}$ is modified using the ANS concept with sampling points for which curvature locking do not occur. This is true for the points $A$, $B$, $C$ and $D$ corresponding to the plane $\zeta = 0$ in figure 2.7 and the new $E_{33}$ term reads,

$$E_{33}^{ANS} = \bar{N}_A \bar{E}_{33}^A + \bar{N}_B \bar{E}_{33}^B + \bar{N}_C \bar{E}_{33}^C + \bar{N}_D \bar{E}_{33}^D = \sum_{K=A}^{D} \bar{N}_K \bar{E}_{33}^K$$  \hspace{1cm} (2.28)

with $\bar{N}_K$ being the shapefunction evaluated in the midplane $\zeta = 0$,

$$\bar{N}_K = \frac{1}{4}(1 + \xi_K \xi)(1 + \eta_K \eta) \quad \text{for} \quad K = A, \ldots, D$$  \hspace{1cm} (2.29)

In [17] and [16] they mention that many ANS formulations only uses linear interpolation between two sampling points instead of bilinear interpolation between four. The authors argue that using this approach is better for the stability of the element when reduced integration is present. Using the ANS concept on the Green Lagrangian strain components $E_{33}$, $E_{13}$ and $E_{23}$ concentrically leads to the corresponding modification of the virtual components $\delta E_{33}$, $\delta E_{13}$ and $\delta E_{23}$, they are therefore interpolated in exactly the same fashion.

### 2.6 Transformation Matrix in Polynomial Form

The transformation matrix $T$ in (2.17) which transforms components from the contravariant basis to the Cartesian is a matrix containing products of components from the inverse Jacobian in (2.12). As mentioned in the previous section, the Green Lagrangian strain and its corresponding virtual component will be approximated using a Taylor expansion around the center of the element, therefore it is advantageous to establish a polynomial expression for $T$ with enough polynomial components to represent the transformation with sufficient accuracy. In order to achieve this it is essential to derive a polynomial expression for the inverse Jacobian with enough accuracy.

Using the nodal approximation in (2.6) together with the shape functions derived in (2.7) it is possible to rewrite the Jacobian matrix (2.10) in polynomial form. Calculating the derivatives of the shapefunctions result in a polynomial structure given by,

$$J = J^0 + \xi J^\xi + \eta J^\eta + \zeta J^\zeta + \xi \eta J^{\xi\eta} + \eta \zeta J^{\eta\zeta} + \xi \zeta J^{\xi\zeta}$$  \hspace{1cm} (2.30)
with $J^{\xi}$ and $J^{\xi, \xi_i}$ being constant matrix coefficients. For the sake of completeness these matrix coefficients are tabulated in appendix A, expression (A2) and (A3). For later derivations it is convenient to introduce notations for the columns of the Jacobian $J$ in the following manner,

$$J = [J_1, J_2, J_3]$$

$$\begin{align*}
J_1 &= J^0_1 + \eta J^\eta_1 + \zeta J^\zeta_1 \\
J_2 &= J^0_2 + \xi J^\xi_2 + \zeta J^\zeta_2 \\
J_3 &= J^0_3 + \xi J^\xi_3 + \eta J^\eta_3 + \xi \eta J^{\eta \xi}_3
\end{align*}$$

(2.31)

and it is a trivial polynomial task to extract these columns from the full expression in (2.30). The exact same polynomial format can be constructed for the quantity $D$ in (2.18) using the interpolation of the displacements in (2.8) and the shape functions in (2.7),

$$D = D^0 + \xi D^{\xi} + \eta D^{\eta} + \zeta D^{\zeta} + \xi \eta D^{\eta \xi} + \xi \zeta D^{\xi \zeta}$$

(2.32)

with the resulting matrix coefficients being tabulated in appendix A, expression (A4) and (A5). It is also useful to introduce the notation $D_1$, $D_2$ and $D_3$ for the columns of the $D$ matrix in the same fashion as with the Jacobian matrix. The Jacobian of the current configuration $\tilde{J}$ is given as the sum of the Jacobian $J$ and the $D$ matrix. This results in the following polynomial format,

$$\tilde{J} = \tilde{J}^0 + \xi \tilde{J}^{\xi} + \eta \tilde{J}^{\eta} + \zeta \tilde{J}^{\zeta} + \xi \eta \tilde{J}^{\eta \xi} + \xi \zeta \tilde{J}^{\xi \zeta}$$

(2.33)

By using the relation $\tilde{J} = J + D$ it is a trivial task to derive the matrix coefficients and they are therefore not included here. Furthermore the current Jacobian is split into columns $\tilde{J} = [\tilde{J}_1, \tilde{J}_2, \tilde{J}_3]$ in a completely analogous manner as with $J$ and $D$.

To obtain the desired polynomial form of the inverse Jacobian a linear Taylor expansion is performed with respect to the center of the element,

$$J^{-1} \approx (J^{-1})_{\xi=0} + \sum_{i=1}^3 (J^{-1})_{\xi_i=0} \cdot \xi_i$$

(2.34)

in this expression the convention $(\xi_1, \xi_2, \xi_3) = (\xi, \eta, \zeta)$ is adopted. There is a convenient way to represent the term $(J^{-1})_{\xi_i=0}$ by use of the Taylor expansion,

$$J \cdot J^{-1} \approx (J J^{-1})_{\xi=0} + \sum_{i=1}^3 ((J J^{-1})_{\xi_i})_{\xi=0} \cdot \xi_i$$

Taking the partial derivative of this expansion and exploiting the identity statement $J \cdot J^{-1} = I$ results in,

$$(I)_{\xi_i} = 0 \approx (J_{\xi_i})_{\xi=0} \cdot (J^{-1})_{\xi=0} + (J)_{\xi=0} \cdot (J^{-1})_{\xi=0}$$

from this expression the sought out term reads,

$$(J^{-1})_{\xi=0} = - (J^0)^{-1} \cdot J_{\xi_i} \cdot (J^0)^{-1}$$

were use was made of the relations,

$$(J_{\xi_i})_{\xi=0} = J_{\xi_i}, \quad (J^{-1})_{\xi=0} = (J^0)^{-1} \quad \text{and} \quad (J)_{\xi=0} = J^0$$
resulting from the polynomial form of the Jacobian in (2.30). The final polynomial expression for the inverse Jacobian in (2.34) is now given by,
\[
J^{-1} \approx (J^{-1})^0 + (J^{-1})^\xi \xi + (J^{-1})^\eta \eta + (J^{-1})^\zeta \zeta \tag{2.35}
\]
with \((J^{-1})^0 = (J^0)^{-1}\) and \((J^{-1})^\xi = -(J^0)^{-1} J^\xi (J^0)^{-1}\).

This expression is convenient because the inverse Jacobian need to only be calculated at the center of the element. The transformation matrix \(T\) given by (2.17) is containing products between components \(j_{ij}\) of the inverse Jacobian matrix. A component of the inverse Jacobian can also be expressed in polynomial form using (2.35),
\[
j_{ij} = (j_{ij})^0 + (j_{ij})^\xi \xi + (j_{ij})^\eta \eta + (j_{ij})^\zeta \zeta \tag{2.36}
\]
Calculating the product between two components of the inverse Jacobian results in,
\[
j_{ij} j_{kl} = (j_{ij})^0 (j_{kl})^0 + \sum_{n=1}^3 (j_{ij})^0 (j_{kl})^\xi_n + (j_{ij})^\xi_n (j_{kl})^0 \xi_n + \sum_{m=1}^3 \sum_{n=1}^3 O(\xi_n \xi_m)
\]
with \(O\) representing higher order quadratic terms. In [16] the authors show that it is enough to consider linear terms to pass the patch test, the expression then reads,
\[
j_{ij} j_{kl} \approx (j_{ij})^0 (j_{kl})^0 + \sum_{n=1}^3 (j_{ij})^0 (j_{kl})^\xi_n + (j_{ij})^\xi_n (j_{kl})^0 \xi_n \tag{2.37}
\]
Using relation (2.37) in expression (2.17) a linear polynomial structure is obtained,
\[
T = T^0 + T^\xi \xi + T^\eta \eta + T^\zeta \zeta \tag{2.38}
\]
with \(T^\xi\) and \(T^0\) being constant matrix coefficients, they are tabulated in appendix A, expressions (A6)-(A9) for the sake of completeness.

### 2.7 Taylor Expansion of Second Piola Kirchhoff Stress

The element contribution to the internal work \(g_{int}\) from the principle of virtual work (2.5) require an integration over the element volume \(\beta_e\) in material configuration. Transforming the integrals to isoparametric coordinates is then convenient because they are aligned with the element configuration. For a fully integrated element, gauss integration is performed with respect to the isoparametric configuration and the points of integration corresponds to both the in-plane and out-of-plane direction. An example of a reduced isoparametric element is the one point quadratial element with only one integration point at the center of the element. Elements based on reduced integration are obviously faster then fully integrated elements but apart from this they can sometimes also perform better. This is due to the fact that a finite element problem is a stiff approximation resulting from the constrain introduced by the discretization. Reduced integration counteract this effect by softening the elements [13]. The problem with elements based on reduced integration is that spurious zero energy modes can occur corresponding to modes of deformation which are not rigid body modes. Modes of this kind are called hourglass modes and for the quadratial one point element there exist twelve such hourglass modes [2] and four of them corresponding to the
Figure 2.9: Illustration of hourglass modes in $\xi$-direction

$\xi$-direction are illustrated in figure 2.9. The existence of hourglass modes can be observed by analysing the stiffness matrix. It turns out that elements with reduced integration has a stiffness matrix with a nullspace of both rigid body modes and hourglass modes. In order to remove the hourglass modes it is therefore necessary to apply a method in such a way that the kernal for the stiffness matrix only contains the proper nullspace corresponding to rigid body modes. It is also common to use the terminology of full rank when referring to the proper stiffness matrix and an hourglass control method introduces stabilization terms in such a way that the rank remains full.

The shell element of interest in this thesis aims to only perform gauss integration in the out-of-plane direction $\xi^* = (0, 0, \zeta)^T$, referring to figure 2.10 with the number of gauss points being able to vary in order to correctly model a shell like structure using only one element in the thickness direction. The authors in [17] construct hourglass stabilization terms in such a way that they can be integrated analytically which implies no dependence on the material behaviour at the gauss points. In order to achieve this a Taylor expansion with respect to the out-of-plane direction is performed for the second Piola Kirchhoff stress $\hat{S}$ and an expansion around the center is computed for the Green Lagrange strain $\hat{E}$, both in Voigt notation. Furthermore it is convenient to split these quantity's into the following

Figure 2.10: Integration points in the out-of-plane direction $\zeta^*$
format,

\[(\bullet) = (\bullet)^* + (\bullet)^{hg}\]  \hspace{1cm} (2.39)

in which \((\bullet)^*\) is containing all terms with dependence on only the out-of-plane coordinate \(\zeta\). This term is the important one for both \(\hat{E}\) and \(\hat{S}\) because the numerical integration will be performed with respect to \(\zeta\) and the constitutive law will therefore only enter terms related to these quantity's. The remaining terms from both Taylor expansions are stored in the \((\bullet)^{hg}\) part and the purpose is to model them in an efficient way to prevent hourglass modes (not destroying full rank) while not providing an impact on the physical solution.

Starting with a Taylor expansion of the Green Lagrangian Strain around the center of the element result in,

\[
\hat{E} = \hat{E}^0 + \zeta \hat{E}^\zeta + \zeta^2 \hat{E}^{\zeta\zeta} + \xi \hat{E}^\xi + \eta \hat{E}^\eta + \eta \zeta \hat{E}^{\eta\zeta} + \zeta \xi \hat{E}^{\xi\zeta}
\]  \hspace{1cm} (2.40)

in this expression the following convention is adopted,

\[(\bullet)^{\xi_i} = \frac{\partial (\bullet)}{\partial \xi_i} \hspace{1cm} \text{and} \hspace{1cm} (\bullet)^{\xi_i\xi_i} = \frac{\partial^2 (\bullet)}{\partial \xi_i^2}\]  \hspace{1cm} (2.41)

The expansion in (2.40) includes linear and bilinear terms within the shell plane and one quadratic term \(\zeta^2\) for the thickness direction, this term is included to accurately capture the behaviour of thick shells. A numerical study strengthening this assumption is done in [17]. Using the explicit formula for \(\bar{E}_{ij}\) in (2.19) with the ANS concept in (2.28), (2.24) and (2.26), the final Voigt format \(\hat{E}\) is established using (2.14). Transforming this expression to the Cartesian base vectors \(\hat{E}\) is done by applying the polynomial form of the transformation matrix \(T\) in (2.38). The polynomial coefficients for the Taylor expansion in (2.40) is then calculated using the expression for \(\hat{E}\) and computing the derivatives according to the convention in (2.41), the coefficients are tabulated in appendix (A10)-(A17). Transferring the polynomial expression (2.40) into the format explained in (2.39) result in the following,

\[
\hat{E} = \hat{E}^* + \hat{E}^{hg}
\]  \hspace{1cm} (2.42)

in which the out-of-plane and hourglass term reads,

\[
\hat{E}^* = \hat{E}^0 + \zeta \hat{E}^\zeta + \zeta^2 \hat{E}^{\zeta\zeta}
\]

\[
\hat{E}^{hg} = \xi \hat{E}^\xi + \eta \hat{E}^\eta + \eta \zeta \hat{E}^{\eta\zeta} + \zeta \xi \hat{E}^{\xi\zeta}
\]  \hspace{1cm} (2.43)

The exact same Taylor expansion and split is adopted to the corresponding virtual quantity \(\delta \hat{E}\), using the \(B\) matrix to separate the virtual displacements the following format is achieved,

\[
\delta \hat{E} = \delta \hat{E}^* + \delta \hat{E}^{hg} = \left( B^* + B^{hg} \right) \delta U_e
\]  \hspace{1cm} (2.44)

with the polynomial form of the \(B\) matrix being split into,

\[
B^* = B^0 + \zeta B^\zeta + \zeta^2 B^{\zeta\zeta}
\]

\[
B^{hg} = \xi B^\xi + \eta B^\eta + \eta \zeta B^{\eta\zeta} + \zeta \xi B^{\xi\zeta}
\]  \hspace{1cm} (2.45)

The polynomial coefficients for the \(B\) matrix can be calculated by first constructing the Voigt format (2.14) for the corresponding non-orthogonal components given by (2.23), this is achieved utilizing the expressions (2.22) and (2.33) in conjunction with the shapefunctions
in (2.7). Then the ANS concept, explained in previous section, is applied to components of the B-matrix corresponding to the quantity’s $\delta \bar{E}_{33}$, $\delta \bar{E}_{23}$ and $\delta \bar{E}_{13}$. When the Voigt format for the non-orthogonal components are constructed the corresponding Cartesian format is achieved by applying the polynomial form of the transformation matrix $T$ in (2.38). Finally the polynomial coefficients of the B-matrix in (2.45) are derived by computing the derivatives in accordance with (2.41), the resulting expressions are tabulated in appendix (A18)-(A26).

For the second Piola Kirchhoff stress $\hat{S}$ a Taylor expansion around the out-of-plane direction $\xi^* = (0, 0, \zeta)^T$ is performed in the following manner,

$$\hat{S} \approx \hat{S}\bigg|_{\xi^*} + \frac{\partial \hat{S}}{\partial \hat{E}} \frac{\partial \hat{E}}{\partial \xi} \bigg|_{\xi^*} \xi + \frac{\partial \hat{S}}{\partial \hat{E}} \frac{\partial \hat{E}}{\partial \eta} \bigg|_{\xi^*} \eta \quad (2.46)$$

The term $\hat{S}\bigg|_{\xi^*}$ already has the desired structure to match the out-of-plane term $\hat{S}^*$ in (2.39) while the remaining terms in (2.46) need to be modified to match the structure of the hourglass part $\hat{S}^{hg}$. Applying the polynomial expression for the Green Lagrangian strain in (2.40) the following expression is identified at the present state,

$$\hat{S}^* = \hat{S}\bigg|_{\xi^*}, \quad \hat{S}^{hg} = \left. \frac{\partial \hat{S}}{\partial \hat{E}} \right|_{\xi^*} \left( E^\xi \xi + E^\eta \eta + E^\zeta \zeta + E^{\eta \zeta} \eta \zeta \right) \quad (2.47)$$

The problem with the hourglass term is the tangent $\left. \frac{\partial \hat{S}}{\partial \hat{E}} \right|_{\xi^*}$ which is both material and deformation dependent, in order to get an efficient element modifications this quantity need to be addressed which is done in the next chapter.

Volumetric locking is cured for the out-of-plane terms by applying the ANS concept in combination with the enhanced assumed strain method (EAS) which will be discussed in later sections. This type of locking is still present for the hourglass terms and in order to cure this behaviour the B-Bar method [16] is applied to the hourglass terms which implies working with the deviatoric part,

$$\hat{S}^{hg} := \hat{S}^{hg\text{dev}}, \quad B^{hg} := B^{hg\text{dev}}, \quad \hat{E}^{hg} := \hat{E}^{hg\text{dev}} \quad (2.48)$$

The product between two matrices in which one has deviatoric character results in a deviatoric quantity. Therefore to achieve the corresponding deviatoric quantity to $\hat{E}^{hg}$ and $B^{hg}$ only the polynomial coefficients to the transformation matrix need to be constructed as deviatoric and applied to the expressions in (A10) and (A19).

### 2.8 Hourglass Stiffness Matrix

As mentioned in the previous section, the tangent matrix $\left. \frac{\partial \hat{S}}{\partial \hat{E}} \right|_{\xi^*}$ present in the hourglass part of the second Piola Kirchhoff stress given by the expression (2.47) is a very demanding quantity. It contains both a material part, which in it self can be very demanding for a complex constitutive model, and a geometrical nonlinear part. Such a complex quantity cannot be allowed in the hourglass part and the authors in [17] suggest replacing $\left. \frac{\partial \hat{S}}{\partial \hat{E}} \right|_{\xi^*}$ with
an isotropic linear elastic material tangent. This quantity should also be deviatoric according to (2.48) and the proposal is then to substitute the tangent $\frac{\partial \hat{S}}{\partial \hat{E}}|_{\xi^*}$ with the following,

$$ C^{hg} = \mu_{eff}^h I^{dev} $$

(2.49)

with $I^{dev}$ being the second order deviatoric identity tensor defined as,

$$ I^{dev} = \begin{bmatrix}
\frac{4}{3} & -\frac{2}{3} & -\frac{2}{3} & 0 & 0 & 0 \\
-\frac{2}{3} & \frac{4}{3} & \frac{4}{3} & 0 & 0 & 0 \\
-\frac{2}{3} & \frac{4}{3} & \frac{4}{3} & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix} $$

(2.50)

and $\mu_{eff}^h$ is the effective hourglass shear module. When the response is elastic and isotropy is present, the effective shear modulus is the regular isotropic shear modulus given by $\mu = \frac{E}{2(1+\nu)}$ with $E$ being the elastic modulus and $\nu$, Poisson’s ratio. When plasticity occurs the elastic shear modulus produces a to stiff response and the authors in [17] suggest using the constitutive relation $S^{hg \, dev} = 2 \mu_{eff}^h E^{hg \, dev}$. This relation results in an adaptive shear modulus given by the following expression,

$$ \mu_{eff}^h = \frac{1}{2} \int_{-1}^{1} \frac{S^{s \, dev}}{E^{s \, dev}} \, d\zeta $$

(2.51)

with $S^{s \, dev} = \sqrt{S^{s \, dev}_{ij} S^{s \, dev}_{ij}}$ and $E^{s \, dev} = \sqrt{E^{s \, dev}_{ij} E^{s \, dev}_{ij}}$

The effective shear modulus in (2.51) requires numerical integration with respect to the out-of-plane direction, the details behind this integration will be introduced in later sections.

The final form of the hourglass split for the second Piola Kirchhoff stress reeds,

$$ \hat{S} = \hat{S}^s + \hat{S}^{hg} $$

(2.52)

with

$$ \hat{S}^s = \hat{S}^s|_{\xi^*}, \quad \hat{S}^{hg} = C^{hg} \left( E^{\xi \, dev} \xi + E^{\eta \, dev} \eta + E^{\xi \zeta \, dev} \xi \zeta + E^{\eta \zeta \, dev} \eta \zeta \right) $$

(2.53)

### 2.9 Enhanced Assumed Strain Formulation

In the previous section the ANS concept was used on the transverse normal strain $\bar{E}_{33}$ in (2.28) to make the quantity bilinear within the shell plane, but it is still constant with respect to the out-of-plane direction $\xi^* = (0,0,\zeta)^T$. This constant feature give rise to locking for the bending scenario in figure 2.6 in which the analytical solution produces a linear traversal strain $\bar{E}_{33}$ with respect to the out-of-plane $\xi^*$ direction if the Poisson ratio $\nu$ is non-vanishing. The locking phenomena is called Poisses thickness locking [16] and in order to cure this behaviour some method need to be applied to make this strain linear in $\xi^*$ direction. Another locking phenomena called volumetric locking occurs when the normal strains $\bar{E}_{11}, \bar{E}_{22}$ and $\bar{E}_{33}$ are being represented by polynomials of different degrees and the state of deformation is approaching incompressibility [16]. This phenomena also requires
In order to establish this linear out-of-plane feature the "enhanced assumed strain" (EAS) procedure is embedded into the formulation. In the enhanced strain concept new so called enhanced degrees of freedom here denoted $W$ are introduced into the Green Lagrangian strain tensor $E$ consequently splitting it into one part $E_e$ (enhanced part) only dependent on the enhanced degrees of freedom and another part $E_c$ (compatible part) only dependent on the displacement degrees of freedom,

$$E = E_c + E_e$$

$$E_c = E_c(U)$$

$$E_e = E_e(W)$$

The exact same splitting procedure is applied to the corresponding virtual quantity $\delta E = \delta E_c + \delta E_e$. All previously established quantity’s related to the Green Lagrangian strain tensor (2.42) and (2.44) are based on displacement degrees of freedom and therefore all those quantities are stored within the compatible part of the strain tensors $E_c$ and $\delta E_c$. Applying the splitting of the virtual strain tensor to (2.5), the principle of virtual work equation can be decomposed into two equations at element ($\beta_e$) level,

$$g_1 = \int_{\beta_e} \delta \hat{E}_e^T \hat{S} dV + g_{\text{ext}} = 0$$

$$g_2 = \int_{\beta_e} \delta \hat{E}_c^T \hat{S} dV = 0$$

where Voigt matrix format for the decomposed virtual green Lagrangian strain tensor and the second Piola Kirchhoff stress has been adopted.

In the virtual equations (2.55), (2.56) it is assumed that the second Piola Kirchhoff stress can be written by the constitutive model as a sole function of the Green Lagrangian strain tensor,

$$\hat{S} = \hat{S}(E)$$

therefore $g_1$ and $g_2$ are functions of both $W$ and $U$. In the framework of enhanced strain formulations the strategy is to use the two equations $g_1$ and $g_2$ to eliminate the dependence of $W$ in order to avoid it entering the physical solution, in context of the explicit formulation this will be more clearly demonstrated in the forthcoming chapters.

In order to establish the linear feature of the term $\hat{E}_{33}$ in the out-of-plane direction $\zeta$ only one enhanced degree of freedom $W_e$ need to be implemented in the following manner,

$$\hat{E}_e = \hat{B}_e W_e$$

with the corresponding enhanced contravariant $\hat{B}_e$ matrix being defined as,

$$\hat{B}_e = [0, 0, \zeta, 0, 0, 0]^T$$

The contravariant enhanced Green Lagrangian strain in (2.58) need to be transferred into the Cartesian basis by using the transformation matrix in (2.38). But implementing the full polynomial expression of $T$ will result in a non-zero contribution for $g_2$ in (2.56) when
applying a constant stress field. In order to avoid this the transformation of (2.58) into
the Cartesian basis is chosen to only include the constant term $T^0$ from the polynomial
expression in (2.38). The final Cartesian format reads as follows,

$$\hat{E}_e = \hat{E}_e^* = T^0 \hat{B}_e W_e$$

(2.60)

where the $(\bullet)^*$ notation is adopted to emphasize the fact that it is only dependent on the
out-of-plane direction $\xi^* = (0, 0, \zeta)^T$. The corresponding virtual quantity have the exact
same structure and for the sake of completeness the expression is tabulated here as,

$$\delta \hat{E}_e = \delta \hat{E}_e^* = T^0 \hat{B}_e \delta W_e$$

(2.61)

### 2.10 Discretized Weak Form

The volume integral in the material domain for equation (2.55) and (2.56) are transformed
by the determinant of the Jacobian matrix in (2.30) to the isoparametric domain. This
procedure is quite demanding for the full polynomial expression in (2.30). Luckily in the
case of shell like structures with the thickness dimension being significantly smaller than
the in-plane dimensions this volume is approximated with sufficient accuracy using only the
linear polynomial term in $T$ i.e.

$$dV \approx J^0 d\Omega_e$$

(2.62)

with $d\Omega_e = d\xi d\eta d\zeta$ being the infinitesimal volume quantity in the isoparametric domain
and $J^0$ being the shorthand notation for the determinant of the linear Jacobian component
$J$.

Introducing in (2.55) the hourglass decomposition for the compatible part of the virtual
Green Lagrangian strain (2.42) and the second Piola Kirchhoff stress in (2.52) followed by
utilizing the isoparametric mapping of the volume element in (2.62) lead to the following
expression,

$$g_1 \approx \int_{\Omega_e} \left( \delta \hat{E}_e^* + \delta \hat{B}_e^{hg} \right)^T \left( \hat{S}^* + \hat{S}^{hg} \right) J^0 \, d\Omega_e + g_{ext} = 0$$

(2.63)

When computing the integrals above the cross terms $(\bullet)^* \cdot (\bullet)^{hg}$ will vanish because of the
fact that $(\bullet)^{hg}$ is linear with respect to the natural coordinates $\xi$, $\eta$ and $\zeta$ while $(\bullet)^*$ is
independent of $\xi$ and $\eta$,

$$g_1 \approx \int_{\Omega_e} \delta \hat{E}_e^{*T} \hat{S}^* J^0 \, d\Omega_e + \int_{\Omega_e} \left( \delta \hat{B}_e^{hg} \right)^T \hat{S}^{hg} J^0 \, d\Omega_e + g_{ext}$$

(2.64)

$$= [\text{applying (43) and introducing the external forces}]$$

$$= \delta U_e^T \left( \int_{\Omega_e} \hat{B}_e^{*T} \hat{S}^* J^0 \, d\Omega_e + \int_{\Omega_e} \left( \hat{B}_e^{hg} \right)^T \hat{S}^{hg} J^0 \, d\Omega_e - F_{ext} \right) = 0$$

with $F_{ext}$ being the external force vector. Using the fact that the virtual displacements can be
chosen arbitrarily in the above equation the following residual format is obtained,

$$G_u = R_u^* + R_{u^{hg}} - F_{ext} = 0$$

(2.65)
where the short hand notations for the integrals was introduced,

\[
\begin{align*}
R_u^* &= \int_{\Omega_e} \hat{B}_c^T \hat{S}^* J^0 d\Omega_e \\
R_{uhg}^* &= \int_{\Omega_e} (\hat{B}_{c}^{hg})^T \hat{S}_{hg} J^0 d\Omega_e
\end{align*}
\]  

(2.66)

with the subscript \((\bullet)_u\) indicating that the derivation is based on the compatible, displacement based part of the virtual work equation. The hourglass part of the residual do not depend on the constitutive modelling for the stress tensor and can therefore be calculated directly using the deviatorical form of (2.45) and (2.53),

\[
\begin{align*}
R_{uhg}^* &= \frac{8}{3} \left( B_c^{\xi \text{dev}} C^{hg} E_c^{\xi \text{dev}} + B_c^{\eta \text{dev}} C^{hg} E_c^{\eta \text{dev}} \right) J^0 \\
&\quad + \frac{8}{9} \left( B_c^{\eta \zeta \text{dev}} C^{hg} E_c^{\eta \zeta \text{dev}} + B_c^{\xi \zeta \text{dev}} C^{hg} E_c^{\xi \zeta \text{dev}} \right) J^0
\end{align*}
\]  

(2.67)

In contrast to the hourglass part, the residual vector \(R_u^*\) is depending on the stress tensor evaluated along the \(\zeta\) direction. Therefore a numerical integration with respect to the out-of-plane direction is eventually necessary. Performing the analytical integration for (2.66a) with respect to the in-plane directions and introducing the polynomial representation (2.45) results in,

\[
R_u^* = \int_{-1}^{1} \left( B_c^0 + \zeta B_c^\xi + \zeta^2 B_c^\xi \zeta \right)^T \hat{S}^* d\zeta 4 J^0
\]  

(2.68)

The exact same procedure is implemented for the virtual work equation corresponding to the enhanced degree of freedom (2.56) by using (2.53), (2.61) and (2.62)

\[
\begin{align*}
g_2 &= \int_{\Omega_e} \delta \hat{E}_e^T \hat{S} dV \\
&= \int_{\Omega_e} \delta \hat{E}_e^T \left( \hat{S}^* + \hat{S}_{hg} \right) J^0 d\Omega_e \\
&= \int_{\Omega_e} \delta \hat{E}_e^T \hat{S}^* J^0 d\Omega_e \\
&= \delta W_e^T \left( \int_{\Omega_e} B_c^T \hat{S}^* J^0 d\Omega_e \right)
\end{align*}
\]  

(2.69)

The virtual enhanced degree of freedom in the above expression can be chosen arbitrarily. Using the arbitrary state of \(W_e\) and preforming the in-plane analytical integration result in the following residual equation,

\[
G_w = R_w = R_{w}^* = \int_{-1}^{1} B_c^T \hat{S}^* 4 J^0 d\Omega_e = 0
\]  

(2.70)

The necessary residual equations are now in place and numerical integration is required for the residuals \(G_w\) in (2.70), \(G_u\) in (2.65) and if plastic response is present then \(\mu_{hg}^{\text{eff}}\) in (2.51). Numerical integration is done by using the method of Gauss which approximates integrals in the following manner,

\[
\int_{-1}^{1} (\bullet) d\zeta \approx \sum_{i=1}^{n_{ip}} (\bullet)|_{\zeta=\zeta_i} \omega_i
\]  

(2.71)
with \( n_{\text{ip}} \) being the number of gauss points \( \zeta_i \) along the out-of-plane direction \( \xi^* = (0, 0, \zeta)^T \) and \( \omega_i \) are the matching weights to the gauss points. The points corresponding to the integration are schematically illustrated in figure 2.10 and they are allowed to vary in the formulation to accurately model the behaviour of thick shells.

### 2.11 Fully Explicit Finite-Element-Formulation

In previous sections the starting point for the element-formulation has been the static form of the virtual work equation. To include the dynamical contribution in the formulation an element massmatrix \( M_e \) acting on the nodal accelerations \( \ddot{U}_e \) are introduced into the displacement-based residual equation (2.65). After utilizing the assembling process for all elements the global equation reads,

\[
G^M \ddot{U} + G^R_u^* + G^{hg} - G^F_{\text{ext}} = 0 \quad \text{or} \quad G^M \ddot{U} = -G^G_u
\]

(2.72)

where the superscript \( G(\cdot) \) indicates that the given quantity is assembled into the global framework. A fully explicit finite element formulation as the one implemented in the commercial software Abaqus [7] require the mass matrix to be diagonal. The simplest way of constructing a diagonal massmatrix is to do the following lumping procedure at the element level,

\[
M_e = \rho J^0 I_{24 \times 24}
\]

(2.73)

with \( I_{24 \times 24} \) being the identity matrix and \( \rho \) the mass density for the element.

The equation in (2.72) then becomes trivial and the nodal accelerations are computed given the residual \( G^G_u \). When the nodal accelerations are given the solver uses explicit time integration to get the displacements in the next timestep. While this procedure is fast the drawback is that it usually requires very small timesteps to converge.

When the massmatrix is constructed the explicit algorithm only requires the calculation of the right hand side \( G_u \) in (2.65) for a given displacement \( \bar{U}_e \) at element level but this equation is also a function of the out-of-plane stress \( \hat{S}^* \) which is dependent on the enhanced degree of freedom \( W_e \). The displacement given by the time integration \( \bar{U}_e \) is then to be considered fixed and the corresponding enhanced degree of freedom \( W_e \) can be calculated from residual \( G_w \) in (2.70) resulting in,

\[
G_w(W_e) = G_w(\bar{U}_e, W_e) = \int_{-1}^{1} B_e^T \hat{S}^* \ 4 J^0 d\zeta = 0
\]

with \( \hat{S}^* = \hat{S}^*(\bar{U}_e, W_e) = \hat{S}^*(W_e) \)

(2.74)

If the material is nonlinear with respect to \( \zeta \) this equation is consequently nonlinear with respect to \( W_e \) and it should be solved using an iterative procedure. The iterative method employed in this work when solving the equation \( G_w \) in a precise way to obtain \( W_e \) is the bisection algorithm. The bisection method is one of the most robust algorithms to find a root to a unimodule scalar equation. No derivatives of the function is required but the procedure is quite time consuming compared to many derivative based methods with quadratic convergence. More about the bisection algorithm can be found in [4].

To speed up the simulation process the authors in [17] proposed to use the previous value
for \( W_e \) in the current step and to do an explicit estimate for \( W_e \) in the next step. This explicit estimate was constructed using one Newton Raphson step in which the residual in (2.74) is linearised with respect to \( W_e \) resulting in

\[
\tilde{G}_w + \tilde{S}_{ww}^* dW_e = 0 \tag{2.75}
\]

\[
\tilde{S}_{ww}^* = \int_{-1}^{1} B_e^T C_e^* B_e 4 J^0 d\zeta , \quad C_e^* = \frac{d\tilde{S}_e^*}{dE^*} \tag{2.76}
\]

and the value to be used in the next timestep is given by,

\[
W_e = W_e + dW_e \tag{2.77}
\]

with

\[
dW_e = -\tilde{G}_w/\tilde{S}_{ww}^* \tag{2.78}
\]

An explicit estimate of this kind will certainly give some error to the residual \( G_w \) but the argument is that the explicit formulation work with such small timestep that this incremental procedure will still be a valid choice. Apart from the fact that no iterations are necessary, this explicit procedure requires only one loop through the gauss points for the entire system in such a way that \( G_u \) and \( \mu_{eff} \) can be calculated in the same loop as the quantity’s in (2.76). The explicit estimate of this kind seems to work well for the problems studied in [17] although the authors conclude that this method needs to be investigated further with a larger range of examples.

The most time consuming part of this strategy is that it requires the construction of the algorithmic tangent matrix \( C_e^* = \frac{d\tilde{S}_e^*}{dE^*} \) which can be a non-trivial task for a complex constitutive model. As a possible remedy one can propose to reduce the statement even more and use one linearised Euler forward step for the incremental change \( dW_e \) in (2.77) which then results in the following expression,

\[
dW_e = \frac{h \cdot G_w(W_e)}{G_w(W_e) - G_w(W_e + h)} \quad \text{with} \quad h << 1 \tag{2.79}
\]

Using the Euler forward procedure requires two loops throughout the gauss points but no material tangent is needed. In this thesis the use of one Euler forward estimate in (2.79) will be compared to the bisection procedure of finding a precise value for \( W_e \).

### 2.12 Finite Elasticity

Apart from trying to combine the paperboard model with the solid shell element a material model based on isotropic finite elasticity will also be considered to validate the element implementation and to investigate the explicit estimate in (2.77). The model is hyper elastic which implies [14] that the stress can be obtained from a strain energy function \( W \) in the following manner,

\[
S = \frac{\partial W}{\partial E} \tag{2.80}
\]

The strain energy is chosen to be Neo-Hookean,

\[
W = \frac{1}{2} k \left[ \frac{1}{2}(\det C - 1) - \ln(\sqrt{\det C}) \right] + \frac{1}{2} \mu \left[ \text{tr}(C)(\det C)^{-1/3} - 3 \right] \tag{2.81}
\]
which can be found c.f. [10]. The quantity $C$ is the right Cauchy-Green tensor related to the green Lagrangian strain in the following way,

$$ C = 2E + I $$

(2.82)

$k$ and $\mu$ are the bulk and shear modulus defined as,

$$ k = \frac{E}{3(1 - 2\nu)}, \quad \mu = \frac{E}{2(1 + \nu)} $$

(2.83)

When using the bisection method or the explicit Euler estimate to update $W_e$ no material tangent is needed, only the stress corresponding to the gauss points need to be addressed. The second Piola Kirchhoff stress is obtained from the potential $W$ and the resulting expression reads,

$$ S = \frac{1}{2} k (\det C - 1) C^{-1} + \mu (\det C)^{-2/3} \left[ I - \frac{1}{3} \text{tr}(C) C^{-1} \right] $$

(2.84)
Chapter 3

Modelling of Paperboard

3.1 Introduction

The problem of modelling paperboard is a highly complex task especially when used in the processing industry were both large deformations and rotations occurs. From a material point of view paperboard is for instance sensitive to moisture, nonlinear in the elastic region, large plastic deformations and is highly anisotropic. The anisotropic nature of paperboard is a consequence of the manufacturing process where fibers are continuously sprayed in one direction, Machine Direction (MD). Stiffness in the MD direction is about 2-3 times the stiffness of the Cross Direction, here denoted CD, and about 100 times larger than the out-of-plane direction ZD, figure 3.1 illustrates the adopted notations. Paperboard is then modelled as being orthotropic having three planes of symmetry characterized by the three normal vectors in MD, CD and ZD. One successful continuum model to capture the

Figure 3.1: Adopted convention for the directions of paperboard. MD being the machine direction, CD is the cross direction and ZD the out-of-plane z-direction.

behaviour of paperboard is the one developed by Borgqvist et.al in [5]. The model builds on ideas established in [18] where the author were able to establish a continuum framework to capture the in-plane behaviour of paperboard while the out-of-plane response was modelled by applying an interface structure. One of the modifications done in [5] was to establish a more rigorous mathematical framework, for instance applying thermodynamics and to capture the out-of-plane behaviour in a fully continuum based framework. This section is dedicated to describing this model which is later implemented into the shell element formulation discussed in the previous sections, to the authors knowledge no anisotropic continuum model have previously been implemented in combination with this particular solid shell element.
3.2 Kinematics

The model is based on the spatial configuration utilizing the deformation gradient $F$ as the deformation quantity while the energy conjugate stress measure to the deformation gradient is the Kirchhoff stress denoted $τ$. The deformation gradient can be split into two parts, one part corresponding to the elastic part of the deformation $F^e$ and one part related to the permanent plastic deformations $F^p$,

$$F = F^e F^p$$

(3.1)

One important quantity utilized in the thermodynamical framework is the spatial velocity gradient defined as,

$$l = \dot{F} F^{-1} = l^e + F^e L^p F^{e-1} = l^e + l^p$$

with $l^e = \dot{F}^e F^{e-1}$ and $L^p = \dot{F}^p F^{p-1}$

(3.2)

The plastic spatial velocity gradient can be further split into one symmetric part and one skew symmetric part,

$$l^p = F^e \dot{F}^p F^{p-1} F^{e-1} = \text{sym}(l^p) + \text{skew}(l^p) = d^p + \omega^p$$

(3.3)

The skew symmetric part in (3.3) is called the Eulerian plastic spin and special consideration is later adopted for this quantity. In order to handle the highly anisotropic characteristics of paperboard the material directions illustrated in figure 3.1 is embedded into the formulation. An orthogonal basis is adopted in the undeformed (reference) configuration consisting of three vectors $v^{(1)}_0$, $v^{(2)}_0$ and $v^{(3)}_0$ where the fist one is parallel to MD, the second one is parallel to CD and the last one pointing in the out-of-plane direction in the same manner as ZD. The vectors for the in-plane directions are chosen to deform with respect to the elastic part of the deformation gradient,

$$v^{(1)} = F^e v^{(1)}_0$$

$$v^{(2)} = F^e v^{(2)}_0$$

(3.4)

while the out-of-plane direction is deformed in such a way that orthogonality always holds with respect to the in-plane directions,

$$v^{(3)} = F^e n^{(3)}_0$$

with $n^{(3)} = J^e F^{e-1} n^{(3)}_0$ and $n^{(3)}_0 = v^{(1)}_0 \times v^{(2)}_0$

(3.5)

This particular choice for the out-of-plane vector is motivated by assuming that paperboard acts like a deck of cards when being subject to an idealized shearing situation, cf. [5]. For the sake of convenience it is also practical to define the following set out second order structural tensors,

$$m^{(1)} = v^{(1)} \otimes v^{(1)}$$,  $$m^{(2)} = v^{(2)} \otimes v^{(2)}$$,  $$m^{(3)} = n^{(3)} \otimes n^{(3)}$$

(3.6)

3.3 Modelling with Thermodynamic Framework

When doing constitutive modelling it is convenient to not only consider experimental evidence but also apply fundamental physical principals like thermodynamics. Applying the second law of thermodynamics it is possible to derive the so called dissipation inequality
often used within constitutive modelling [14]. Assuming an isothermal setting and introducing Helmholtz free energy per unit mass $\Psi$ the dissipation inequality states,

$$\gamma = \tau : d - \rho_0 \dot{\Psi} \geq 0 \quad (3.7)$$

with $\rho_0$ being the density in the reference configuration and $\gamma$ being the notation for dissipation. For an idealized reversible situation no dissipation occurs and equality in equation (3.7) is obtained. In order to continue, it is necessary to introduce variables that characterize the state of the system. The model adopts the structural tensors in (3.6) to be such variables. Plasticity is included in the model and internal variables, $\kappa$, will be used as state variables. Finally the last state variable is a deformation measurement chosen as the left Cauchy-Green tensor defined as,

$$b^e = F^e F^{eT} \quad (3.8)$$

It is now postulated that Helmholtz free energy is a function of the state variables $\Psi(m^{(i)}, \kappa, b^e)$. Using this in the dissipation inequality (3.7) and applying arguments used in [6] it is shown in [5] that the following relation holds for the Kirchhoff stress tensor,

$$\tau = 2\rho_0 \left( \frac{\partial \Psi}{\partial b^e} b^e + \frac{\partial \Psi}{\partial m^{(1)}} m^{(1)} + \frac{\partial \Psi}{\partial m^{(2)}} m^{(2)} - \frac{\partial \Psi}{\partial m^{(3)}} m^{(3)} + \left( \frac{\partial \Psi}{\partial m^{(3)}} : m^{(3)} \right) I \right) \quad (3.9)$$

It is also assumed that Helmholtz free energy can be additively split into one elastic and one plastic part. Furthermore the elastic part is split into the following format,

$$\rho_0 \Psi^e = \rho_0 \Psi^{ip} + \rho_0 \Psi^{op} \quad (3.10)$$

with $\Psi^{(ip)}$ being the in-plane contribution and $\Psi^{(op)}$ the out-of-plane contribution to the energy. To be able to conveniently identify the in-plane and out-of-plane energies in (3.10) from an experimental setting the following invariants are introduced,

$$I_{11} = \sqrt{m^{(1)}} : I, \quad I_{12} = \sqrt{m^{(2)}} : I, \quad I_{13} = \frac{1}{J_e} \sqrt{m^{(3)} : b^e b^e} \quad (3.11)$$

Using the definitions in (3.6), (3.8) in (3.11) it can be shown that the invariants $I_{11}$, $I_{12}$ and $I_{13}$ characterize the stretch in MD CD and ZD respectively. It is also possible to relate $I_{23}$ to the deformation of an area element with a vector normal in ZD direction while the last invariant $J^e$ is a measurement for the volumetric deformation.

The following anzats is made for the in-plane Helmholtz energy,

$$\rho_0 \Psi^{ip} = A_1 \left( I_{11} + \frac{1}{I_{11}} \right) + A_2 \left( I_{12} + \frac{1}{I_{12}} \right) + A_4 \left( I_{11} + I_{12} \right) \left( \frac{1}{I_{11}} + \frac{1}{I_{12}} \right) + A_5 \left( I_{11} + I_{12} + \frac{1}{I_{23}} \right) \quad (3.12)$$

with $A_i$ being positive elastic parameters which are obtainable from experiments performed for the in-plane directions. Every factor corresponding to an elastic parameter $A_i$ in expression (3.12) will approach infinity for both unlimited compression and tension which is to be expected. The first two terms in (3.12) relates to pure tension and compression in MD and CD directions respectively. The third term corresponding to the elastic parameter $A_4$ is contributing to the coupling between the in-plane directions while the last term is representing the change for the in-plane area.
The out-of-plane part of Helmholtz free energy $\Psi^{\text{op}}$ is postulated to have the following structure,

$$\rho_0 \Psi^{\text{op}} = H^+ \rho_0 \Psi^{\text{top}} + (1 - H^+) \rho_0 \Psi^{\text{cop}} + \rho_0 \Psi^{\text{sop}}$$

(3.13)

where the energy is split into three parts corresponding to out-of-plane behaviour for compression $\Psi^{\text{top}}$, tension $\Psi^{\text{cop}}$ and shear $\Psi^{\text{sop}}$. Also a switch is introduced in order to distinguish between tensile and compression,

$$H^+ = \begin{cases} 
1 & \text{if } (I_{13} - 1) \geq 0 \\
0 & \text{otherwise} 
\end{cases}$$

(3.14)

It should be noted that $I_{13}$ is the elastic stretch in the out-of-plane direction therefore (3.14) is one for tensile deformation and zero in compression. The ansätze for the three components in (3.13) is made in the following manner,

$$\rho_0 \Psi^{\text{top}} = A_3 \left( I_{13} + \frac{1}{I_{13}} \right)$$

$$\rho_0 \Psi^{\text{cop}} = A_7 \left( (I_{13})^2 + \frac{1}{I_{13}} e^{-A_6(I_{13})^2 - 1} \right)$$

$$\rho_0 \Psi^{\text{sop}} = A_6 \left( I_{11} + I_{12} + I_{13} - J^e \right)$$

(3.15)

The tensile part is modelled in the same fashion as the in plane directions while the compression part is modelled with a stiffening behaviour represented by the exponential term. The elastic parameters can also be calibrated using out-of-plane experiments in the laboratory. Applying the ansätze functions from (3.15), (3.13) and (3.12) into (3.10) result in an expression for Helmholtz free energy furthermore using this in the relation for the Kirchhoff stress in (3.9) results in the final expression for the Kirchhoff stress in (3.16),

$$\tau = P_1 m^{(1)} + P_2 m^{(2)} + P_3 m^{(3)} + P_4 I + P_5 \frac{1}{(J^e)^2} b^e m^{(3)} b^e$$

(3.16)

In the above expression for $\tau$ the following parameters has been introduced to have an aesthetically pleasing formulation,

$$P_1 = \frac{1}{I_{11}^2} \left( A_1 + A_5 + A_6 + A_4 \left( \frac{1}{I_{11}} + \frac{1}{I_{12}} \right) \right) - \frac{1}{(I_{11})^3} (A_1 + A_4(I_{11} + I_{12}))$$

$$P_2 = \frac{1}{I_{12}^2} \left( A_2 + A_5 + A_6 + A_4 \left( \frac{1}{I_{12}} + \frac{1}{I_{11}} \right) \right) - \frac{1}{(I_{12})^3} (A_2 + A_4(I_{12} + I_{11}))$$

$$P_3 = \frac{A_5}{(I_{23})^3}$$

$$P_4 = -\frac{A_5}{I_{23}} - A_6 J^e$$

$$P_5 = \frac{A_6}{I_{13}} + H^+ A_3 \left( \frac{1}{I_{13}} - \frac{1}{(I_{13})^3} \right) + (1 - H^+) 2A_7 \left( 1 - e^{A_6((I_{13})^2 - 1)} \right)$$

(3.17)

### 3.4 Plasticity

It has been observed in experiments [9] that permanent deformations occurs when unloading paperboard from a certain critical load, this observation validates the use of plasticity
theory. Modelling of plasticity in a one dimensional setting is straightforward, measure the point for yielding in a stress strain diagram, the process is quite complex for an arbitrary stress state. For an arbitrary stress state it is common to postulate a so called yield surface \( f \) which is a function of some stress invariants. This function have the property of being less then zero when pure elasticity is present and equal to zero when entering the plastic region. When plasticity occurs this yield surface needs to deform in some manner to fulfil the criteria \( f = 0 \). A simple way to model this behaviour is to assume isotropic hardening when the yield surface expands proportionally in the given stress space. One example of a yield surface is the von Mises yield surface which is used for modelling of isotropic materials [14]. For anisotropic materials the most common yield surface is probably the one developed by Hill (1948). The yield surface used for the paperboard model discussed in this section is building on the work done in [18] and it utilizes six subsurfaces for in-plane direction and six subsurfaces for the out-of-plane direction. The explicit expression for the yield surface is the following,

\[
f(\tau, n_s^e, K^e) = \sum_{v=1}^{12} \chi^{(v)} \left( \frac{\tau : n_s^{(v)}}{\tau^{(v)}} \right)^{2k} - 1 \quad (3.18)
\]

were \( n_s^{(v)} \) represent the normal to the given yield surface,

\[
n_s^{(v)} = \sum_{i=1}^{3} \sum_{j=1}^{3} N_{ij}^{(v)} \bar{u}^{(i)} \otimes \bar{v}^{(j)} \quad \text{with} \quad \bar{v}^{(k)} = \frac{1}{|v^{(k)}|} v^{(k)}, \quad k = 1, 2, 3 \quad (3.19)
\]

The parameters \( N_{ij}^{(v)} \) in (3.19) is the coefficients to the yield normals \( \bar{v}^{(k)} \) and they are chosen in such a way that the following normalization condition is fulfilled,

\[
\sqrt{n_s^{(v)} : I} = 1 \quad (3.20)
\]

In order to determine if a given subsurface is active the following switch function is introduced in (3.18),

\[
\chi^{(v)} = \begin{cases} 
1 & \text{if} \quad \tau : n_s^{(v)} > 0 \\
0 & \text{otherwise.} 
\end{cases} \quad (3.21)
\]

The exponent \( k \) in (3.18) is a material parameter while \( \tau^{(v)} \) represents the hardening stress for the given subsurface defined as,

\[
\tau^{(v)} = K_0^{(v)} + K^{(v)} \quad (3.22)
\]

with \( K_0^{(v)} \) being the initial value for the hardening parameters related to the initial yield stress which can be determined in the laboratory. \( K^{(v)} \) is the hardening variables representing the change in distance for the given subsurface when plastic deformation occurs. Most of the subsurfaces are modelled using idealized plasticity in which the hardening variable is zero. The exceptions are the following,

\[
\begin{align*}
K_0^{(v)} &= a_v \ln(b_v \kappa^{(v)} + 1) & v = \{1, 2, 3, 7\} \\
K^{(v)} &= a_v \kappa^{(v)} & v = 7
\end{align*} \quad (3.23)
\]
with $a_v$ and $b_v$ being material parameters and $\kappa^{(v)}$ are the conjugated internal hardening variables corresponding to the hardening variables $K^{(v)}$. The model is assuming associated plasticity in which the following evolution laws are present,

$$
\begin{align*}
\dot{d}^p &= \dot{\lambda} \frac{\partial f}{\partial \tau} \\
\dot{\kappa}^{(v)} &= -\dot{\lambda} \frac{\partial f}{\partial K^{(v)}} \\
\end{align*}
$$

(3.24)

where equations includes the so called plastic multiplier $\dot{\lambda}$. Utilizing the equations of associated plasticity in (3.24) the following system is obtained,

$$
\begin{align*}
\dot{d}^p &= \dot{\lambda} \sum_{\gamma=1}^{12} \chi^{(\gamma)} \frac{2k\Lambda^{2k-1}_v}{\tau^{(\gamma)}} \text{sym}(n^{(\gamma)}_s) \\
\dot{\kappa}^{(v)} &= \dot{\lambda} \chi^{(v)} \frac{2k\Lambda^{2k}_v}{\tau^{(v)}} \\
\text{with} \quad \Lambda^{2k}_v &= \frac{\tau : n^{(v)}_s}{\tau^{(v)}} \\
\end{align*}
$$

(3.25)

for more detail regarding the derivation see [5]. In order to obtain a fully functional model it is necessary to address the Eulerian plastic spin $\omega^p$ previously introduced as the skew symmetric part in (3.3). The Eulerian plastic spin is responsible for determining the direction of the permanent plastic deformations and it is postulated in [5] that this quantity has the following structure,

$$
\omega^p = \sum_{\gamma=1}^{12} \chi^{(\gamma)} \frac{2k\Lambda^{2k-1}_v}{\tau^{(\gamma)}} \text{skew}(n^{(\gamma)}_s)
$$

(3.26)

### 3.5 Integrating Plasticity Equations

By using the Eulerian plastic spin (3.26) and the equations of associated plasticity (3.25) in combination with (3.3) and (3.1) it is possible to write the equations of plasticity in the following general form,

$$
\begin{align*}
\dot{F}^p &= \dot{\lambda} N^p \cdot F^p \\
\dot{k} &= -\dot{\lambda} n^k \\
\dot{\lambda} f &= 0, \quad \dot{\lambda} \geq 0, \quad f \leq 0
\end{align*}
$$

(3.27)

with $\kappa$ being a vector of the hardening parameters while $N^p$ and $n^\kappa$ are the plastic flow directions.

The Abaqus material routine applied in this thesis is designed by Tetra Pak to work fast in explicit simulations. In such simulations the timestep is extremely small which implies that the equations of plasticity in (3.27) can be integrated using a method of approximation without much loss. The choice for integration in [1] was to use an Euler forward integration scheme in which the following updating procedure was obtained,

$$
\begin{align*}
F^p_{\text{new}} &= F^p_{\text{old}} + \Delta \lambda (N^p \cdot F^p)_{\text{old}} \\
\kappa_{\text{new}} &= \kappa_{\text{old}} - \Delta \lambda (n^k)_{\text{old}} \\
f_{\text{new}}((F^p_{\text{new}}(\Delta \lambda), \kappa_{\text{new}}(\Delta \lambda))) &= 0
\end{align*}
$$

(3.28)
When the plastic deformation gradient and the new plastic history variables are obtained from the integration, the current value for the Kirchhoff stress is calculated using expression (3.16).
Chapter 4

Combining Paperboard Model with the Solid Shell Element

This section is describing some problems encountered when trying to combine the paperboard model with the solid shell element described in previous chapter.

4.1 Pullback to Material Configuration

The paperboard model described in the previous section is implemented in the spatial configuration utilizing the deformation gradient \( F \) as the measure of strain and the corresponding energy conjugate Kirchhoff stress \( \tau \) as the measure of stress. This poses a problem when trying to combine the model with the solid shell element which operates in the material configuration with the Green Lagrangian strain \( E \) and the second Piola Krichhoff stress \( S \).

If no element technology (ANS, EAS and Taylor expansion) were to be used apart from the approximation of the inverse Jacobian in (2.35), the deformation gradient corresponding to the out-of-plane gauss points would be calculated using (2.35),(2.32) and (2.2) which results in

\[
F = I + \left( D^0 + \zeta D^\zeta \right) \left( (J^{-1})^0 + \zeta (J^{-1})^\zeta \right) \tag{4.1}
\]

Using a polar decomposition of the deformation gradient reads,

\[
F = RU \tag{4.2}
\]

with \( U \) being the right stretch tensor corresponding to the stretch of the deformation and \( R \) is an orthogonal tensor containing the rotational part of the deformation. The element technology used in the solid shell element to strengthen the Green Lagrangian strain is corresponding to the part of the deformation \( U \) representing the stretch. The rotational part \( R \) will therefore remain the same with and without element technology. To obtain \( R \) the first step is to compute the right Cauchy-Green tensor \( C \) and apply the following polar decomposition,

\[
C = F^T F = U^T R^T R U = U^T U = U^2 \tag{4.3}
\]

By using a spectral decomposition of \( C \), the right stretch tensor can be written as

\[
U = \sum_{i=1}^{3} \lambda_i N_i N_i^T \tag{4.4}
\]
with \( \lambda_i \) and \( N_i \) being the eigenvalues and eigenvectors (principal stretch and direction) of the right Cauchy-Green deformation tensor \( C \). The rotational part \( R \) is now obtained by inverting the polar decomposition,

\[
R = F U^{-1}
\]  
(4.5)

Same procedure is applied to find the right stretch tensor with element technology \( U^{tec} \). The right Cauchy-Green tensor with element technology \( C^{tec} \) is related to the Green Lagrangian strain \( E \) in the following way,

\[
C^{tec} = 2E + I
\]  
(4.6)

and \( U^{tec} \) is computed in complete analogy to the previous procedure,

\[
U^{tec} = \sum_{i=1}^{3} \lambda_i^{tec} N_i^{tec} N_i^{tecT}
\]  
(4.7)

with \( \lambda_i^{tec} \) and \( N_i^{tec} \) being the eigenvalues and eigenvectors (principal stretch and direction) of the right Cauchy-Green deformation tensor with element technology \( C^{tec} \). The final expression for the deformation tensor with element technology included is now given by,

\[
F^{tec} = RU^{tec}
\]  
(4.8)

By using the strengthen version of the deformation gradient \( F^{tec} \), the pullback procedure from the Kirchhoff stress configuration \( \tau \) to second Piola Kirchhoff configuration \( S \) is given as, cf. [10],

\[
S = (F^{(tec)})^{-1} \tau (F^{(tec)})^{-T}
\]  
(4.9)

### 4.2 Anisotropic Hourglass Matrix

The hourglass matrix in (2.49) with the effective shear modulus in (2.51) is based on a isotropic linear elastic material tangent. It is not certain that such a matrix will work when combined with the highly anisotropic paperboard model. As an alternative to the isotropic matrix an anisotropic version is proposed based on the initial paperboard stiffness in [5],

\[
C = \frac{\partial \tau}{\partial F} F^T \Big|_{F=I} \quad \text{with} \quad F = F^e
\]  
(4.10)

Using (3.16) this expression can be written in Voigt notation for the Cartesian system with base vectors MD, CD and ZD, the resulting matrix reads,

\[
C = \begin{bmatrix}
2A_1+2A_4 & 2A_5-2A_1-A_6 & -A_6 \\
A_5-2A_1-A_6 & 2A_2+2A_4+2A_5 & -A_6 \\
-A_6 & -A_6 & 2A_3H^++4A_7A_8H^-
\end{bmatrix}
\]  
(4.11)

To simplify the hourglass matrix both switches \( H^+ \) and \( H^- \) were considered to be active. Furthermore applying the B-Bar method implies working with the deviatoric part which
results in the following anisotropic hourglass matrix,

\[
C_{hg} = \begin{pmatrix}
\frac{4}{3} A_1 + 2 A_4 + \frac{2}{9} A_6 & -\frac{2}{3} A_2 - 3 A_4 - \frac{2}{3} A_6 & -\frac{2}{3} A_3 - \frac{1}{3} A_6 - \frac{1}{3} A_7 A_8 \\
-\frac{2}{3} A_1 - 2 A_4 - \frac{1}{3} A_6 & \frac{1}{3} A_2 + 2 A_4 + \frac{2}{3} A_6 & -\frac{2}{3} A_3 - \frac{1}{3} A_6 - \frac{1}{3} A_7 A_8 \\
-\frac{2}{3} A_1 - A_3 - \frac{1}{3} A_6 & -\frac{2}{3} A_2 - 2 A_4 - \frac{1}{3} A_6 & \frac{2}{3} A_3 + \frac{1}{3} A_7 A_8 + 2 A_6
\end{pmatrix}
\] (4.12)

If the configuration of the fibers MD, CD and ZD in the element is not aligned with the global Cartesian system \((e_x, e_y, e_z)\) an orthogonal transformation of the \(C_{hg}\) should be performed. Such a transformation between Cartesian configurations is trivial and can for instance be found in [14].
Chapter 5

Implementation in Abaqus

The solid shell element has been implemented in the commercial software Abaqus explicit using a user element subroutine of the type VUEL (see [7]) and the subroutine was combined with a highly efficient code from Tetra Pak to calculate the stress response from the paperboard model. This section is describing some practical aspects concerning the implementation of the element in Abaqus.

5.1 Simulations with User Defined Elements

The procedure for running simulations with user written elements in Abaqus is rather tedious because of two reasons. One is that the modelling tree in Abaqus do not support user written elements, the only way to apply such an element is to directly modify the input file and to run the simulation from an external terminal. Three modifications to the input file is necessary, the first one is to include the following line,

```
*USER ELEMENT, NODES=8, TYPE=VU3, PROPERTIES=6, COORDINATES=3, VARIABLES=55
1,2,3
```

which is providing information regarding the VUEL subroutine. The second thing to modify in the input file is regarding the previous element used to mesh the structure in Abaqus. This element should be replaced in the input file with a reference to the user element in the following manner,

```
*Element, type=VU3, elset=vuelset
```

The last modification to the input file is to add properties to the user element by including,

```
*UEL PROPERTY, elset=vuelset
1e-8, 2, 1, 3666, 0.3
```

somewhere in the input file. The second row of this command is referring to some specific properties used for this particular job.

The other obstacle is that Abaqus does not support any visualization of user defined elements. The recommended method in the Abaqus manual [7] is to overlap the user element mesh with so called dummy elements. A dummy element should kinematically be of the same type as the user element with the same number of nodes and degrees of freedom. Furthermore the dummy element should be assigned to a material with very low properties.
in such a way that the element do not contribute to the result of the simulation. An overlapped mesh can be achieved by creating two identical parts and regarding one of them as the dummy part. Then use the same mesh density for both but apply reduced integrated elements to the dummy part and fully integrated ones to the other. The overlapped mesh can now be obtained by adding both parts into the assembly tree in Abaqus and use the merge operation. Finally when the problem is properly defined and the input file is written the fully integrated elements are replaced by the user elements as previously outlined.

5.2 Node Numbering in Abaqus

The ordering of nodes for a specific mesh in Abaqus does not automatically identify the thickness direction. This poses a problem when using the solid shell which require a node convention of the type shown in figure 2.10 to ensure that the numerical integration is performed with respect to the thickness direction $\zeta$. To overcome this problem the strategy used in [16] is adopted which consists of determining the thickness direction at element level by examine the columns of the Jacobian $J_0^1$, $J_0^2$ and $J_0^3$ evaluated at the center of the element. If the element mesh is not highly distorted they represent the stretch of the natural directions $\xi$, $\eta$ and $\zeta$ between the isoparametric reference cube and the real domain illustrated in figure 2.4. There exist two cases when $\zeta$ is not the thickness direction for the element and they are identified using the following procedure,

\begin{align}
\text{Case 1} & : |J_0^1| < |J_0^2|, |J_0^1| < |J_0^3| \\
\text{Case 2} & : |J_0^2| < |J_0^3|, |J_0^2| < |J_0^3| 
\end{align}

and if case 1 or 2 is fulfilled then the renumbering of nodes are done according to figure 5.1.

![Figure 5.1: Renumbering of nodes if $\zeta$ is not thickness direction in Abaqus](image)

5.3 Stable Time Increment in Explicit Formulation

In order to get convergence when working with an explicit time integration of the residual equation in (2.72) it is necessary to apply very small time steps. An upper bound for the stable time increment is mathematically given by the so called Courant-Friedrichs number which is related to the highest eigenvalue produced by the system. When implementing the solid shell element in Abaqus using a VUEL subroutine it is necessary to provide a value to
this stable time increment, otherwise only fixed time integration can be used in Abaqus. A conservative estimate for this number is given in Abaqus documentation [7] and it states the following,

\[ \Delta t = \min \left( \frac{L_c}{c_d} \right) \]  

(5.2)

with \( \Delta t \) being the upper bound for the stable time increment, \( L_c \) is the smallest characteristic length of the element and \( c_d \) is the speed of the dilatational stress wave. The fraction between \( L_c \) and \( c_d \) is an element based value and the global time estimate \( \Delta t \) is chosen to be the smallest one of these element fractions. For elasticity the dilatational wave speed is given by,

\[ c_d = \sqrt{\frac{\lambda + 2 \mu}{\rho}} \]  

(5.3)

with the following Lame parameters,

\[ \mu = \frac{E}{2(1 + \nu)}, \quad \lambda = \frac{E \nu}{(1 + \nu)(1 - 2\nu)} \]  

(5.4)

For a linear elastic material tangent \( C \), the Lame parameters can be used to represent the matrix in the following convenient manner,

\[
C = \begin{bmatrix}
\lambda + 2\mu & \lambda & \lambda \\
\lambda & \lambda + 2\mu & \lambda \\
\lambda & \lambda & \lambda + 2\mu \\
\end{bmatrix}
\]  

(5.5)

When using the paperboard model a very conservative estimate for the dilatational wave speed \( c_d \) is archived using the same expression (5.3) and replacing \( \lambda + 2\mu \) with the initial paperboard stiffness corresponding to the stiffest direction, i.e. the MD direction. Comparing the matrix (5.5) with the initial paperboard stiffness in (4.11) and identifying the part corresponding to the MD direction results in the following conservative estimate,

\[ c_d = \sqrt{\frac{2A_1 + 2A_2 + 2A_5}{\rho}} \]  

(5.6)
Chapter 6

Results

A number of examples has been studied regarding the shell element discussed in the previous sections. From this point forward the solid-shell element is denoted Q1STs in the same fashion as the authors did in [17]. The notation 'Q1' is referring to the first order quadrilateral isotropic framework in which the elements is fundamentally based on while 'ST' is shorthand notation for stabilization based on Taylor expansion. The short case letter 's' is implying the usefulness for problems with a shell like structure.

6.1 Elastic Pinched Cylinder

The solid shell element Q1STs was implemented in the commercial software Abaqus [7] using an VUEL subroutine. To assess the usefulness of the element and to validate the explicit implementation, the pinched cylinder from [11] was considered. This is a benchmark problem with geometric non-linearities and the problem was also studied by the authors of the implicit version of the Q1STs element in [17]. The problem consists of a cylinder pulled in opposite directions resulting in a sealing of the cylinder. The geometry is illustrated in figure 6.1.
The length of the cylinder is $L = 10.35\, mm$, the radius to the inner boundary is $R = 4.953\, mm$ and the thickness of the shell structure is $t = 0.094\, mm$. The material is considered elastic with the module of elasticity and Poisson's ratio being $E = 10.5\, MN/mm^2$ and $\nu = 0.3125$, furthermore the density is taken to be $\rho = 2.8 \cdot 10^{-8}\, Ns^2/mm^4$. Due to symmetry of the problem only one eight of the structure need to be meshed with the boundary conditions applied according to figure 6.2.
The authors in [17] for the implicit version of Q1STs used a force driven formulation applying a total force of $F = 40\, kN$ for both directions. For an explicit analysis this would require a very long simulation time to get the problem to converge towards the static solution, therefore a displacement driven formulation was considered in which the maximum displacement of the pinched node would reach $u_y^A = 2.8\, mm$ referring to figure 6.2. For the implicit formulation of the Q1STs element in [17] the requirement for very good convergence was 16 elements along the length direction and 24 elements along the radius referring to figure 6.2 and only two gausspoints were needed.

Figure 6.3 is showing result of the simulation, plotting the magnitude of the vertical component of the reaction force $F_y^A$ in node A against the magnitude of the vertical displacement $u_y^A$ for node A and the magnitude of the horizontal displacements $u_x^C$ and $u_x^B$ for node C and B respectively. The simulation for the explicit version of Q1STs was done with the same mesh density which resulted in convergence for the implicit version and using the same number of gauss points. The explicit Q1STs element was then compared with both the static reference solution in [11] and results using the Abaqus solid shell element SC8R with higher mesh density, 32 elements along the length and 48 along the radius. There were no apparent difference to the solution using the explicit estimate of the enhanced degree of freedom $W_e$ based on the Euler forward method in (2.79) compared to using an iterative bisection method and the computational speed was approximately 50% faster with the explicit estimate. The final state of deformation for cylinder is illustrated in figure 6.4.
Figure 6.3: Magnitude of the vertical reaction force in A against displacements of node A, B and C. Simulation using the explicit solid shell Q1STs is compared to the static reference solution and results using Abaqus SC8R continuum based solid shell element.
6.2 Simple Deformations with Paperboard Model

In this section the Q1STs element was combined with the highly anisotropic model for paperboard previously discussed in the theory section. In order to validate the response some simple deformation fields where considered and studied using one Q1STs element and the results were compared with a fully eight node integrated continuum element C3D8, present in Abaqus standard library. For the simple fields of deformations presented in this section the C3D8 element is providing a good reference for the solution. The specimen considered in this section had the dimensions of one millimetre for the in-plane directions and the thickness direction was one tenth of the in-plane directions.

Uniaxial tension was simulated along the paperboard Machine Direction (MD), Cross Direction (CD) and 45° between MD and CD. The displacement \( u \) was normalized against the initial length \( L_0 \) to resemble strain and the reaction force \( F \) was normalized against the initial area \( A_0 \) to represent the corresponding stress. The result for the in-plane tension is given in figure 6.5 in which the Q1STs element using two gauss points is compared to the C3D8 Abaqus element and a very good match in obtained. For the out-of-plane direction (ZD) both tension and compression is also accurately captured by the solid shell element with two gauss points in figure 6.5 and 6.7. There where no apparent difference to the simulations of Q1STs in figure 6.5, 6.6 and 6.7 using the anisotropic hourglass matrix in (4.12) and the isotropic one in (2.49).
Out-of-plane shearing of the specimen was considered in which the bottom nodes were fixed and the upper nodes sheared towards the CD-direction on the surface with normal in ZD-direction. The normalized force against displacement for the shearing simulation is shown in figure 6.8 in which the continuum and solid shell element with isotropic hourglass matrix is compared. While the result is matching quite well there is a slight difference. Visualizing the final deformation with ten times magnification for the displacements in figure 6.9 the problem is revealed in form of an hourglass mode for the solid shell element. Using the anisotropic deviatoric hourglass matrix proposed in (4.12) the hourglass mode is removed and a very good match is obtained for the simulation in figure 6.10.

In the out-of-plane shearing situation the paperboard will obtain an increased thickness with the deformation. Therefore a simple shearing in the out-of-plane direction was performed in which the upper boundary is fixed in the ZD direction. The result is given in figure 6.11 in which the Abaqus C3D8 element is compared with the solid shell element using both the isotropic hourglass matrix in (2.49) and the anisotropic proposal in (4.12). In this example the solid shell with linear hourglass matrix is failing quite early into the plastic region while the anisotropic version has a good match with the Abaqus C3D8 element. The final deformation for the Q1STs element with linear hourglass matrix is shown in figure 6.11 and it is apparent that the cause of failure is due to the development of an hourglass mode. Figure 6.13 is showing the evolution of the adaptive effective shear modulus for plasticity $\mu_{eff}^h$ proposed in (2.51) and highlights the value in which the hourglass mode start to propagate. This value is approximately equal to 70 MPa which seems to be in the vicinity of the initial shear modulus for the out-of-plane direction which is 78 MPa for this calibration of paperboard. In figure 6.14 the effective shear modulus is kept fixed and varied until convergence occurs with the anisotropic hourglass matrix, a decent match is obtained with shear modulus equal to 640 MPa.

There were no apparent difference to any simulations in this section using the bisection algorithm to obtain $W_e$ or applying one explicit Euler estimate as proposed in (2.79).
Figure 6.5: Normalized force against displacement for in-plane tension tests along the Machine Direction (MD), Cross Direction (CD) and \(45^\circ\) between CD and MD. Comparison is made for the solid-shell (Q1STs) and Abaqus continuum element (C3D8).

Figure 6.6: Normalized force against displacement for tension test in the out-of-plane direction (ZD). Comparison is made between the solid-shell (Q1STs) and Abaqus continuum element (C3D8).
Figure 6.7: Normalized force against displacement for compression test in the out-of-plane direction (ZD). Comparison is made between the solid-shell (Q1STs) and Abaqus continuum element (C3D8).

Figure 6.8: Normalized force against displacement for shear in out-of-plane direction (ZD) along the Cross Direction (CD). The solid shell (Q1STs) is compared with Abaqus (C3D8) element
Figure 6.9: Final deformation for the shear simulation with ten times magnification of displacements. The solid shell element Q1STs is shown in (a) and Abaqus continuum element C3D8 in (b).

Figure 6.10: Zoom in for the last deformation of the out-of-plane (ZD) shearing simulation. Abaqus continuum element (C3D8) is compared against the solid shell element (Q1STs) with isotropic and anisotropic hourglass matrix.
Figure 6.11: Simple shearing situation for the out-of-plane (ZD) direction in which ZD is fixed. Comparison is made between Abaqus C3D8 element and the solid shell element Q1STs with isotropic hourglass matrix and with anisotropic hourglass matrix.

Figure 6.12: Final deformation in the simple shearing situation with fixed ZD using the Q1STs element with linear hourglass matrix.
Figure 6.13: Evolution history for the adaptive effective shear modulus $\mu_{\text{eff}}^{\text{hg}}$ used in the isotropic hourglass matrix. The example is simple shearing in the out-of-plane direction with fixed ZD. Hourglass mode occurs around $\mu_{\text{eff}}^{\text{hg}} = 70$ MPa.

Figure 6.14: Simple shearing in out-of-plane direction keeping ZD fixed. The effective hourglass shear module $\mu_{\text{eff}}^{\text{hg}}$ is varied and compared to the anisotropic hourglass matrix.
6.3 Paperboard Subject to Bending

In this section the paperboard model in combination with the Q1STs shell element is studied in a bending situation. The problem is described in figure 6.15 in which the shell like structure is fixed in one end and pulled downwards at the bottom nodes of the opposite end until the magnitude of the horizontal displacement $u_A^z = 4 \text{ mm}$ is reached.

In order to obtain a reference solution for the problem a convergence study was investigated using Abaqus C3D8 elements. The sum of the reaction force for the end nodes subject to the horizontal pull is plotted against the absolute vertical displacements for node A, B and C referring to figure 6.15. The result is given in figure 6.16 and convergence using the C3D8 element was achieved for a mesh of 48 elements along the length of the structure and 10 element along the thickness. Only two elements along the width was considered because this dimension is not being deformed.

When simulating the problem using the Q1STs element with isotropic hourglass matrix and adaptive shear modulus the simulation is failing immediately ($|u_A^z| \approx 10^{-7} \text{ mm}$) because of hourglass propagation which is demonstrated in figure 6.17.

Using the anisotropic hourglass matrix in (4.12) with the Q1STs element the hourglass modes were removed and simulations throughout the entire deformation could be obtained without a crash in the simulation. Figure 6.16 is showing simulations in which the number of gauss points for the thickness direction are varied and the mesh of the element is kept fixed with only six elements along the length direction, one element in thickness and two elements in width. Figure 6.18 also includes the reference solution obtained for the convergence study in 6.16. In figure 6.19 the same type of study was done with twelve elements along the length direction. Decent results are obtained compared to the reference solution using six elements in length and eight gausspoints and a good match is achieved with twelve elements in length and eight gausspoints.

No apparent difference on the result was obtained using the bisection method or the explicit estimate based on the Euler-forward scheme in (2.79). Using the explicit method the computational gain in simulation time for eight gauss points and twelve elements amounted to roughly 12% of the simulation time when using the bisection method.
Figure 6.15: Problem formation for bending of paperboard
Figure 6.16: Sum of reaction force for the pulled nodes against the absolute vertical displacements of node A, B and C. Different mesh density for Abaqus C3D8 element is simulated. Convergence is obtained for 48 elements along the length direction and 10 elements along the thickness.
Figure 6.17: Showing the state of deformation before the Q1STs element with linear hourglass and adaptive shear is crashing. The magnification of the displacements are $10^5$. 
Figure 6.18: Sum of reaction force for the pulled nodes against the absolute displacements of node A, B and C. The solid shell element Q1STs is meshed with six elements along the length dimension and the number of gauss integration points are varied. The result is compared with the convergent solution using the Abaqus C3D8 element.
Figure 6.19: Sum of reaction force for the pulled nodes against the absolute displacements of node A, B and C. The solid shell element Q1STs is meshed with twelve elements along the length dimension and the number of gauss integration points are varied. The result is compared with the convergent solution using the Abaqus C3D8 element.
Chapter 7

Discussion and Conclusions

When the explicit solid shell element Q1STs was investigated in the pinched cylinder problem the result was given in figure 6.3. In this figure there is a slight difference between the static reference solution and the Q1STs explicit element and furthermore also a slight difference between the Abaqus continuum shell SC8R. The implicit version of the Q1STs was able to obtain a perfect match for the same mesh which then should also be the case for the explicit version. Looking closely at the graph in figure 6.3 the solid shell in Abaqus and Q1STs element has a very close match at the start of the deformation while the static reference is slightly off even at this early state. This would indicate that there exist a slight difference in the modelling of this specific problem as opposed to something wrong in the implementation of the Q1STs element.

When using the Q1STs element with the isotropic hourglass matrix in (2.49) and the adaptive effective shear modulus in (2.51) the result were poor when combined with the paperboard model. While using an isotropic matrix for the hourglass matrix might work with the paperboard model as indicated by the study in figure 6.14, the use of the adaptive method in (2.51) is certainly not able to hinder the development of hourglass modes according to figure 6.9, 6.12 and 6.17. It is interesting to note from figure 6.9 that the hourglass mode occurs when the adaptive efficient shear modulus approaches the value for the initial out-of-plane shear modulus which is 78 MPa. One possible explanation why the adaptive method fails could be because of the significant difference of the initial shear stiffness between the in-plane (78 MPa) and the out-of-plane (1333 MPa) direction which makes the adaptive method unstable.

The anisotropic hourglass matrix in (4.12) applied to the Q1STs element was able to remove hourglass modes with no visual influence on the solution for the examples studied in this work. Furthermore the usefulness of the element when applied to the paperboard model with anisotropic hourglass matrix was demonstrated in the bending example in which only six element in the length direction was required to obtain decent results referring to figure 6.18. Although it is problematic that more then two gausspoints is required to achieve a good result for this simple bending example which is to be considered as a thin shell problem. As such two gausspoints should be enough to represent a convergent solution, but when using the paperboard a good accuracy was only obtained using eight gausspoints.

The possibility of introducing one Euler forward step (2.79) when using the explicit estimate of $W_e$ in (2.77) was investigated and the results did not differ for any examples when
compare with using the iterative bisection method on equation $G_w$ to obtain $W_e$. While the bisection method was certainly not optimized the speed of the Euler forward version could be as much as eight times faster which is quite substantial. Using the euler forward method is new compared to the article in [15] were the authors used one Newton Raphson step in the explicit estimate which require the calculation of the material tangent $C^*$ referring to (2.78). Although the material tangent is not needed in the Euler estimate this method does require one more loop throughout the gausspoints.

It should admittedly be stated that from a fundamental point of view this element might not be the most optimal solid shell to combine with the complex paperboard model. This is because the material model is developed in the spatial configuration while the element is constructed using the material configuration. To be able to combine the two requires use of the pullback procedure in (4.9) which in turn consists of solving two eigenvalue (vector) problems corresponding to the spectral decompositions in (4.4) and (4.7). This procedure is required for each gausspoint and can potentially be quite time consuming.

Although this element might not be optimal with the paperboard model it could still be interesting for future work to investigate a broader range of examples. One such example could be the sealing of a Tetra Pak container similar to the pinched cylinder example investigated with elasticity in this work. Such an example was considered by the author in this work but some programming difficulties arouse with having different fiber directions (MD,CD,ZD) for the elements in the mesh and the investigation was cancel due to lack of time.
Chapter 8

Appendix

8.1 Appendix A

The polynomial form of the tri-linear shape functions established in equation (2.7) have the following structure,

\[ N(\xi) = [N_1, \ldots, N_8]^T = r + \xi g_1 + \eta g_2 + \zeta g_3 + \xi \eta h_1 + \eta \zeta h_2 + \xi \zeta h_3 + \xi \eta \zeta h_4 \]

And the polynomial coefficients in the above expression reads,

\[ r = \frac{1}{8}[1, 1, 1, 1, 1, 1, 1, 1]^T \]
\[ g_1 = \frac{1}{8}[-1, 1, -1, -1, 1, 1, 1, 1]^T \]
\[ g_2 = \frac{1}{8}[-1, 1, 1, -1, 1, -1, 1, 1]^T \]
\[ g_3 = \frac{1}{8}[-1, -1, 1, 1, 1, 1, 1, 1]^T \]
\[ h_1 = \frac{1}{8}[1, -1, 1, -1, 1, 1, -1, 1]^T \]
\[ h_2 = \frac{1}{8}[1, 1, 1, -1, 1, -1, 1, 1]^T \]
\[ h_3 = \frac{1}{8}[1, -1, 1, 1, 1, 1, -1, 1]^T \]
\[ h_4 = \frac{1}{8}[-1, -1, 1, 1, 1, 1, 1, 1]^T \] (A1)

The Jacobian matrix was rewritten into polynomial form with the following structure

\[ \mathbf{J} = \mathbf{J}^0 + \xi \mathbf{J}^\xi + \eta \mathbf{J}^\eta + \zeta \mathbf{J}^\zeta + \xi \eta \mathbf{J}^{\xi \eta} + \eta \zeta \mathbf{J}^{\eta \zeta} + \xi \zeta \mathbf{J}^{\xi \zeta} \]

and the matrix coefficients corresponding to the constant and linear terms are given by,

\[ \mathbf{J}^0 = \begin{bmatrix} g_1^T X_{1e} & g_2^T X_{1e} & g_3^T X_{1e} \\ g_1^T X_{2e} & g_2^T X_{2e} & g_3^T X_{2e} \\ g_1^T X_{3e} & g_2^T X_{3e} & g_3^T X_{3e} \end{bmatrix}, \quad \mathbf{J}^\xi = \begin{bmatrix} 0 & h_1^T X_{1e} & h_2^T X_{1e} \\ 0 & h_1^T X_{2e} & h_2^T X_{2e} \\ 0 & h_1^T X_{3e} & h_2^T X_{3e} \end{bmatrix} \]

\[ \mathbf{J}^\eta = \begin{bmatrix} h_1^T X_{1e} & 0 & h_2^T X_{1e} \\ h_1^T X_{2e} & 0 & h_2^T X_{2e} \\ h_1^T X_{3e} & 0 & h_2^T X_{3e} \end{bmatrix}, \quad \mathbf{J}^{\xi \eta} = \begin{bmatrix} h_1^T X_{1e} & h_2^T X_{1e} & 0 \\ h_1^T X_{2e} & h_2^T X_{2e} & 0 \\ h_1^T X_{3e} & h_2^T X_{3e} & 0 \end{bmatrix} \]

\[ \mathbf{J}^{\eta \zeta} = \begin{bmatrix} h_1^T X_{1e} & h_2^T X_{1e} & 0 \\ h_1^T X_{2e} & h_2^T X_{2e} & 0 \\ h_1^T X_{3e} & h_2^T X_{3e} & 0 \end{bmatrix}, \quad \mathbf{J}^{\xi \zeta} = \begin{bmatrix} h_1^T X_{1e} & h_2^T X_{1e} & 0 \\ h_1^T X_{2e} & h_2^T X_{2e} & 0 \\ h_1^T X_{3e} & h_2^T X_{3e} & 0 \end{bmatrix} \] (A2)
while the bilinear terms are the following

\[
J^{\xi \eta} = \begin{bmatrix}
0 & 0 & h^T_1 X_{1e} \\
0 & 0 & h^T_1 X_{2e} \\
0 & 0 & h^T_1 X_{3e}
\end{bmatrix}, \quad J^{\eta \zeta} = \begin{bmatrix}
h^T_1 X_{1e} & 0 & 0 \\
h^T_1 X_{2e} & 0 & 0 \\
h^T_1 X_{3e} & 0 & 0
\end{bmatrix}, \quad J^{\zeta \xi} = \begin{bmatrix}
0 & h^T_1 X_{1e} & 0 \\
0 & h^T_1 X_{2e} & 0 \\
0 & h^T_1 X_{3e} & 0
\end{bmatrix}
\]

The polynomial form of the \( D \) matrix is constructed in a completely analogous manner to the Jacobian matrix,

\[
D = J^0 + \xi D^\xi + \eta D^\eta + \zeta D^\zeta + \xi \eta D^{\xi \eta} + \eta \zeta D^{\eta \zeta} + \xi \zeta D^{\zeta \xi}
\]

with the constant and linear matrix terms given by,

\[
D^0 = \begin{bmatrix}
g_1^T U_{1e} & g_2^T U_{1e} & g_3^T U_{1e} \\
g_1^T U_{2e} & g_2^T U_{2e} & g_3^T U_{2e} \\
g_1^T U_{3e} & g_2^T U_{3e} & g_3^T U_{3e}
\end{bmatrix}, \quad D^\xi = \begin{bmatrix}
0 & h^T_1 U_{1e} & h^T_2 U_{1e} \\
0 & h^T_1 U_{2e} & h^T_2 U_{2e} \\
0 & h^T_1 U_{3e} & h^T_2 U_{3e}
\end{bmatrix}
\]

\[
D^\eta = \begin{bmatrix}
h^T_1 U_{1e} & 0 & h^T_2 U_{1e} \\
h^T_1 U_{2e} & 0 & h^T_2 U_{2e} \\
h^T_1 U_{3e} & 0 & h^T_2 U_{3e}
\end{bmatrix}, \quad D^\zeta = \begin{bmatrix}
h^T_1 U_{1e} & h^T_2 U_{1e} & 0 \\
h^T_1 U_{2e} & h^T_2 U_{2e} & 0 \\
h^T_1 U_{3e} & h^T_2 U_{3e} & 0
\end{bmatrix}
\]

while the corresponding bilinear terms are,

\[
D^{\xi \eta} = \begin{bmatrix}
0 & 0 & h^T_1 U_{1e} \\
0 & 0 & h^T_1 U_{2e} \\
0 & 0 & h^T_1 U_{3e}
\end{bmatrix}, \quad D^{\eta \zeta} = \begin{bmatrix}
h^T_1 U_{1e} & 0 & 0 \\
h^T_1 U_{2e} & 0 & 0 \\
h^T_1 U_{3e} & 0 & 0
\end{bmatrix}, \quad D^{\zeta \xi} = \begin{bmatrix}
0 & h^T_1 U_{1e} & 0 \\
0 & h^T_1 U_{2e} & 0 \\
0 & h^T_1 U_{3e} & 0
\end{bmatrix}
\]

The polynomial form of the transformation matrix \( T \) in expression (2.38) reads,

\[
T = T^0 + \sum_{n=1}^{3} T^{\xi_n} \zeta_n \quad \text{with} \quad (\xi_1, \xi_2, \xi_3) = (\xi, \eta, \zeta)
\]

By introducing the following notation,

\[
\alpha^{0}_{ijkl} = (j_{ij})^0 (j_{kl})^0 \quad \text{and} \quad \alpha^{\xi_n}_{ijkl} = (j_{ij})^0 (j_{kl})^{\xi_n} + (j_{ij})^{\xi_n} (j_{kl})^0
\]

the matrix coefficients for \( T \) are given by,

\[
T^0 = \begin{bmatrix}
\alpha_{1111}^0 & \alpha_{2121}^0 & \alpha_{3131}^0 & \alpha_{1121}^0 & \alpha_{1231}^0 & \alpha_{1131}^0 \\
\alpha_{1212}^0 & \alpha_{2222}^0 & \alpha_{3232}^0 & \alpha_{1222}^0 & \alpha_{2232}^0 & \alpha_{1232}^0 \\
\alpha_{1313}^0 & \alpha_{2323}^0 & \alpha_{3333}^0 & \alpha_{1323}^0 & \alpha_{2333}^0 & \alpha_{1333}^0 \\
2\alpha_{1121}^0 & 2\alpha_{2112}^0 & 2\alpha_{3132}^0 & \alpha_{1221}^0 + \alpha_{1122}^0 & \alpha_{2231}^0 + \alpha_{1213}^0 & \alpha_{1231}^0 + \alpha_{1132}^0 \\
2\alpha_{1213}^0 & 2\alpha_{2223}^0 & 2\alpha_{3233}^0 & \alpha_{1322}^0 + \alpha_{1223}^0 & \alpha_{2332}^0 + \alpha_{2233}^0 & \alpha_{1332}^0 + \alpha_{1233}^0 \\
2\alpha_{1113}^0 & 2\alpha_{2113}^0 & 2\alpha_{3133}^0 & \alpha_{1231}^0 + \alpha_{1123}^0 & \alpha_{2331}^0 + \alpha_{2233}^0 & \alpha_{1331}^0 + \alpha_{1133}^0
\end{bmatrix}
\]
and

\[
T^{\xi_n} = \begin{bmatrix}
\alpha_{11}^{\xi_n} & \alpha_{21}^{\xi_n} & \alpha_{31}^{\xi_n} & \alpha_{12}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{32}^{\xi_n} \\
\alpha_{21}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{12}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{32}^{\xi_n} \\
\alpha_{31}^{\xi_n} & \alpha_{32}^{\xi_n} & \alpha_{33}^{\xi_n} & \alpha_{13}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{33}^{\xi_n} \\
\alpha_{12}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{12}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{32}^{\xi_n} \\
\alpha_{22}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{33}^{\xi_n} & \alpha_{22}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{33}^{\xi_n} \\
\alpha_{13}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{33}^{\xi_n} & \alpha_{13}^{\xi_n} & \alpha_{23}^{\xi_n} & \alpha_{33}^{\xi_n}
\end{bmatrix}
\]  

(A9)

The polynomial form of the Green Lagrangian strain in Voigt format for the Cartesian basis is given in expression (2.40) and the coefficients reads,

\[
\begin{align*}
\dot{E}^0 &= T^0 \hat{E}^0 \\
\dot{E}^{\xi\xi} &= T^\xi \hat{E}^{\xi\xi} + T^\xi \hat{E}^\xi \\
\dot{E}^\eta &= T^\eta \hat{E}^\eta + T^\eta \hat{E}^\eta \\
\dot{E}^{\eta\xi} &= T^\eta \hat{E}^{\eta\xi} + T^\eta \hat{E}^\xi + T^\xi \hat{E}^\eta
\end{align*}
\]

(A10)

where the covariant coefficients are given by,

\[
\dot{E}^0 = \begin{bmatrix}
J_1^{0T} D_1^0 + 1/2 D_1^{0T} D_1^0 \\
J_2^{0T} D_2^0 + 1/2 D_2^{0T} D_2^0 \\
1/4 \sum_{K=A}^D (J_3^{KT} D_3^K + 1/2 D_3^{KT} D_3^K) \\
J_1^{0T} D_2^0 + J_2^{0T} D_1^0 + D_1^{0T} D_2^0 \\
1/4 \sum_{K=E}^H (J_3^{KT} D_3^K + J_3^{KT} D_2^K + D_2^{KT} D_3^K) \\
1/4 \sum_{K=J}^M (J_3^{KT} D_3^K + J_3^{KT} D_2^K + D_2^{KT} D_3^K)
\end{bmatrix}
\]

(A11)

\[
\dot{E}^{\xi\xi} = \begin{bmatrix}
J_1^{\xi T} D_1^\xi + J_1^{\xi T} D_1^0 + D_1^{\xi T} D_1^\xi \\
J_2^{\xi T} D_2^\xi + J_2^{\xi T} D_2^0 + D_2^{\xi T} D_2^\xi \end{bmatrix}
\]

(A12)
\[ \hat{E}^{\zeta} = \begin{bmatrix} J_1^T D_1^\zeta + 1/2 D_1^T D_1^\zeta \\ J_2^T D_2^\zeta + 1/2 D_2^T D_2^\zeta \\ 0 \\ J_1^T D_2^\zeta + J_2^T D_1^\zeta + D_1^T D_2^\zeta \\ 0 \\ 0 \end{bmatrix} \]  
(A13)

\[ \hat{E}^{\xi} = \begin{bmatrix} 0 \\ J_2^T D_2^\xi + J_2^T D_0^\xi + D_2^T D_2^\xi \\ 1/4 \sum_{K=A}^{D} \xi^K (J_3^K D_3^K + 1/2 D_3^K D_3^K) \\ J_1^T D_2^\xi + J_2^T D_1^\xi + D_1^T D_2^\xi \\ 1/4 \sum_{K=E}^{H} \xi^K (J_2^K D_3^K + J_3^K D_2^K + D_2^K D_3^K) \\ 0 \end{bmatrix} \]  
(A14)

\[ \hat{E}^{\eta} = \begin{bmatrix} J_1^T D_1^\eta + J_1^T D_1^\eta + D_1^T D_1^\eta \\ 0 \\ 1/4 \sum_{K=A}^{D} \eta^K (J_3^K D_3^K + 1/2 D_3^K D_3^K) \\ J_2^T D_1^\eta + J_1^T D_0^\eta + D_2^T D_1^\eta \\ 0 \\ 1/4 \sum_{K=J}^{M} \eta^K (J_1^K D_3^K + J_3^K D_1^K + D_1^K D_3^K) \end{bmatrix} \]  
(A15)
The polynomial coefficients for the $B$ in (2.45) are calculated by first introducing the following split,

$$B^0 = \begin{bmatrix} B_1^0, \ldots, B_9^0 \end{bmatrix}$$

$$B^\xi = \begin{bmatrix} B_1^\xi, \ldots, B_9^\xi \end{bmatrix}$$

$$B^{\xi_i} = \begin{bmatrix} B_1^{\xi_i}, \ldots, B_9^{\xi_i} \end{bmatrix}$$

with $(\xi_1, \xi_2, \xi_3) = (\xi, \eta, \zeta)$ and $I = 1, \ldots, 8$

then the Cartesian sub-matrices are given by,

$$B_I^0 = T^0 B_I^0$$

$$B_I^\xi = T^0 B_I^\xi + T^\xi B_I^\xi$$

$$B_I^{\xi_i} = T^0 B_I^{\xi_i} + T^\xi B_I^{\xi_i}$$

(A18)
and the corresponding covariant form of the sub-matrices reads,

\[
\bar{B}^0_I = \begin{pmatrix}
g_{11} \tilde{J}_1^0T \\
g_{21} \tilde{J}_2^0T \\
1/4 \sum_{K=A}^{D} N^K_{I,\xi} \tilde{J}_3^K T \\
g_{11} \tilde{J}_2^0T + g_{21} \tilde{J}_1^0T \\
1/4 \sum_{K=E}^{H} (N^K_{I,\eta} \tilde{J}_3^K T + N^K_{I,\zeta} \tilde{J}_2^K T) \\
1/4 \sum_{K=J}^{M} (N^K_{I,\xi} \tilde{J}_3^K T + N^K_{I,\zeta} \tilde{J}_2^K T)
\end{pmatrix}
\tag{A20}
\]

\[
\bar{B}^\zeta_I = \begin{pmatrix}
h_{31} \tilde{J}_1^0T + g_{11} \tilde{J}_1^\zeta T \\
h_{21} \tilde{J}_2^0T + g_{21} \tilde{J}_2^\zeta T \\
0 \\
h_{21} \tilde{J}_1^0T + h_{31} \tilde{J}_2^0T + g_{21} \tilde{J}_1^\zeta T + g_{11} \tilde{J}_2^\zeta T \\
1/4 \sum_{K=E}^{H} \zeta^K (N^K_{I,\eta} \tilde{J}_3^K T + N^K_{I,\zeta} \tilde{J}_2^K T) \\
1/4 \sum_{K=J}^{M} \zeta^K (N^K_{I,\xi} \tilde{J}_3^K T + N^K_{I,\zeta} \tilde{J}_2^K T)
\end{pmatrix}
\tag{A21}
\]

\[
\bar{B}^{\zeta\zeta}_I = \begin{pmatrix}
h_{31} \tilde{J}_1^\zeta T \\
h_{21} \tilde{J}_2^\zeta T \\
0 \\
h_{21} \tilde{J}_1^\zeta T + h_{31} \tilde{J}_2^\zeta T \\
0 \\
0
\end{pmatrix}
\tag{A22}
\]
\[ \bar{B}_i^\xi = \begin{pmatrix} 0 & h_{11}\bar{J}_2^{\eta T} & g_{21}\bar{J}_2^{\xi T} \\ & & \frac{1}{4} \sum_{K=A}^{D} \xi^K N_{1,\xi}^K \bar{J}_3^{KT} \\ & h_{11}\bar{J}_1^{\eta T} & g_{11}\bar{J}_2^{\xi T} \\ & & \frac{1}{4} \sum_{K=E}^{H} \xi^K (N_{1,\xi}^K \bar{J}_3^{KT} + N_{1,\zeta}^K \bar{J}_2^{KT}) \end{pmatrix} \] (A23)

\[ \bar{B}_i^\eta = \begin{pmatrix} h_{11}\bar{J}_1^{\eta T} & g_{21}\bar{J}_2^{\xi T} \\ 0 & 0 \\ \frac{1}{4} \sum_{K=A}^{D} \xi^K N_{1,\xi}^K \bar{J}_3^{KT} \\ h_{11}\bar{J}_2^{\eta T} & g_{11}\bar{J}_2^{\xi T} \\ 0 & \frac{1}{4} \sum_{K=J}^{M} \eta^K (N_{1,\xi}^K \bar{J}_3^{KT} + N_{1,\zeta}^K \bar{J}_1^{KT}) \end{pmatrix} \] (A24)

\[ \bar{B}_i^{\xi\zeta} = \begin{pmatrix} h_{11}\bar{J}_1^{\eta T} & h_{31}\bar{J}_1^{\eta T} & h_{11}\bar{J}_1^{\xi T} & g_{11}\bar{J}_1^{\xi CT} & 0 \\ 0 & 0 \\ h_{11}\bar{J}_2^{\eta T} & h_{31}\bar{J}_2^{\eta T} & h_{11}\bar{J}_2^{\xi T} & g_{11}\bar{J}_2^{\xi CT} & 0 \\ 0 & 0 \\ \frac{1}{4} \sum_{K=J}^{M} \eta^K \zeta^K (N_{1,\xi}^K \bar{J}_3^{KT} + N_{1,\zeta}^K \bar{J}_1^{KT}) \end{pmatrix} \] (A25)

\[ \bar{B}_i^{\eta\zeta} = \begin{pmatrix} 0 & h_{41}\bar{J}_2^{\xi T} & h_{11}\bar{J}_2^{\xi T} & g_{11}\bar{J}_2^{\xi CT} \\ 0 & 0 \\ h_{41}\bar{J}_1^{\xi T} & h_{31}\bar{J}_2^{\xi T} & h_{11}\bar{J}_2^{\xi T} & g_{11}\bar{J}_2^{\xi CT} \\ 0 & 0 \\ \frac{1}{4} \sum_{K=E}^{H} \xi^K \zeta^K (N_{1,\xi}^K \bar{J}_3^{KT} + N_{1,\zeta}^K \bar{J}_2^{KT}) \end{pmatrix} \] (A26)
Bibliography


