Understanding the deformation gradient in Abaqus and key guidelines for anisotropic hyperelastic user material subroutines (UMATs)

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Abstract

This tutorial paper provides a step-by-step guide to developing a comprehensive understanding of the different forms of the deformation gradient used in Abaqus, and outlines a number of key issues that must be considered when developing an Abaqus user defined material subroutine (UMAT) in which the Cauchy stress is computed from the deformation gradient. Firstly, we examine the "classical" forms of global and local deformation gradients. We then show that Abaqus/Standard does not use the classical form of the local deformation gradient when continuum elements are used, and we highlight the important implications for UMAT development. We outline the key steps that must be implemented in developing an anisotropic fibre-reinforced hyperelastic UMAT for use with continuum elements and local orientation systems. We also demonstrate that a classical local deformation gradient is provided by Abaqus/Standard if structural (shell and membrane) elements are used, and by Abaqus/Explicit for all element types. We emphasise, however, that the majority of biomechanical simulations rely on the use of continuum elements with a local coordinate system in Abaqus/Standard, and therefore the development of a hyperelastic UMAT requires an in-depth and precise understanding of the form of the non-classical deformation gradient provided as input by Abaqus. Several worked examples and case studies are provided for each section, so that the details and implications of the form of the deformation gradient can be fully understood. For each worked example in this tutorial paper the source files and code (Abaqus input files, UMATs, and Matlab script files) are provided, allowing the reader to efficiently explore the implications of the form of the deformation gradient in the development of a UMAT.

Keywords: finite element analysis; abaqus; anisotropic; fibers

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Nomenclature

$\boldsymbol{G}_i$ global basis vector in the i direction.

$\boldsymbol{E}_i$ material basis vector in the reference configuration in the i direction.

$\boldsymbol{e}_i$ material basis vector in the current configuration in the i direction.

$\boldsymbol{I}$ identity matrix.

$\boldsymbol{\chi}$ deformation motion.

$\boldsymbol{X}$, $\boldsymbol{x}$ position vector in the reference and current configuration respectively.

$\boldsymbol{F}$ deformation gradient tensor.

$F_{ij}^{\boldsymbol{EE}}$ components of the "global" deformation gradient in a global $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$ basis system.

$F_{ij}^{\boldsymbol{eE}}$ components of a classical "local" deformation gradient in a local $\boldsymbol{e}_i \otimes \boldsymbol{E}_j$ basis system.

F_{ij}^{al} components of an "Abaqus local" deformation gradient when a local coordinate system is specified with continuum elements.

J determinant of the deformation gradient

$\boldsymbol{R}$ rotational part of the deformation gradient, in co-rotational system used to map $\boldsymbol{E}_i$ to $\boldsymbol{e}_i$.

$\boldsymbol{U}$, $\boldsymbol{V}$ right and left stretch tensors, respectively

$\boldsymbol{U}^{al}$ Abaqus definition of local right stretch tensor

$\overline{\boldsymbol{U}}$ isochoric part of the right stretch tensor

$\boldsymbol{C}$ right Cauchy-Green deformation tensor

$\boldsymbol{C}'$ classical definition of the local right Cauchy-Green deformation tensor

$\boldsymbol{C}^{al}$ Abaqus definition of the local right Cauchy-Green deformation tensor

$\boldsymbol{B}$ left Cauchy-Green deformation tensor

$\boldsymbol{B}'$ classical definition of the local left Cauchy-Green deformation tensorsdfsdfsdf

$\boldsymbol{B}^{al}$ Abaqus definition of the local left Cauchy-Green deformation tensor

$\overline{\boldsymbol{B}}$ isochoric part of the left Cauchy-Green deformation tensor

$\boldsymbol{\theta}$, $\boldsymbol{Q}$, $\boldsymbol{\Phi}$, $\boldsymbol{\rho}$ generic rotation matrix

$\boldsymbol{\sigma}$ Cauchy stress tensor

$\boldsymbol{A}_\beta$, fibre vector in the reference configuration, the subscript β denotes its basis system.

$\boldsymbol{a}_\beta$, fibre vector in the current configuration, the subscript β denotes its basis system.

I_f fibre invariant, square of the stretch of the fibre

1 Introduction

The implementation of new constitutive laws through user defined material subroutines (UMATs) in the finite element software Abaqus represents a powerful tool for researchers in the fields of solid mechanics, biomechanics, structural mechanics and material science. A UMAT is called at each integration point with the deformation gradient matrix provided as input. The user must compute the Cauchy stress tensor as the output from the UMAT (a consistent tangent matrix must also be provided for UMATS (Abaqus/Standard), but not for VUMATs (Abaqus/Explicit)). While the logarithmic strain tensor is also provided as input to a UMAT, it should be noted in hyperelastic constitutive laws for large deformation kinematics that the Cauchy stress tensor is usually constructed from the deformation gradient. Examples include constitutive laws for soft tissue (Holzapfel et al., 2000; Weiss et al., 1996), elastomers and rubber (Mooney, 1940; Rivlin, 1948).

It is often necessary or convenient to define a local material coordinate system (basis) whose orientation varies spatially across a body. For example, in a model of an aneurysm, it is useful to define a local basis system where the basis vectors are tangential to the aneurysm wall so that circumferential and axial stresses may be easily analysed. A local coordinate basis co-rotates along with any rigid body rotation or rotational deformations as the material deforms from the reference to the current configuration. This change of basis throughout the simulation must be accounted for.

A finite element model in Abaqus is defined by an input file which contains all of the relevant information required to run the simulation. An input file consists of several keywords which the Abaqus compiler recognises and interprets. A keyword is usually proceeded by numerical data, for example the position of a node in 3D space, or a switching variable which turns a simulation feature on or off. When viewing an input file, a keyword is easily identified by the asterisk character (*) which precedes it. A local coordinate system is specified in an input file by using the `*orientation` keyword. If this keyword is not present then a global basis scheme is used throughout the simulation (Abaqus Analysis User's Guide; 2.2.5 Orientations, 2019; Abaqus Keywords Reference Guide; *orientation, 2019).

In this paper we demonstrate that the form of the deformation gradient depends on the choice of coordinate basis system (i.e. local or global) and on the element type. The form of the deformation gradient provided as input to an Abaqus user defined material subroutine has not previously been systematically outlined, to the best of our knowledge. In particular we demonstrate that if a local coordinate system is used in conjunction with continuum elements, the form of the deformation gradient provided as input to a UMAT is different to the classical definition of a local deformation gradient matrix. In Section 2 we outline the key differences between the classical form of a local deformation gradient matrix and that provided as input to a UMAT. In Section 3 we then systematically outline the key steps that must be taken by the user in order to develop a UMAT where the local Cauchy stress must be constructed from the deformation gradient using the example of an isotropic hyperelastic material.

The use of anisotropic hyperelastic constitutive models based on structural tensors has become widespread in biomechanics in the past two decades (Holzapfel et al., 2000; Spencer, 1984; Weiss et al., 1996). This class of constitutive model has been used to simulate soft tissues such as: arterial (Creane et al., 2012; Famaey et al., 2013; Ghasemi et al., 2018; Nolan and McGarry, 2015), tendon (Khayyeri et al., 2016; Shearer, 2015) , cartilage (Nagel and Kelly, 2010), skin (Annaidh et al., 2012), myocardium (McEvoy et al., 2018), annulus fibrosis (Eberlein et al., 2004) to name but a few. These constitutive models are based on fibre vectors which indicate the direction in which structurally important fibres are orientated, for example collagen or elastin fibres in arterial tissues (Gaul et al., 2017; Whelan et al., 2019). This offers an attractive, intuitive method to define the anisotropy of a material. The findings of the current study are also relevant to several other fields of biomechanics modelling, including anisotropic deformation of bone behaviour (Feerick and McGarry, 2012) , stress fibre formation in cells (Reynolds et al., 2014), and collagen alignment in tissue engineered scaffolds (Wang et al., 2015).

Fibre vector based constitutive models often take advantage of local coordinate systems as it allows directional mechanical properties determined in straightforward mechanical tests to be deployed in complex geometries. For example, one can calibrate a two-fibre hyperelastic model using biaxial and uniaxial mechanical testing data on arterial tissue in the circumferential and axial directions. If one wishes to simulate an arch shaped artery whose diameter is decreasing along its axial length, a local coordinate system will allow the use of this directionally calibrated model in this complex geometry. In Section 4 we demonstrate the key steps that must be taken by the user to correctly account for fibre rotations in the construction of an anisotropic hyperelastic UMAT.

The creation of advanced UMATs is not straightforward. One must have a strong command of solid mechanics and a comprehensive knowledge of how a constitutive model must be implemented. Additionally, one must be familiar with Fortran, a coding language in which it is easy to make minor but consequential mistakes and is difficult to debug by modern standards. This tutorial paper has been created for three purposes: a) to introduce the reader to the important differences in the continuum mechanics of a body where a global basis system or a local basis system is used, b) to highlight some issues we have found where a local basis system is used in conjunction with continuum elements in Abaqus, c) to provide materials which will act as a starting point to readers who wish to create their own UMATs.

1.1 Document structure

This tutorial paper is intended as a step-by-step guide to developing a comprehensive understanding of the construction of Abaqus UMATs in which the Cauchy stress is computed from the deformation gradient.

In Section 2 we examine the "Classical" forms of global and local deformation gradients. We then show that Abaqus does not use the classical form of the local deformation gradient when continuum elements are used. We highlight the important implications this has for writing user-defined material subroutines (UMATs) for isotropic hyperelastic material laws (Section 3), and anisotropic fibre-reinforced hyperelastic material laws (Section 4).

Further case studies are presented in Section 5 highlighting the errors which will occur if the local deformation gradient in Abaqus is not correctly managed. Several worked examples are provided for each section. The user is provided with all required code (Abaqus input files, UMATs, and Matlab script files) to systematically work through each example.

1.2 Access to Codes

The codes created for this tutorial paper are stored and will be maintained at the GitHub site https://github.com/LallyLabTCD/localBasisAbaqus/releases/tag/1.3. Additionally, the codes have been archived at zenodo.org and have the DOI: https://doi.org/10.5281/zenodo.1968356

2 Lesson A: The deformation gradient in global and local coordinate systems

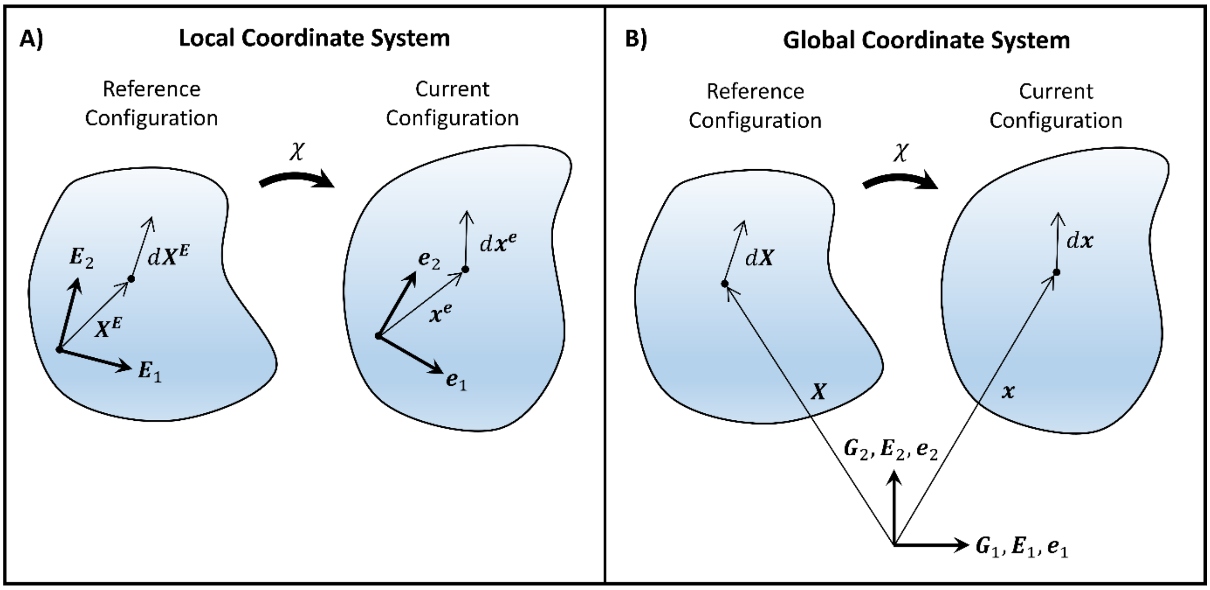

Figure 1: 2-D schematic demonstrating the coordinate bases used in the reference and current configurations in Abaqus. The basis $\boldsymbol{G}_i$ is the global basis, $\boldsymbol{E}_i$ is the basis in the reference configuration at the material point defined by position vector $\boldsymbol{X}$, and $\boldsymbol{e}_i$ is the basis in the current configuration of the same material point which has undergone a motion χ; this point is defined by position vector $\boldsymbol{x}$. **A)** In the case where a local coordinate basis is used, this basis need not be orthogonal to the global basis in the reference configuration; i.e. $\boldsymbol{E}_i$ need not be orthogonal to $\boldsymbol{G}_i$. Importantly, under a motion χ the local basis co-rotates with any rigid body rotations. **B)** The default setting in Abaqus where the global coordinate basis is used throughout the simulation. Both $\boldsymbol{E}_i$ and $\boldsymbol{e}_i$ are *colinear* to the global basis $\boldsymbol{G}_i$.

Figure 1 shows the typical kinematic setup in large deformation continuum mechanics where we consider a generic body in two configurations. The first is the reference configuration which is the starting position of the body. In this paper we assume that in the reference configuration the body is undeformed and holds no stress or strain (while this convention is widely adapted, it should be noted that it is not necessary that the reference configuration is a stress/strain free configuration). Next, as shown in Figure 1, starting from the reference configuration a deformation χ is applied to the body, after which we consider the deformed body to be in the current configuration.

In this paper we refer to three distinct coordinate systems (orthogonal basis vector systems) which are shown in Figure 1. Firstly, there is the set of global basis vectors $\boldsymbol{G}_i$ where i is the number of spatial dimensions; this is typically a Cartesian coordinate system. Secondly, we describe a set of orthogonal basis vectors at a material point in the reference configuration which we denote as $\boldsymbol{E}_i$. Finally, we define a set of orthogonal basis vectors at a material point in the current configuration which we denote as $\boldsymbol{e}_i$.

Figure 1 illustrates the key difference between global and local coordinate systems in terms of the relationship between the basis vector systems and the material deformation. When a local scheme is used (Figure 1A), one may define a uniquely orientated local orthogonal material basis system $\boldsymbol{E}_i$ at any point in the body in the reference configuration. This local basis system maps to the local basis system in the current configuration $\boldsymbol{e}_i$ which may have its own unique orientation. In a co-rotational system, $\boldsymbol{e}_i$ is determined by a rotational transformation of $\boldsymbol{E}_i$ based on the rotational deformation of the material. In the following sections we attempt to provide an in-depth explanation and understanding of the implications of such transformation of the basis vectors. In Abaqus, a local orthogonal material basis system $\boldsymbol{E}_i$ is defined using the `*orientation` keyword.

In the case of a global scheme (Figure 1B) the relationship is straightforward; material basis vectors in the reference and current configurations $\boldsymbol{E}_i$ and $\boldsymbol{e}_i$ are colinear with the global basis vectors $\boldsymbol{G}_i$. Essentially, $\boldsymbol{E}_i = \boldsymbol{e}_i = \boldsymbol{G}_i$ regardless of deformations.

2.1 Basic kinematics

The deformation gradient is the fundamental unit of deformation in finite strain and hyperelastic continuum mechanics. It is defined as,

$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}, \tag{1}$$

where $\boldsymbol{X}$ is a position vector in the reference configuration, and $\boldsymbol{x}$ is a position vector in the current configuration (Abaqus Theory Guide; 1.4.1 Deformation, 2019). The deformation gradient may be multiplicatively decomposed into two parts, one representing the rotational part of the deformation and the other representing the stretching part. This is known as a polar decomposition and is given as,

$$\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U} = \boldsymbol{V} \cdot \boldsymbol{R} \tag{2}$$

where the rotational part of the deformation gradient is the rotation matrix $\boldsymbol{R}$, and the stretching part of the deformation with respect to (w.r.t) the reference configuration is the right stretch tensor $\boldsymbol{U}$ and the stretching part of the deformation w.r.t. the current configuration is the left stretch tensor $\boldsymbol{V}$.[1]

The right Cauchy-Green deformation tensor, commonly used in finite deformation continuum mechanics and hyperelasticity, is given as

$$\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F} \tag{3}$$

Using (2), this can be written in terms of the right stretch tensor,

[1] Both $\boldsymbol{U}$ and $\boldsymbol{V}$ are symmetric tensors, and any rotation matrix $\boldsymbol{R}$ has the property $\boldsymbol{R}^{-1} = \boldsymbol{R}^T$.

$$C = U^T \cdot R^T \cdot R \cdot U = U \cdot U. \tag{4}$$

Similarly, the left Cauchy-Green deformation tensor, is given as

$$B = F \cdot F^T \tag{5}$$

Using (2), this can be written in terms of the right stretch tensor,

$$B = R \cdot U \cdot U^T \cdot R^T = R \cdot C \cdot R^T. \tag{6}$$

2.2 Local and global basis vectors and deformation gradient components

Consider a local scheme, as shown in Figure 1A, whereby the basis vectors $\boldsymbol{e}_i$ used to describe deformed material points in the current configuration are not the same as the basis vectors $\boldsymbol{E}_i$ used to describe the corresponding material points in the undeformed reference configuration (i.e. $\boldsymbol{e}_i \neq \boldsymbol{E}_i$). In a local scheme the basis vectors $\boldsymbol{E}_i$ are fixed, while $\boldsymbol{e}_i$ can change as the material deforms/rotates. Assuming that $\boldsymbol{E}_i = \boldsymbol{G}_i \neq \boldsymbol{e}_i$, the deformation gradient can be computed as follows (Bonet and Wood, 2008)[2]:

$$\boldsymbol{F} = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} (\boldsymbol{e}_i \otimes \boldsymbol{E}_j) = \sum_{i,j=1}^{3} F_{ij}^{\boldsymbol{eE}} (\boldsymbol{e}_i \otimes \boldsymbol{E}_j); \tag{7}$$

where the superscripts are introduced to emphasise that the coordinates $x_i^{\boldsymbol{e}}$ of the deformed position vector $\boldsymbol{x}$ are w.r.t. the basis vectors $\boldsymbol{e}_i$ and the coordinates $X_i^{\boldsymbol{E}}$ of the undeformed position vector $\boldsymbol{X}$ are w.r.t. the basis vectors $\boldsymbol{E}_i$, whereby $\boldsymbol{x} = x_i^{\boldsymbol{e}} e_i$ and $\boldsymbol{X} = X_i^{\boldsymbol{E}} E_i$. It should be noted that the deformation gradient is a two-point tensor, given that it refers to both the reference configuration (with vectors $\boldsymbol{E}_i$) and the deformed configuration (with vectors $\boldsymbol{e}_i$).

In a global scheme, as shown in Figure 1B, the same basis system is used for the reference and current configurations, i.e. $\boldsymbol{E}_i = \boldsymbol{e}_i = \boldsymbol{G}_i$, such that $\boldsymbol{x} = x_i^E E_i$ and $\boldsymbol{X} = X_i^E E_i$. In a global scheme $\boldsymbol{e}_i$ $(= \boldsymbol{E}_i)$ is fixed and does not rotate with the material, in contrast to a local scheme. The deformation gradient can be computed as,

$$\boldsymbol{F} = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}} (\boldsymbol{E}_i \otimes \boldsymbol{E}_j) = \sum_{i,j=1}^{3} F_{ij}^{\boldsymbol{EE}} (\boldsymbol{E}_i \otimes \boldsymbol{E}_j); \tag{8}$$

Noting that the dyadic product $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$ has a value of one at the $(i,\ j)$ component and zero everywhere else, the components of $\boldsymbol{F}$ in a global scheme are given as $\frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}}$.

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[2]Unless otherwise stated we assume that $\boldsymbol{E}_i = \boldsymbol{G}_i$. In Section 2.6 we consider the special case where $\boldsymbol{E}_i \neq \boldsymbol{G}_i$.

Returning again to the general case of a local system where $\boldsymbol{e}_i \neq \boldsymbol{E}_i$ (as illustrated in Figure 1B), the basis vectors of the current and reference configuration can be related through a standard transformation such that

$$\boldsymbol{e}_i = \boldsymbol{\theta} \cdot \boldsymbol{E}_i$$

or in index notation,

$$\boldsymbol{e}_i = \sum_{k=1}^{3} \theta_{ki} \boldsymbol{E}_k \tag{9}$$

Substituting into (8) we can relate the deformation gradient components in the local $\boldsymbol{e}_i \otimes \boldsymbol{E}_j$ basis system and the global $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$ system,

$$\boldsymbol{F} = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} \left(\boldsymbol{e}_i \otimes \boldsymbol{E}_j\right) = \sum_{i,j,k=1}^{3} \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} \theta_{ki} \boldsymbol{E}_k \otimes \boldsymbol{E}_j = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}} \left(\boldsymbol{E}_i \otimes \boldsymbol{E}_j\right) \tag{10}$$

Expanding the third and fourth expressions in equation (10) above it is straightforward to show (see Appendix A.1) that,

$$\sum_{k=1}^{3} \theta_{ik} \frac{\partial x_k^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} = \frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}} \tag{11}$$

$$F_{ij}^{\boldsymbol{EE}} = \theta_{ik} F_{kj}^{\boldsymbol{eE}} \tag{12}$$

If we drop the i, j, k index notation we can write (12) using tensor notation

$$\boldsymbol{F}^{\boldsymbol{EE}} = \boldsymbol{\theta} \cdot \boldsymbol{F}^{\boldsymbol{eE}} \tag{13}$$

Or the reverse relationship,

$$\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{\theta}^{T} \cdot \boldsymbol{F}^{\boldsymbol{EE}} \tag{14}$$

And it should also be noted that,

$$\boldsymbol{F}^{\boldsymbol{EE}} = \boldsymbol{F} \tag{15}$$

A key point to note from equation (13) is that, because the deformation gradient is a two-point tensor, formed from the reference configuration (with basis vectors $\boldsymbol{E}_i$) and the current configuration (with basis vectors $\boldsymbol{e}_i$), only one operation is required to transform $\boldsymbol{F}^{\boldsymbol{EE}}$ to $\boldsymbol{F}^{\boldsymbol{eE}}$. In other words, it is clearly not correct to state that transformation of the deformation gradient requires two operations, i.e. $\boldsymbol{F}^{\boldsymbol{eE}} \neq \boldsymbol{\theta}^T \cdot \boldsymbol{F}^{\boldsymbol{EE}} \cdot \boldsymbol{\theta}$, in contrast to a conventional second order tensor $\boldsymbol{S}$ (e.g. Cauchy stress) where the standard transformation is given as $\boldsymbol{S}^{\boldsymbol{ee}} = \boldsymbol{\theta}^T \cdot \boldsymbol{S}^{\boldsymbol{EE}} \cdot \boldsymbol{\theta}$. We shall return to this important point in Section 2.3.

2.2.1 Co-rotational local system:

In a *co-rotational system*, the rotation of the basis vectors is given by $\boldsymbol{R}$ from the polar decomposition $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$, the current basis vector is given by,

$$\boldsymbol{e}_i = \boldsymbol{R} \cdot \boldsymbol{E}_i \tag{16}$$

Following from (9) and (13) above, we can write,

$$\boldsymbol{F}^{\boldsymbol{EE}} = \boldsymbol{R} \cdot \boldsymbol{F}^{\boldsymbol{eE}} \tag{17}$$

Noting that the rotation matrix $\boldsymbol{R}$ is orthogonal, we can write the co-rotational local deformation gradient $\boldsymbol{F}^{\boldsymbol{eE}}$ as

$$\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{R}^T \cdot \boldsymbol{F}^{\boldsymbol{EE}} = \boldsymbol{R}^T \cdot \boldsymbol{R} \cdot \boldsymbol{U} = \boldsymbol{U} \tag{18}$$

This demonstrates that in a co-rotational system the local deformation gradient is the Cauchy-Green stretch tensor. This result is expected, given that a co-rotational system is not affected by rigid body rotations.

The right and left Cauchy-Green deformation tensors can be written in terms of the local basis system using the definitions in (3), (5), (18) and the polar decomposition in (2),

$$\boldsymbol{B}^{\boldsymbol{ee}} = \boldsymbol{F}^{\boldsymbol{eE}} \cdot (\boldsymbol{F}^{\boldsymbol{eE}})^T \tag{19}$$

$$\boldsymbol{B}^{\boldsymbol{ee}} = \boldsymbol{R}^T \cdot \boldsymbol{F}^{\boldsymbol{EE}} \cdot (\boldsymbol{F}^{\boldsymbol{EE}})^T \cdot \boldsymbol{R}$$

$$\boldsymbol{B}^{\boldsymbol{ee}} = \boldsymbol{R}^T \cdot \boldsymbol{R} \cdot \boldsymbol{U} \cdot \boldsymbol{U}^T \cdot \boldsymbol{R}^T \cdot \boldsymbol{R} = \boldsymbol{U} \cdot \boldsymbol{U}$$

where once again the superscripts indicate the basis vectors of the tensor. Similarly,

$$\boldsymbol{C}^{\boldsymbol{EE}} = (\boldsymbol{F}^{\boldsymbol{eE}})^T \cdot \boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{U} \cdot \boldsymbol{U} \tag{20}$$

Therefore,

$$\boldsymbol{C}^{\boldsymbol{EE}} = \boldsymbol{B}^{\boldsymbol{ee}} \tag{21}$$

2.3 Abaqus/Standard form of the local deformation gradient for continuum elements in a local basis system

When continuum elements are used in Abaqus/Standard (Abaqus Analysis User's Guide; 28.1 General Purpose Continuum Elements, 2019) in conjunction with a user defined material subroutine (UMAT), the deformation gradient and other tensors are provided as input to the UMAT are defined w.r.t. the global basis system, provided that a local basis system is *not* defined through a `*orientation` statement[3]. Essentially, at all material points $\boldsymbol{E}_i = \boldsymbol{e}_i = \boldsymbol{G}_i$, as shown in Figure 1A. Importantly, the deformation gradient components that are input to the UMAT are correctly given as $\frac{\partial x_i^E}{\partial X_j^E}$ and are fully consistent with the expression for $\boldsymbol{F}$ given in equation (8).

In Abaqus one may define a local coordinate frame where the basis vectors in the reference configuration, $\boldsymbol{E}_i$, are directly specified by the user. This feature is invoked when the `*orientation` keyword is used. In such a scheme, the basis vectors in the current configuration $\boldsymbol{e}_i$ co-rotate with the material, as described in equation (18). We denote $\boldsymbol{F}^{al}$ as the deformation gradient that is passed to a UMAT when such a local coordinate system is used in conjunction with continuum elements in Abaqus/Standard. The superscript "al" denotes "abaqus local". As we will describe in the following, $\boldsymbol{F}^{al}$ does not correspond to the classical form of a global ($\boldsymbol{F}^{\boldsymbol{EE}}$, equation (8)) or local ($\boldsymbol{F}^{\boldsymbol{eE}}$, equation (11)) deformation gradient. Instead, $\boldsymbol{F}^{al}$ is related to the global deformation gradient $\boldsymbol{F}$ (in the $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$) basis system through the following operation:

$$\boldsymbol{F}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R} \tag{22}$$

As discussed in Section 2.2 above, such a transformation is only appropriate for a single basis tensor (Cauchy stress is an example of such a tensor) whose basis is to be changed from $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$ to $\boldsymbol{e}_i \otimes \boldsymbol{e}_j$, rather than a two-point tensor where the basis is given as $\boldsymbol{e}_i \otimes \boldsymbol{E}_j$. Recalling equation (14), we once again emphasise that the correct transformation of the deformation gradient from a global to a local co-rotational scheme is given as $\boldsymbol{F}' = \boldsymbol{R}^T \cdot \boldsymbol{F} = \boldsymbol{U}$.

The unconventional form of $\boldsymbol{F}^{al}$ has important consequences for the calculation of deformation tensors and for fibre vector kinematics. Consider, for example, the Cauchy-Green deformation tensors,

$$\boldsymbol{C}^{al} = (\boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R})^T \cdot (\boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R}) \tag{23}$$

$$\boldsymbol{C}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R} = \boldsymbol{R}^T \cdot \boldsymbol{C} \cdot \boldsymbol{R} = \boldsymbol{R}^T \cdot \boldsymbol{U} \cdot \boldsymbol{U} \cdot \boldsymbol{R}$$

and

[3] In an Abaqus/Standard UMAT the deformation gradient components are stored under the variable names `DFGRAD1` (current increment) and `DFGRAD0` (previous increment).

$$\boldsymbol{B}^{al} = (\boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R}) \cdot (\boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R})^{\boldsymbol{T}} \tag{24}$$

$$\boldsymbol{B}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{F}^T \cdot \boldsymbol{R} = \boldsymbol{R}^T \cdot \boldsymbol{B} \cdot \boldsymbol{R}$$

so that

$$\boldsymbol{B}^{al} = \boldsymbol{U} \cdot \boldsymbol{U}^T = \boldsymbol{U} \cdot \boldsymbol{U} \tag{25}$$

Therefore, in contrast with the classical definition of the local deformation tensors in (21), in Abaqus,

$$\boldsymbol{C} = \boldsymbol{B}^{al} \neq \boldsymbol{C}^{al} \tag{26}$$

This result has important consequences for the implementation of hyperelastic constitutive models and it is crucial that mechanicians writing user-defined materials in Abaqus are aware of it. The difference between $\boldsymbol{F}'$ and $\boldsymbol{F}^{al}$ also has important consequences for the use of the Abaqus utility subroutine `sprind`, as discussed in Appendix A.2.

2.3.1 Relating the classical local deformation gradient $\boldsymbol{F}^{\boldsymbol{eE}}$ to the abaqus local deformation gradient $\boldsymbol{F}^{al}$

Let us probe a little further into (22), using (2),

$$\boldsymbol{F}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R} = \boldsymbol{R}^T \cdot \boldsymbol{R} \cdot \boldsymbol{U} \cdot \boldsymbol{R} = \boldsymbol{U} \cdot \boldsymbol{R} \tag{27}$$

Contrast this with the classical expression for the local deformation gradient in (18). Though (27) is similar to the polar decomposition in outlined in (2), the ordering of $\boldsymbol{U}$ and $\boldsymbol{R}$ is incorrect.

A relationship for the local right stretch tensor can also be established using (27),

$$\boldsymbol{F}^{al} = \boldsymbol{R} \cdot \boldsymbol{U}^{al} = \boldsymbol{U} \cdot \boldsymbol{R} \tag{28}$$

$$\boldsymbol{U}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{U} \cdot \boldsymbol{R}$$

(Note that no such relationship exists in the classical description of local basis system, whereby $\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{U}$)

One straightforward approach to writing an isotropic hyperelastic UMAT in Abaqus/Standard when a local orientation system is used in conjunction with continuum elements is as follows:

(i) Perform a polar decomposition of $\boldsymbol{F}^{al}$ (which is provided as input to the UMAT) in order to determine $\boldsymbol{R}$.

(ii) Compute $\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{U} = \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T$.

(iii) From $\boldsymbol{F}^{\boldsymbol{eE}}(= \boldsymbol{U})$, compute the Cauchy stress in the deformed local coordinate system.

We will now step through some examples which will underscore the theoretical aspects outlined in this section.

2.4 Worked Example #1: Structural Elements versus Continuum Elements

We will now go through a worked example to illustrate the implications of the use of global and local coordinates in Abaqus. Complementary Abaqus and Matlab files are included in the supplementary data in the folder called "Lesson A - deformation gradient" which will aid in understanding this example.

We first highlight the difference between the treatment of the deformation gradient in structural elements (Abaqus Analysis User's Guide; 29.6 Shell Elements, 2019) such as a shell element, and in continuum elements. Specifically, we compare a four noded shell element to a four noded plane stress element, given that the out of plane stress is zero for both element types.

For direct comparison with a plane stress element, the shell element is constructed in the x-y plane and is constrained to deform only in this plane. A uniaxial stretch with a 45° rotation is imposed on the element, as shown in Figure 2. In the case of the membrane the following components of the deformation gradient is passed to a UMAT, regardless of whether an orientation is prescribed in the membrane section:

$$\boldsymbol{F}^{eE} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1.1 & 0 \\ 0 & 0 & 0.9091 \end{bmatrix} \tag{29}$$

Clearly this deformation gradient matrix corresponds to the right stretch tensor $\boldsymbol{U}$, and is correct for a local co-rotational $\boldsymbol{e}_i \otimes \boldsymbol{E}_j$ basis system. In other words, for membrane elements a default local coordinate system that rotates with the element is always used, so that the resultant *local deformation gradient* does not contain any information on material rotation. It should be noted that the value of $F_{33} = 0.9091$ is simply a consequence of the default implementation of material incompressibility.

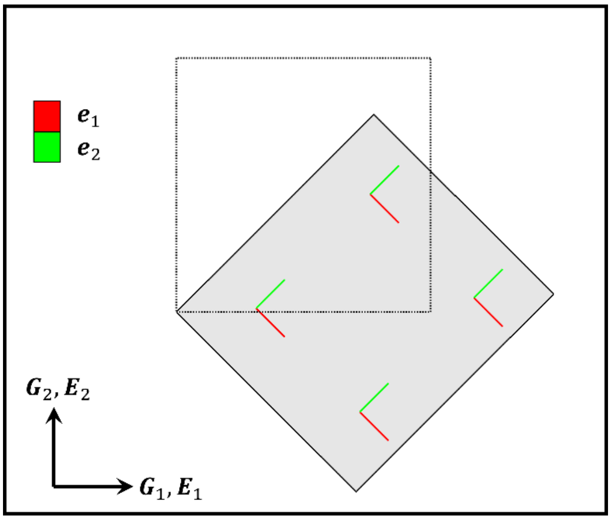

Figure 2 Uniaxial stretch of 10% accompanied by a 45° rotation. This deformation field is applied to membrane and shell element, and to and plane stress and plane strain elements.

In contrast, for a plane stress element, if `*orientation` is not prescribed and an orientation is not prescribed in the solid section, a global scheme is implemented and the following *global* deformation gradient matrix is passed to a UMAT:

$$\boldsymbol{F} = \boldsymbol{F}^{\boldsymbol{EE}} = \begin{bmatrix} 0.7071 & 0.7778 & 0 \\ -0.7071 & 0.7778 & 0 \\ 0 & 0 & 0.9091 \end{bmatrix} \tag{30}$$

A polar decomposition yields,

$$\boldsymbol{U} = \begin{bmatrix} 1. & 0 & 0 \\ 0 & 1.1 & 0 \\ 0 & 0 & 0.9091 \end{bmatrix} \tag{31}$$

And

$$\boldsymbol{R} = \begin{bmatrix} 0.7071 & 0.7071 & 0 \\ -0.7071 & 0.7071 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{32}$$

However, if a *local orientation* is specified in the solid section statement, such that the `*orientation` statements prescribes a local coordinate system that originally coincides with the global system, the following deformation gradient is passed to a UMAT:

$$\boldsymbol{F}^{al} = \begin{bmatrix} 0.7071 & 0.7071 & 0 \\ -0.7778 & 0.7778 & 0 \\ 0 & 0 & 0.9091 \end{bmatrix} \tag{33}$$

As outlined previously, this form of the deformation gradient is related to the global deformation gradient through the following operation:

$$\boldsymbol{F}^{al} = \boldsymbol{R}^{T} \cdot \boldsymbol{F} \cdot \boldsymbol{R} \tag{34}$$

It should be noted that all of the results for plane stress elements outlined above can also be obtained for plane strain elements, with the exception of the F_{33} component, which is equal to 1 due to the imposition of zero out-of-plane strain.

- The Matlab script `Worked_example_1.m` demonstrates the calculation of the Classical and Abaqus definition of the local deformation gradients outlined in Sections 2.2 and 2.3. These correspond to the local deformation gradient when either a structural or continuum element is used respectively.
- The deformation gradient tensor is calculated by a continuum element in Abaqus/Standard with and without the `*orientation` keyword are given in input files `WE1_PStress_Ori.inp` and `WE1_PStress_NoOri.inp`.

- The deformation gradient tensor is calculated by a structural element (shell) in Abaqus/Standard with and without the `*orientation` keyword are given in input files `WE1_Shell_Ori.inp` and `WE1_Shell_NoOri.inp`.

2.4.1 Large rotations and large deformations:

We next consider a uniaxial stretch to a higher nominal strain of 100%, again accompanied by a 45° rigid body rotation, as shown in Figure 3A.

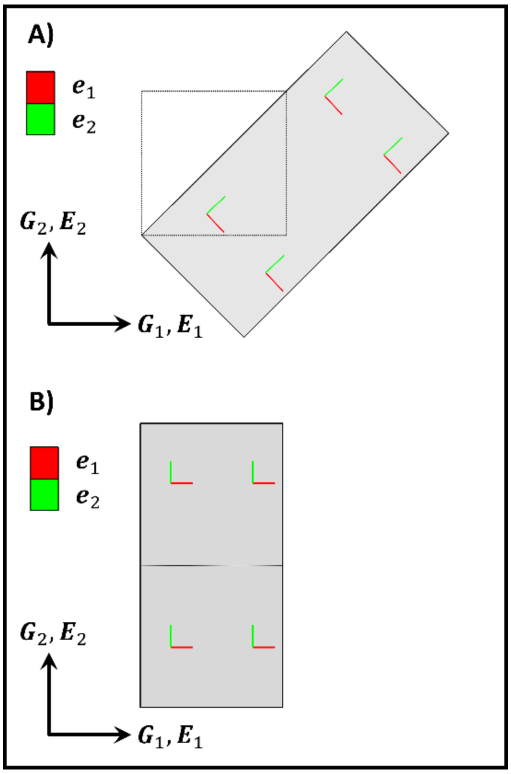

Figure 3 **(A)** Uniaxial stretch of 100% accompanied by a 45° rotation. **(B)** Uniaxial stretch of 100% without rotation.

As expected, a membrane or shell element return the correct local deformation gradient of

$$\boldsymbol{F}^{eE} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \tag{35}$$

regardless of whether `*orientation` is specified in the shell or membrane section statement.

Similarly, in the case of a plane stress continuum element, it a local orientation is not specified in the solid section statement, Abaqus passes the following global deformation to a UMAT:

$$\boldsymbol{F} = \boldsymbol{F}^{EE} = \begin{bmatrix} 0.7071 & 1.4142 & 0 \\ -0.7071 & 1.4142 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \tag{36}$$

Clearly a polar decomposition such that $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$ yields

$$\boldsymbol{U} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \tag{37}$$

And

$$\boldsymbol{R} = \begin{bmatrix} 0.7071 & 0.7071 & 0 \\ -0.7071 & 0.7071 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{38}$$

However, if a local orientation is specified, the following deformation gradient is passed to a UMAT

$$\boldsymbol{F}^{al} = \begin{bmatrix} 0.7312 & 0.6846 & 0 \\ -1.4367 & 1.3902 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \tag{39}$$

In this case, some errors are introduced such that $\boldsymbol{F}^{al} \neq \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R}$**.** The magnitude of the error can be determined from the relationship $\boldsymbol{F}^{al} = \boldsymbol{U}^{al} \cdot \boldsymbol{R}$**,** so that the inaccurate stretch matrix is given as:

$$\boldsymbol{U}^{al} = \begin{bmatrix} 1.0011 & -0.0329 & 0 \\ -0.0329 & 1.9989 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \tag{40}$$

The following additional points should be noted:

(i) Such inaccurate values for $\boldsymbol{F}^{al}$ (and, as a result, for $\boldsymbol{U}^{al}$) are provided by Abaqus for plane stress, plane strain and 3D continuum elements when a local orientation is specified and large deformations are accompanied by large rotations. Such inaccuracies are not observed for large deformations without rotations (e.g. for the deformation shown in Figure 3B, $\boldsymbol{F}^{al} = [1\ 0; 0\ 2]$ as expected).

(ii) Despite the inaccuracy in the values of $\boldsymbol{F}^{al}$, accurate values of log strain and nominal strain are provided by Abaqus. In the example above, accurate values of maximum principal log strain (0.6931) and maximum principal nominal strain (1.0) are obtained, regardless of the choice of element or global/local basis system.

For the accompanying files review the deformation given in (35):

- The Matlab script `Worked_example_1_largeDef.m` demonstrates the calculation of the Classical and Abaqus definition of the local deformation gradients outlined in Sections 2.2 and 2.3. These correspond to the local deformation gradient when either a structural or continuum element is used respectively.
- The deformation gradient tensor is calculated by a continuum element in Abaqus/Standard with the `*orientation` keyword is given in input file `WE1_PStress_Ori_largeDef.inp`.

- The deformation gradient tensor is calculated by a structural (shell) element in Abaqus/Standard with the `*orientation` keyword is given in input file `WE1_Shell_Ori_largeDef.inp`.

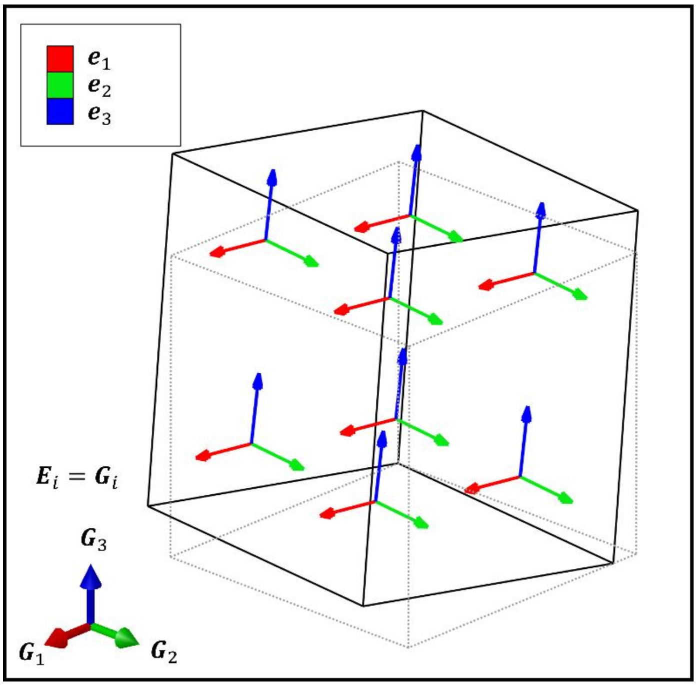

Figure 4 Schematic outlining the reference and current configuration of a unit cube highlighting the relevant basis systems for Worked Example #2. The global basis vectors are $\boldsymbol{G}_i$, and in this particular scenario the material basis vectors in the reference configuration are colinear with the global basis, $\boldsymbol{E}_i = \boldsymbol{G}_i$. The basis vectors in the current configuration $\boldsymbol{e}_i$ are shown at each of the integration points in the unit cube.

2.5 Worked Example #2: Abaqus local deformation gradient in a 3-D continuum element

Consider a unit cube which is subjected to a motion $\boldsymbol{\chi}$ which entails a rotation component, and is described in the global coordinate system by the deformation gradient,

$$\boldsymbol{F}^{\boldsymbol{EE}} = \begin{bmatrix} 1.10 & 0.10 & 0.00 \\ 0.05 & 0.90 & 0.15 \\ 0.20 & 0.00 & 1.20 \end{bmatrix} \tag{41}$$

We now wish to calculate the deformation gradient when a local basis is used. Assuming the local basis is aligned with the global basis in the reference configuration, using (18) the following is obtained[4],

$$\boldsymbol{R} = \begin{bmatrix} 0.995 & 0.035 & -0.089 \\ -0.029 & 0.997 & 0.077 \\ 0.091 & -0.074 & 0.993 \end{bmatrix} \tag{42}$$

$$\boldsymbol{F}^{al} = \begin{bmatrix} 1.114 & 0.105 & 0.011 \\ 0.053 & 0.896 & 0.123 \\ 0.212 & -0.025 & 1.190 \end{bmatrix} \tag{43}$$

To verify that this is indeed the deformation gradient that Abaqus uses when a local coordinate system is invoked, we created a simple FE model of a single 3D unit cube element with full

[4] All presented values have been rounded to 3 decimal places.

integration being deformed according to deformation gradient in (41). The displacement at each node is calculated using $\boldsymbol{u} = \boldsymbol{F} \cdot \boldsymbol{X} - \boldsymbol{X}$, where $\boldsymbol{u}$ is the displacement of a node whose position in the reference configuration is given by $\boldsymbol{X}$.

Figure 4 shows the global basis $\boldsymbol{G}_i$ which in this case is equal to the local material basis in the reference configuration $\boldsymbol{E}_i$ in the unit cube. Also shown is the rotated local material basis $\boldsymbol{e}_i$ in the current configuration.

Figure 5 shows the values of the deformation gradient output to the Abaqus .dat file (see Appendices for how to output the deformation gradient). When a global coordinate system is used we obtain the global deformation gradient given in (41), and when a local coordinate system is used we get the result (43).

- The Matlab script `Worked_example_2.m` demonstrates the calculation of the global and local deformation gradients outlined above.
- The global deformation gradient tensor is calculated by the Abaqus/Standard input file `WE2_global.inp`.
- The local deformation gradient tensor is calculated by the Abaqus/Standard input file `WE2_local.inp`.
- The post-processing file `plotLocalCoordinates.py` plots the material basis vectors in resulting output database (.odb) file from `WE2_local.inp`.

A)

E L E M E N T   O U T P U T

THE FOLLOWING TABLE IS PRINTED FOR ALL ELEMENTS WITH TYPE C3D8 AT THE INTEGRATION POINTS

ELEMENT	PT	FOOT-NOTE	DG11	DG22	DG33	DG12	DG13	DG23	DG21	DG31	DG32
1	1		1.100	0.9000	1.200	0.1000	0.000	0.1500	5.0000E-02	0.2000	0.000
1	2		1.100	0.9000	1.200	0.1000	-8.6736E-18	0.1500	5.0000E-02	0.2000	-3.4694E-18
1	3		1.100	0.9000	1.200	0.1000	6.9389E-18	0.1500	5.0000E-02	0.2000	0.000
1	4		1.100	0.9000	1.200	0.1000	2.0817E-17	0.1500	5.0000E-02	0.2000	-3.4694E-18
1	5		1.100	0.9000	1.200	0.1000	0.000	0.1500	5.0000E-02	0.2000	4.1633E-17
1	6		1.100	0.9000	1.200	0.1000	-9.5410E-18	0.1500	5.0000E-02	0.2000	-6.9389E-18
1	7		1.100	0.9000	1.200	0.1000	2.0817E-17	0.1500	5.0000E-02	0.2000	1.3878E-17
1	8		1.100	0.9000	1.200	0.1000	1.7347E-17	0.1500	5.0000E-02	0.2000	-6.9389E-18

B)

E L E M E N T   O U T P U T

THE FOLLOWING TABLE IS PRINTED FOR ALL ELEMENTS WITH TYPE C3D8 AT THE INTEGRATION POINTS

ELEMENT	PT	FOOT-NOTE	DG11	DG22	DG33	DG12	DG13	DG23	DG21	DG31	DG32
1	1	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	2	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	3	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	4	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	5	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	6	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	7	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02
1	8	OR	1.114	0.8955	1.190	0.1051	1.1480E-02	0.1228	5.3209E-02	0.2123	-2.5428E-02

Figure 5 Output in the .dat file of the deformation gradient from the Abaqus FE simulation of a cube under deformation using **A)** a global coordinate system, and **B)** a local coordinate system. The deformation gradient output in (A) corresponds to (41) The deformation gradient output in (B) corresponds to (43).

2.6 Worked Example #3: Abaqus local deformation gradient in a 3-D continuum element where $\boldsymbol{E}_i \neq \boldsymbol{G}_i$

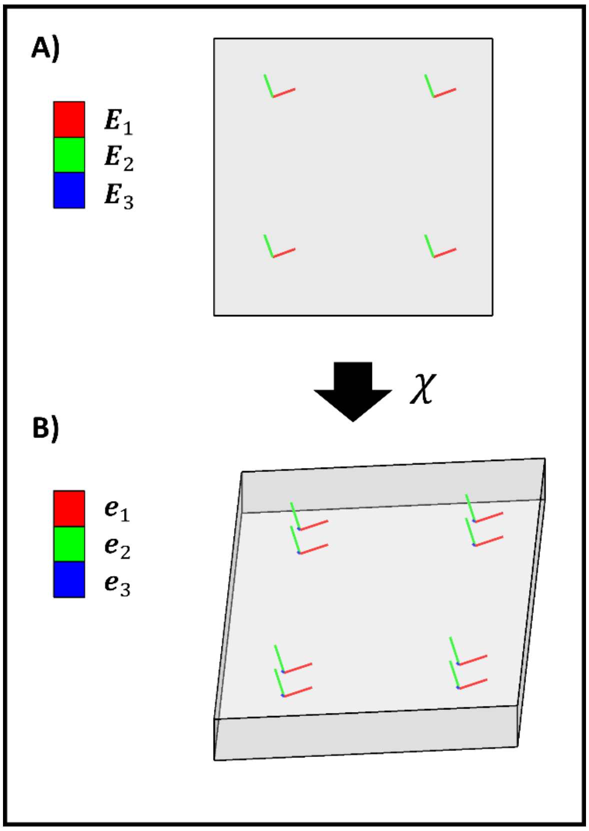

Figure 6 Schematic for Worked Example #3 showing a unit cube in; **A)** the reference configuration with basis vectors $\boldsymbol{E}_i$ rotated 20° about the global $\boldsymbol{G}_3$ basis vector, and **B)** the current configuration showing the co-rotated basis vectors $\boldsymbol{e}_i$.

Next, we consider the same deformation as Worked Example #2, but in this case the reference configuration local coordinate basis is not the same as the global coordinate basis, i.e. $\boldsymbol{E}_i \neq \boldsymbol{G}_i$, instead $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$ are rotated clockwise by 20° about the $\boldsymbol{G}_3$ axis. Starting with the global deformation gradient $\boldsymbol{F}$ given in (41) and using a standard rotation matrix $\boldsymbol{Q}$,

$$\boldsymbol{Q} = \begin{bmatrix} \cos(20°) & -\sin(20°) & 0 \\ \sin(20°) & \cos(20°) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{44}$$

we perform a change of basis of (41) from $\boldsymbol{G}_i$ to the new $\boldsymbol{E}_i$,

$$\boldsymbol{F}_{20}^{EE} = \boldsymbol{Q}^T \cdot \boldsymbol{F}^{GG} \cdot \boldsymbol{Q} \tag{45}$$

where the subscript acts as a reminder that the reference basis vectors are rotated by 20°. The reader will recognise that the transformation in equation (42) above is similar to that for a single point tensor. This is the case because we have merely transformed the global basis vector $\boldsymbol{G}_i \otimes \boldsymbol{G}_j$

to $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$. By performing a polar decomposition on this deformation gradient, $\boldsymbol{F}_{20} = \boldsymbol{R}_{20}\boldsymbol{U}_{20}$, we can calculate the local deformation gradient in this new basis system[5],

$$\boldsymbol{F}_{20}^{al} = (\boldsymbol{R}_{20})^T \cdot \boldsymbol{F}_{20}^{\boldsymbol{EE}} \cdot \boldsymbol{R}_{20} \tag{46}$$

The local deformation gradient, $\boldsymbol{F}_{20}^{al}$, is passed into the UMAT subroutine by Abaqus when a local material basis is used. Abaqus does not provide $\boldsymbol{F}^{\boldsymbol{EE}}$ or $\boldsymbol{F}_{20}^{\boldsymbol{EE}}$.

- The Matlab script `Worked_example_3.m` demonstrates the calculation of the local deformation gradient in the rotated reference material basis outlined above.
- The corresponding Abaqus simulation is performed by running the file `WE3_local.inp`. On inspection of the resulting .dat file from this simulation, one will observe that the deformation gradient is identical to (46).

In the two worked examples above, we start with a global deformation gradient and map to a local deformation gradient. It is important to note that the inverse of this process is achievable, one can start with a local deformation gradient and map back to a global deformation gradient.

[5] On running the Matlab code (`Worked_example_3.m`) you will notice that $\boldsymbol{R}_{20} = \boldsymbol{R}$; this is because the rotation between $\boldsymbol{E}_i$ and $\boldsymbol{e}_i$ is the same in both of these examples.

3 Lesson B: The calculation of stress in an isotropic hyperelastic material

Hyperelastic material models are ideal for use in applications where there are large deformations. Unlike linear elastic or hypoelastic materials, the stress state in a hyperelastic material is a unique function of its deformation, i.e. for a given $\boldsymbol{F}$ there is a unique $\boldsymbol{\sigma}$. Consequently, for a closed-loop deformation, the total work is zero and the starting stress and energy states are recovered. This thermodynamic consistency is evident in the objectivity of stress in hyperelastic materials. This is where the stress state in material is independent of the chosen coordinate system, and no erroneous stresses or stress rates will be computed when the material undergoes rigid body rotation. Practically speaking, one of the easiest ways to ensure that stress objectivity has been preserved when validating a UMAT is to deform a body, then check that the stress invariants[6] remain constant under a subsequent rigid body rotation.

When a user-defined material (UMAT) is used in Abaqus/Standard, the stress which is returned to the FE solver must be given w.r.t. the coordinate basis of that solution increment. As we have seen in the previous lesson, simulations can be posed using a fixed global coordinate basis or a co-rotational local coordinate basis. Regardless of the choice of basis system, for the application of a displacement field $\boldsymbol{\chi}$ must result in the calculation of a unique stress state (in terms of stress invariants) and a unique strain energy density.

In this lesson we will look at the calculation of stress in an isotropic neo-Hookean hyperelastic material. Here, the stress in the global basis is given as,

$$\boldsymbol{\sigma}_{\mathrm{NH}} = \frac{2}{J} C_{10} \left(\overline{\boldsymbol{B}} - \frac{\mathrm{tr}(\overline{\boldsymbol{B}})}{3} \boldsymbol{I} \right) + \frac{2}{D_1} (J-1) \boldsymbol{I} \tag{47}$$

where J is the determinant of the deformation gradient $\boldsymbol{F}$, the left Cauchy-Green tensor $\boldsymbol{B}$ is given in (5) and its isochoric part $\overline{\boldsymbol{B}} = J^{-2/3}\,\boldsymbol{B}$. The material parameters C_{10} and D_1 control the isochoric and volumetric response of the stress respectively. The operator $\mathrm{tr}(\cdot)$ is the trace of a tensor, which in this context is the sum of the diagonal elements.

Let's now consider the construction of the global $\boldsymbol{B}$ tensor in terms of the *Abaqus local* deformation gradient $\boldsymbol{F}^{al}$ that is input to a UMAT when a local orientation is specified for a continuum element. Recalling the definition of $\boldsymbol{F}^{al}$ from Equation (22), the Abaqus local form of the left Cauchy-Green tensor, $\boldsymbol{B}^{al}$, is related to the global $\boldsymbol{B}$ tensor as follows:

$$\boldsymbol{B} = \boldsymbol{F} \cdot \boldsymbol{F}^T = \left(\boldsymbol{R} \cdot \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T\right) \cdot \left(\boldsymbol{R} \cdot \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T\right)^T \tag{48}$$

[6] For example the principal stresses, von Mises stress, and pressure stress are all stress invariants

$$= \quad \boldsymbol{R}\cdot\boldsymbol{F}^{al}\cdot\boldsymbol{R}^T\cdot\boldsymbol{R}\cdot\boldsymbol{F}^{al^T}\cdot\boldsymbol{R}^T$$

$$= \quad \boldsymbol{R}\cdot\boldsymbol{F}^{al}\cdot\boldsymbol{F}^{al^T}\cdot\boldsymbol{R}^T$$

$$= \quad \boldsymbol{R}\cdot\boldsymbol{B}^{al}\cdot\boldsymbol{R}^T$$

So, the left Cauchy-Green tensor $\boldsymbol{B}$ can be mapped from a global to a local coordinate basis in a similar manner as the Cauchy stress is. The isochoric left Cauchy-Green tensor $\overline{\boldsymbol{B}}$ can also be mapped from a global to a local coordinate basis in this manner,

$$\overline{\boldsymbol{B}} = \boldsymbol{R}\cdot\overline{\boldsymbol{B}}^{al}\cdot\boldsymbol{R}^T. \tag{49}$$

If we consider the expression for neo-Hookean stress in (47) in the global basis and substitute for (49) for $\overline{\boldsymbol{B}}$ using (34) we obtain the global stress tensor in terms of the *Abaqus local* deformation tensor $\overline{\boldsymbol{B}}^{al}$,

$$\boldsymbol{\sigma}_{\mathrm{NH}} = \frac{2}{J}C_{10}\left(\boldsymbol{R}\cdot\overline{\boldsymbol{B}}^{al}\cdot\boldsymbol{R}^T - \boldsymbol{R}\cdot\frac{\mathrm{tr}\left(\overline{\boldsymbol{B}}^{al}\right)}{3}\cdot\boldsymbol{R}^T\right) + \frac{2}{D_1}(J-1)\boldsymbol{R}\cdot\boldsymbol{I}\cdot\boldsymbol{R}^T \tag{50}$$

$$= \boldsymbol{R}\cdot\left\{\frac{2}{J}C_{10}\left(\overline{\boldsymbol{B}}^{al} - \frac{\mathrm{tr}\left(\overline{\boldsymbol{B}}^{al}\right)}{3}\boldsymbol{I}\right) + \frac{2}{D_1}(J-1)\boldsymbol{I}\right\}\cdot\boldsymbol{R}^T$$

$$= \boldsymbol{R}\cdot\left\{\boldsymbol{\sigma}_{\mathrm{NH}}^{al}\right\}\cdot\boldsymbol{R}^T$$

The term in the brackets is the local stress which simply follows the rules for the change of basis of a second order tensor. In the context of a UMAT, $\boldsymbol{\sigma}_{\mathrm{NH}}^{al}$ is to be returned to the solver.

Another alternative perspective is to consider the polar decomposition of $\boldsymbol{F} = \boldsymbol{R}\cdot\boldsymbol{U}$, where in much the same way as (48)[7], $\overline{\boldsymbol{B}} = \boldsymbol{R}\cdot\overline{\boldsymbol{U}}^2\cdot\boldsymbol{R}^T$ where $\overline{\boldsymbol{U}} = J^{-1/3}\boldsymbol{U}$. Again, if we consider the expression for neo-Hookean stress in the global coordinate frame,

$$\boldsymbol{\sigma}_{\mathrm{NH}} = \frac{2}{J}C_{10}\left(\boldsymbol{R}\cdot\overline{\boldsymbol{U}}^2\cdot\boldsymbol{R}^T - \boldsymbol{R}\cdot\frac{\mathrm{tr}(\overline{\boldsymbol{U}}^2)}{3}\cdot\boldsymbol{R}^T\cdot\boldsymbol{I}\right) + \frac{2}{D_1}(J-1)\boldsymbol{R}\cdot\boldsymbol{I}\cdot\boldsymbol{R}^T \tag{51}$$

$$= \boldsymbol{R}\cdot\left\{\frac{2}{J}C_{10}\left(\overline{\boldsymbol{U}}^2 - \frac{\mathrm{tr}(\overline{\boldsymbol{U}}^2)}{3}\boldsymbol{I}\right) + \frac{2}{D_1}(J-1)\boldsymbol{I}\right\}\cdot\boldsymbol{R}^T$$

$$= \boldsymbol{R}\cdot\{\boldsymbol{\sigma}_{\mathrm{NH}}^{\mathrm{cr}}\}\cdot\boldsymbol{R}^T$$

The term in brackets is called the co-rotational stress $\boldsymbol{\sigma}_{\mathrm{NH}}^{\mathrm{cr}}$. This is the stress that should be returned to the solver for all elements when using a user-material in Abaqus/Explicit (i.e. via a VUMAT), or for

[7] Note that as $\boldsymbol{U}$ is symmetric, $\boldsymbol{U}\cdot\boldsymbol{U}^T = \boldsymbol{U}\cdot\boldsymbol{U} = \boldsymbol{U}^2$

membrane and shell elements in Abaqus/Standard (i.e. via a UMAT) regardless of whether a local basis is defined in the model. All stress and strain quantities are defined w.r.t. the co-rotational basis. The use of a corotational stress is particularly useful in dynamic and rate dependent simulation as it avoids the computation of erroneous stress rates.

It is noted that the stress in the *Abaqus local* coordinate basis, (50), is the same as the co-rotational stress, (51): i.e. $\boldsymbol{\sigma}_{\mathrm{NH}}^{al} = \boldsymbol{\sigma}_{\mathrm{NH}}^{\mathrm{cr}}$. This is because the local coordinate basis in (50) is the same as a co-rotational basis.

3.1 Worked Example #4: Calculation of the local stress in a continuum element consisting of an isotropic material

We will now go through some of the principles outlined in Lesson B and will calculate the neo-Hookean stress in a material using a global and local basis.

We start with the global deformation gradient $\boldsymbol{F}$ shown in Worked Example #2 and given in (41). Equation (47) is used to calculate the global Cauchy stress tensor using $\overline{\boldsymbol{B}}$, with material properties $C_{10} = 0.2$ MPa and $D_1 = 2.0$ MPa^{-1}. The resulting stress tensor is

$$\boldsymbol{\sigma}_{\mathrm{NH}} = \begin{bmatrix} 0.198 & 0.044 & 0.066 \\ 0.044 & 0.082 & 0.057 \\ 0.066 & 0.057 & 0.276 \end{bmatrix} \tag{52}$$

Using the *Abaqus local* Cauchy-Green deformation tensor $\boldsymbol{B}^{al}$ (48) in the expression for neo-Hookean stress given in (47) we arrive at the expression for the *Abaqus local* stress tensor,

$$\boldsymbol{\sigma}_{\mathrm{NH}}^{al} = \begin{bmatrix} 0.207 & 0.047 & 0.075 \\ 0.047 & 0.077 & 0.041 \\ 0.075 & 0.041 & 0.271 \end{bmatrix} \tag{53}$$

Additionally, the result in (53) is calculated when $\overline{\boldsymbol{U}}^2$ is used in place of $\overline{\boldsymbol{B}}^{al}$ in (47). This is the co-rotational stress. It can also be shown that $\boldsymbol{\sigma}_{\mathrm{NH}}^{al}$ can be directly determined from $\boldsymbol{\sigma}_{\mathrm{NH}}$ using the relationship given in (50).

- The Matlab script `Worked_example_4.m` demonstrates the calculation of the global, local, and co-rotational stress tensors outlined above.
- The global stress tensor is calculated by the Abaqus/Standard input file `WE4_global.inp`.
- The local stress tensor is calculated by the Abaqus/Standard input file `WE4_local.inp`.

3.2 Worked Example #5: Calculation of the local stress in a continuum element consisting of an isotropic material where $\boldsymbol{E}_i \neq \boldsymbol{G}_i$

We now consider the calculation of stress using a neo-Hookean model for the scenario in Worked Example #3. Here the local basis is rotated by 20° about the $\boldsymbol{G}_3$ axis in the reference configuration (refer back to Figure 6), i.e. $\boldsymbol{E}_i \neq \boldsymbol{G}_i$. As we are using the same deformation as Worked Example #4 the global stress is the same as that given in (52). However, in the case of a local basis, we use the deformation gradient $\boldsymbol{F}_{20}^{al}$ given in (46) to calculate the stress, resulting in,

$$\boldsymbol{\sigma}_{\mathrm{NH}}^{al,20} = \begin{bmatrix} 0.222 & 0.006 & 0.084 \\ 0.006 & 0.062 & 0.013 \\ 0.084 & 0.013 & 0.271 \end{bmatrix} \tag{54}$$

The result for the local stress in (54) is also arrived at by using the right stretch tensor $\boldsymbol{U}_{20}$, determined from the polar decomposition of the global deformation gradient in the rotated basis $\boldsymbol{F}_{20}^{\boldsymbol{EE}} = \boldsymbol{R}_{20}\boldsymbol{U}_{20}$, instead of the deformation gradient for the calculation of stress. This is the co-rotational stress and, as noted previously, upon comparison of (50) and (51) the local stress and co-rotational stress are identical, provided they share the same coordinate basis in the reference configuration.

To map the stress calculated in this rotated local basis to the global stress calculated in (52), we may use the transformation,

$$\boldsymbol{\sigma}_{\mathrm{NH}} = \boldsymbol{Q} \cdot \boldsymbol{R}_{20} \cdot \boldsymbol{\sigma}_{\mathrm{NH}}^{al,20} \cdot \boldsymbol{R}_{20}{}^{T} \cdot \boldsymbol{Q}^{T}. \tag{55}$$

where was given previously in (44).

- The Matlab script `Worked_example_5.m` demonstrates the calculation of the local, and co-rotational stress tensors in the rotated reference basis outlined above.
- The local stress tensor is calculated by the Abaqus/Standard input file `WE5_local.inp`.

4 Lesson C: The calculation of stress in an anisotropic hyperelastic material

Lastly, we examine the fibre kinematics and calculation of stress in global and local coordinate bases for a fibre-based anisotropic hyperelastic material. In this scenario, one must take care that the fibre orientation vector is defined w.r.t. the appropriate coordinate basis system.

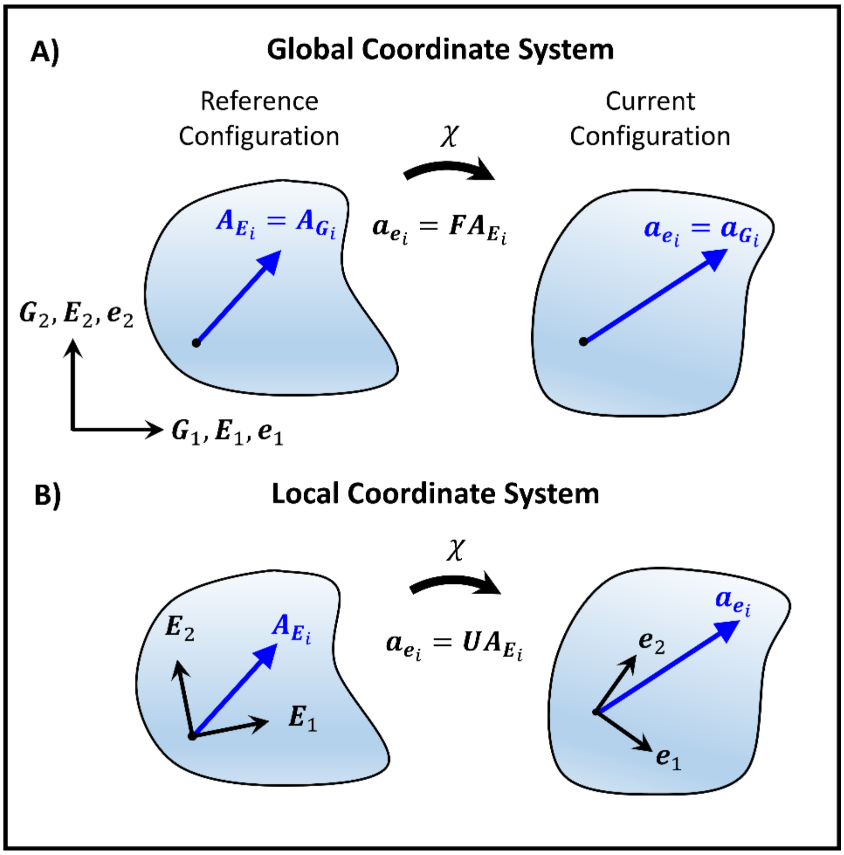

Figure 7: Schematic outlining the key concepts of fibre vector kinematics in a global and local coordinate frame. **A)** Global coordinate frame. As we move from the reference to the current configuration, the basis system does not rotate, $\boldsymbol{e}_i = \boldsymbol{E}_i$. The change of the fibre vector in the reference configuration $\boldsymbol{A}$ to the current configuration $\boldsymbol{a}$ is calculated from the global deformation gradient $\boldsymbol{F}$. **B)** Local coordinate frame. In this case the basis system co-rotates as per (16). The local deformation gradient is (partially) defined w.r.t. this rotated coordinate frame and so too should the deformed fibre vector $\boldsymbol{a}$. This calculated using (58).

4.1 Fibre Kinematics

The orientation of a fibre in the reference configuration is defined by a unit vector $\boldsymbol{A}_\beta$, where we use a capital $\boldsymbol{A}$ to denote that the fibre vector is in the reference configuration, and the subscript β to denote its basis system. As the material is deformed the fibre vector may stretch and rotate in an affine manner such that

$$\boldsymbol{a} = \boldsymbol{F} \cdot \boldsymbol{A}, \tag{56}$$

where lower case $\boldsymbol{a}$ is the fibre vector in the current configuration.

Let us consider the deformation of the fibre vector when a global basis system is used, as illustrated in Figure 7A. The global basis is used in both the reference and current configurations; i.e. $\boldsymbol{E}_i = \boldsymbol{G}_i$. Hence the fibre vector in the current configuration (56) becomes

$$\boldsymbol{a}_{\boldsymbol{E}_i} = \boldsymbol{F}^{\boldsymbol{EE}} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}. \tag{57}$$

In the case of a global scheme in Abaqus/Standard, the user typically defines the fibre direction unit vector $\boldsymbol{A}_{\boldsymbol{E}_i}$ in the global basis, which is typically provided as an input to a UMAT through the user specified material properties. This straightforward approach to the specification of fibre directions is widely used in the literature on fibre based anisotropic hyperelasticity (Gasser et al., 2006; Guo et al., 2006; Holzapfel, 2000; Holzapfel et al., 2000; Weiss et al., 1996).

Figure 7B illustrates the case of a local basis system. In this case the user typically prescribes an undeformed fibre vector $\boldsymbol{A}_{\boldsymbol{E}_i}$ in the reference local coordinate system, $\boldsymbol{E}_i$. The local basis system co-rotates with the material, again with the rotated basis system denoted as $\boldsymbol{e}_i$. Of course, the affine assumption enforces that the fibre also rotates with the material, The deformed fibre vector is then simply obtained using the local deformation gradient such that

$$\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}^{\boldsymbol{eE}} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}. \tag{58}$$

Recall also that $\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{U}$. As previously mentioned, in the case of structural elements in Abaqus/Standard, and in the case of all element types in Abaqus explicit, the user is provided with the classical form of the local deformation gradient $\boldsymbol{F}^{\boldsymbol{eE}} = \boldsymbol{U}$**.** From this, $\boldsymbol{a}_{\boldsymbol{e}_i}$ can be directly calculated.

However, in Abaqus/Standard for the case of a continuum element used with a local basis system (through a `*orientation` statement), a UMAT provides $\boldsymbol{F}^{al} (= \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R} = \boldsymbol{U} \cdot \boldsymbol{R})$ as input, so that the following steps must now be taken to compute $\boldsymbol{a}_{\boldsymbol{e}_i}$:

(i) Perform a polar decomposition of $\boldsymbol{F}^{al}$ (which is provided as input to the UMAT) in order to determine $\boldsymbol{R}$.

(ii) Compute $\boldsymbol{U} = \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T \; (= \boldsymbol{F}')$.

(iii) Compute $\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{U} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}$.

A key component in anisotropic hyperelasticity is the 2nd order structural tensor formed by the operation $\boldsymbol{a} \otimes \boldsymbol{a}$. This operation is written in index notation as, $\boldsymbol{a} \otimes \boldsymbol{a} = a_i a_j$, and may be more simply stated in matrix notation as, $\boldsymbol{a} \otimes \boldsymbol{a} = \boldsymbol{a} \cdot \boldsymbol{a}^T$.

4.2 Anisotropic Structural Tensors, Stress, and Invariant

Once again let us first consider the case of the global coordinate system. The user must compute the structural tensor in the global coordinate system, which follows from Equation (57) as:

$$\boldsymbol{a}_{\boldsymbol{G}_i} \otimes \boldsymbol{a}_{\boldsymbol{G}_i} = \left(\boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i}\right) \cdot \left(\boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i}\right)^T = \boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i} \cdot \boldsymbol{A}_{\boldsymbol{G}_i}{}^T \cdot \boldsymbol{F}^T \tag{59}$$

In standard approaches to modelling fibre reinforced soft tissues (e.g. HGO, Weiss, MA) the stress is given as scalar function of the deformation (let us name it ψ) multiplied by the structural tensor. For a UMAT in a global scheme, the stress is required w.r.t. the global basis system (denoted here as $\boldsymbol{\sigma}_{\boldsymbol{G}_i}$) such that

$$\boldsymbol{\sigma}_{\boldsymbol{G}_i} = \psi(\boldsymbol{F}) \left\{\boldsymbol{a}_{\boldsymbol{G}_i} \otimes \boldsymbol{a}_{\boldsymbol{G}_i}\right\} = \psi(\boldsymbol{F}) \left\{\boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i} \cdot \boldsymbol{A}_{\boldsymbol{G}_i}{}^T \cdot \boldsymbol{F}^T\right\} \tag{60}$$

In a classical corotational local formulation in which the local basis system $\boldsymbol{e}_i$ rotates with the material, such that the global deformation gradient is given as $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$ and the local deformation gradient is simply $\boldsymbol{F}' = \boldsymbol{U}$. In the case of a UMAT in conjunction structural membrane and shell elements in Abaqus/Standard, and for all element types in a VUMAT in Abaqus/Explicit, the user is provided with $\boldsymbol{F}' = \boldsymbol{U}$, and the structural tensor directly follows from equation (58) as follows:

$$\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}' \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{F}'^T = \boldsymbol{U} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{U} \tag{61}$$

In a local scheme the stress is required w.r.t. the deformed local basis system (denoted here as $\boldsymbol{\sigma}_{\boldsymbol{e}_i}$), and is simply given as

$$\boldsymbol{\sigma}_{\boldsymbol{e}_i} = \psi(\boldsymbol{F}') \left\{\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i}\right\} = \psi(\boldsymbol{U}) \left\{\boldsymbol{U} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}{}^T \cdot \boldsymbol{U}^T\right\} \tag{62}$$

Finally, in Abaqus/Standard for the case of a continuum element used with a local basis system (through a `*orientation` statement), a UMAT provides $\boldsymbol{F}^{al}$ as input and $\boldsymbol{\sigma}_{\boldsymbol{e}_i}$ must be computed as output. Recalling that $\boldsymbol{F}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R} = \boldsymbol{U} \cdot \boldsymbol{R}$, such that the deformed fibre vector is given as $\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T \cdot \boldsymbol{A}_{\boldsymbol{E}_i}$, the structural tensor and stress tensor in the deformed local basis system are given as

$$\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{U} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{U}^T = (\boldsymbol{F}^{al} \cdot \boldsymbol{R}^T) \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot (\boldsymbol{R} \cdot \boldsymbol{F}^{al^T}) \tag{63}$$

and

$$\boldsymbol{\sigma}_{\boldsymbol{e}_i} = \psi\left(\boldsymbol{F}^{al}\right) \left\{\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i}\right\} = \psi\left(\boldsymbol{F}^{al}\right) \left\{\boldsymbol{F}^{al} \cdot \boldsymbol{R}^T \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{R} \cdot \boldsymbol{F}^{al^T}\right\} \tag{64}$$

Finally, we examine the scalar anisotropic invariant associated with the fibre vector and resulting structural tensor. In the literature it is commonly referred to as I_4 and here we shall call it I_f, where

f is the fibre vector it is associated with[8]. I_f is defined as the square of the stretch of the fibre vector and is be calculated in a global basis as,

$$I_f = \boldsymbol{A}_{\boldsymbol{G}_i}^T \cdot \boldsymbol{C} \cdot \boldsymbol{A}_{\boldsymbol{G}_i} = \boldsymbol{A}_{\boldsymbol{G}_i}^T \cdot \boldsymbol{F}^T \cdot \boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i} \tag{65}$$

For shell and membrane elements in Abaqus/Standard, and for all elements in Abaqus/Explicit the fibre invariant is computed from

$$I_f = \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{U}^2 \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \tag{66}$$

And finally, for the case of continuum elements with a local basis system in Abaqus/Standard,

$$I_f = \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{C}^{al} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} = \boldsymbol{A}_{\boldsymbol{E}_i}^T \cdot \boldsymbol{F}^{al\,T} \cdot \boldsymbol{F}^{al} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} \tag{67}$$

Clearly the same operations are implemented to compute I_f, regardless of whether a UMAT/VUMAT provides $\boldsymbol{F}^{\boldsymbol{EE}}$, $\boldsymbol{F}^{\boldsymbol{eE}}$ or $\boldsymbol{F}^{al}$ as input.

The invariant may be calculated alternatively by taking the trace of the structural tensor,

$$I_f = \mathrm{tr}\left(\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i}\right) \tag{68}$$

where in the case of the global basis $\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{a}_{\boldsymbol{G}_i}$. As one might expect I_f should remain constant, regardless of the choice of basis system be it global or local. This makes I_f a useful quantity to check when verifying a UMAT as it should not change if the basis system is changed, or if a body is subjected to a simple rigid rotation.

4.3 Specific form of anisotropic hyperelastic constitutive law used in worked examples below:

The expression for stress in fibre-reinforced anisotropic hyperelastic constitutive models can be additively decomposed into isotropic and anisotropic parts, $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\mathrm{iso}} + \boldsymbol{\sigma}_{\mathrm{aniso}}$. We will use the modified anisotropic (MA) model proposed by Nolan et. al (Nolan et al., 2014) to demonstrate local and global implementations. The isotropic part of the Cauchy stress is represented by the neo-Hookean constitutive model given in (47) in either the local or global basis, i.e. $\boldsymbol{\sigma}_{\mathrm{iso}} = \boldsymbol{\sigma}_{\mathrm{NH}}$. The anisotropic part of the stress is given by the second term in (69) below. The summation term indicates that there are two families of fibres ($f = 4, 6$) present in this constitutive model each with their own unique fibre vector. The expression for the total Cauchy stress in the MA model is,

[8] It is possible to have more than one fibre vector in this class of constitutive model.

$$\boldsymbol{\sigma}_{\mathrm{MA}} = \boldsymbol{\sigma}_{\mathrm{NH}} + 2J^{-1}k_1 \sum_{f=4,6} \left(I_f - 1\right) \exp\left[k_2\left(I_f - 1\right)^2\right] \left(\boldsymbol{a}_{\boldsymbol{e}_i}^f \otimes \boldsymbol{a}_{\boldsymbol{e}_i}^f\right), \tag{69}$$

where k_1 and k_2 are material parameters, $\boldsymbol{a}_{\boldsymbol{e}_i}^f$ is the fibre vector in the current configuration for fibre family f; this fibre vector may be in either a local or global basis (in the global case $\boldsymbol{e}_i = \boldsymbol{G}_i$).

4.4 Worked Example #6: Fibre kinematics in a continuum element with a local basis system

We will again consider the same deformation motion χ as the previous Worked Examples and calculate the fibre vector and structural tensor in the current configuration for the cases where global and local bases are used. In this example we will impose the condition that the local basis vectors in the reference configuration are aligned with the global basis vectors, $\boldsymbol{E}_i = \boldsymbol{G}_i$.

Starting with the scenario of a global coordinate basis, we choose the fibre vector in the reference configuration to be a unit vector in the $\boldsymbol{G}_1 - \boldsymbol{G}_2$ plane, at 30° to the $\boldsymbol{G}_1$ axis,

$$\boldsymbol{A}_{\boldsymbol{G}_i} = \begin{bmatrix} \cos(30°) \\ \sin(30°) \\ 0 \end{bmatrix}, \tag{70}$$

The fibre vector in the current configuration $\boldsymbol{a}_{\boldsymbol{G}_i}$ is then calculated using (41) and (70) in (57). So too is the structural tensor, $\boldsymbol{a}_{\boldsymbol{G}_i} \otimes \boldsymbol{a}_{\boldsymbol{G}_i}$, which is calculated using (59). The fibre invariant is calculated using (68),

$$\boldsymbol{a}_{\boldsymbol{G}_i} = \begin{bmatrix} 1.003 \\ 0.493 \\ 0.173 \end{bmatrix}, \qquad \boldsymbol{a}_{\boldsymbol{G}_i} \otimes \boldsymbol{a}_{\boldsymbol{G}_i} = \begin{bmatrix} 1.005 & 0.495 & 0.174 \\ 0.495 & 0.243 & 0.085 \\ 0.174 & 0.085 & 0.030 \end{bmatrix}, \qquad I_f = 1.2786. \tag{71}$$

Next, we examine the local basis case and use the reference configuration fibre vector in (70) as the starting point, setting $\boldsymbol{A}_{\boldsymbol{E}_i} = \boldsymbol{A}_{\boldsymbol{G}_i}$. The fibre vector in the current configuration $\boldsymbol{a}_{\boldsymbol{e}_i}$ is then calculated using (42), (43) and (70) in (58). So too is the structural tensor, $\boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i}$, which is calculated using (63). The fibre invariant is calculated using (68).

$$\boldsymbol{a}_{\boldsymbol{e}_i} = \begin{bmatrix} 1.000 \\ 0.514 \\ 0.121 \end{bmatrix}, \qquad \boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i} = \begin{bmatrix} 0.9995 & 0.5141 & 0.174 \\ 0.5141 & 0.2644 & 0.0623 \\ 0.174 & 0.0623 & 0.0147 \end{bmatrix}, \qquad I_f = 1.2786. \tag{72}$$

- The Matlab script `Worked_example_5.m` demonstrates the calculation of the global and local fibre vectors, structural tensors, and invariants in the scenario outlined above.

4.5 Worked Example #7: Fibre kinematics in a continuum element with a local basis system where $\boldsymbol{E}_i \neq \boldsymbol{G}_i$

Next, we examine the scenario where the local basis system in the reference configuration $\boldsymbol{E}_i$ is rotated by 20° about the $\boldsymbol{G}_3$ axis, as per Worked Example #3. To remain consistent with Worked Example #6, we establish the fibre in the $\boldsymbol{E}_1 - \boldsymbol{E}_2$ plane and to be at 10° w.r.t. the $\boldsymbol{E}_1$ axis. Therefore, in a global sense the fibre is at 30° w.r.t. the $\boldsymbol{G}_1$ axis; the same as in Worked Example #6. The fibre vector in the reference configuration is,

$$\boldsymbol{A}_{\boldsymbol{E}_i} = \begin{bmatrix} \cos(10°) \\ \sin(10°) \\ 0 \end{bmatrix}. \tag{73}$$

Once again, we start by using the change of basis in (45) to map the global deformation gradient in $\boldsymbol{G}_i$ to the global deformation gradient in $\boldsymbol{E}_i$. The local deformation gradient $\boldsymbol{F}_{20}^{al}$ is then computed using (46). Using $\boldsymbol{F}_{20}^{al}$ and the rotation matrix $\boldsymbol{R}_{20}$ (used to map $\boldsymbol{F}_{20}$ to $\boldsymbol{F}_{20}^{al}$) in (58) the fibre vector in the current configuration is calculated. The structural tensor is calculated using (63) and the fibre invariant using (68).

$$\boldsymbol{a}_{\boldsymbol{e}_i} = \begin{bmatrix} 1.115 \\ 0.141 \\ 0.121 \end{bmatrix}, \quad \boldsymbol{a}_{\boldsymbol{e}_i} \otimes \boldsymbol{a}_{\boldsymbol{e}_i} = \begin{bmatrix} 1.2440 & 0.1576 & 0.1351 \\ 0.1576 & 0.0200 & 0.0171 \\ 0.1351 & 0.0171 & 0.0147 \end{bmatrix}, \quad I_f = 1.2786. \tag{74}$$

Note that the fibre invariant remains constant across (71), (72), and (74). This is a result that we should expect as there is the same deformation motion and fibre orientation in all of these scenarios.

- The Matlab script `Worked_example_7.m` demonstrates the calculation of the local fibre vectors, structural tensors, and invariants in the scenario outlined above.

4.6 Worked Example #8: Calculation of stress in a continuum element consisting of an anisotropic material

We will now work through an example of how the Cauchy stress is calculated using the MA constitutive model for the deformation motion we have used for all of the Worked Examples previously. We assume that the material parameters $k_1 = 0.05$ MPa and $k_2 = 2.0$.

Starting with the global case, we assume there are two families of fibres whose vectors are $\pm 20°$ to the $\boldsymbol{G}_1$axis, in the $\boldsymbol{G}_1 - \boldsymbol{G}_2$ plane. The isotropic stress is the same as the neo-Hookean stress in (52), the structural tensor in the current configuration is calculated using (59), and the fibre invariant is calculated using (68). Using these quantities in (69) results in the Cauchy stress,

$$\boldsymbol{\sigma}_{\mathrm{MA}} = \begin{bmatrix} 0.2063 & 0.0456 & 0.0679 \\ 0.0456 & 0.0824 & 0.0576 \\ 0.0679 & 0.0576 & 0.2762 \end{bmatrix} \tag{75}$$

Next, we consider the case of a local coordinate basis where the reference basis $\boldsymbol{E}_i = \boldsymbol{G}_i$. We can use the local deformation gradient given in (43), and the isotropic stress given in (53). The structural tensor in the current configuration is computed using (63) and the fibre invariant using (68). Using these quantities in (69) gives the Cauchy stress,

$$\boldsymbol{\sigma}_{\mathrm{MA}}^{al} = \begin{bmatrix} 0.2168 & 0.0488 & 0.0755 \\ 0.0488 & 0.0779 & 0.0409 \\ 0.0755 & 0.0409 & 0.2708 \end{bmatrix} \tag{76}$$

We can next compute the co-rotational stress using the right stretch tensor $\boldsymbol{U}$ determined from the polar decomposition of the global deformation gradient. When $\boldsymbol{U}$ is used in place of the global deformation gradient in the constitutive equation in (69) we compute the local stress in (76).

Finally, the stress in the local basis can be mapped back to the global stress using the change of basis operation,

$$\boldsymbol{\sigma}_{\mathrm{MA}} = \boldsymbol{R} \cdot \boldsymbol{\sigma}_{\mathrm{MA}}^{al} \cdot \boldsymbol{R}^T \tag{77}$$

- The Matlab script `Worked_example_8.m` demonstrates the calculation of the global, local, and co-rotational stress tensors outlined above.
- The global stress tensor is calculated by the Abaqus/Standard input file `WE8_global.inp` together with the UMAT file `umat_MA_global.for`.
- The local stress tensor is calculated by the Abaqus/Standard input file `WE8_local.inp` together with the UMAT file `umat_MA_local.for`.

4.7 Worked Example #9: Calculation of stress in a continuum element consisting of an anisotropic material

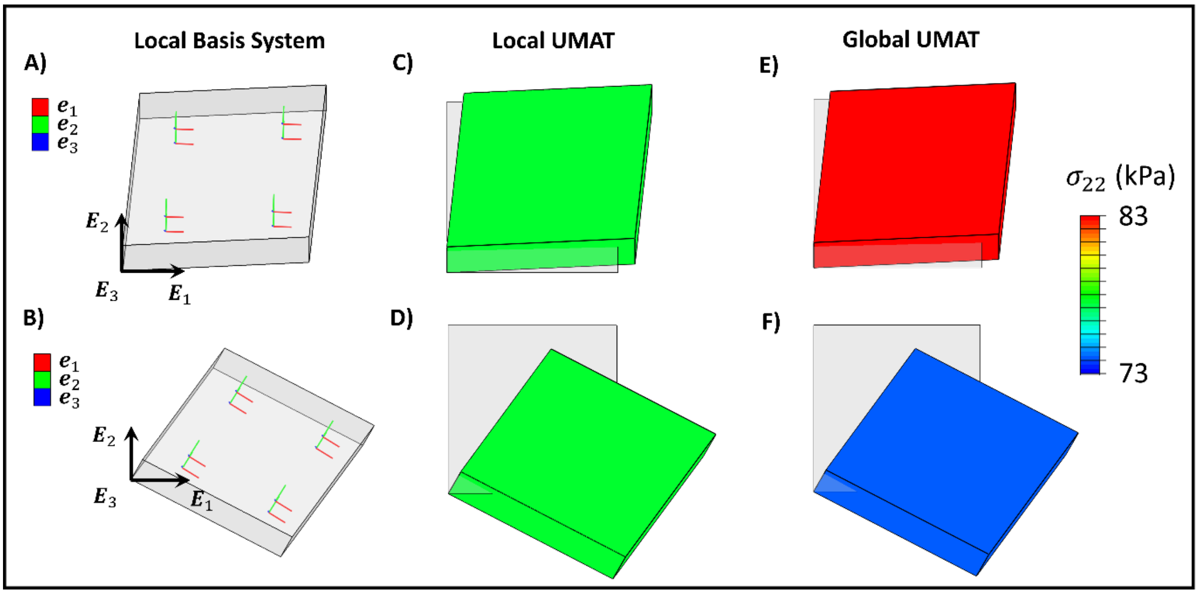

Figure 8 **A)** Deformation of a unit cube according to the deformation gradient in (41). **B)** Rigid body rotation of the deformation in A) given by (78) and (79). Note that the basis vectors in the current configuration $\boldsymbol{e}_i$ have also rigidly rotated. **C)** The stress component σ_{22} when the *local* UMAT is used, for the deformation in A). **D)** The stress component σ_{22} when the local UMAT is used, after the rigid rotation deformation in B). Note that the stress remains constant, as we expect for a rigid body rotation in a co-rotational basis. **E)** The stress component σ_{22} when the *global* UMAT is used, for the deformation in A). **F)** The resulting stress component σ_{22} when the global UMAT is used, after the rigid rotation deformation in B). Note that the stress changes between E) and F), and that this is incorrect. The happens because the global UMAT fails to take account of rotation of the basis system $\boldsymbol{e}_i$.

Finally, we will demonstrate that the principal stresses, deformation and fibre invariants remain constant under a rigid body rotation deformation. In the specific case where a local coordinate system is used, we will show that the stress tensor computed before and after rotation is identical.

We start with the global and local stresses calculated in Worked Example #8 given in (75) and (76) respectively. We shall name $\boldsymbol{F}$ given in (41) to be State 1. This body can be rigidly rotated using a rotation matrix $\boldsymbol{\Phi}$ to a State 2 using,

$$\boldsymbol{F}_2 = \boldsymbol{\Phi} \cdot \boldsymbol{F}_1 \tag{78}$$

where we use the subscript to indicate which state the deformation gradient exists. In this example we rotate the deformed unit cube $-30°$ about the $\boldsymbol{G}_3$ axis.

$$\boldsymbol{\Phi} = \begin{bmatrix} \cos(-30°) & -\sin(-30°) & 0 \\ \sin(-30°) & \cos(-30°) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{79}$$

When $\boldsymbol{F}_2$ is used to calculate stress in the MA constitutive model using the same parameters as the global case in Worked Example #8 we calculate the tensor,

$$\boldsymbol{\sigma}_{\mathrm{MA}} = \begin{bmatrix} 0.2148 & -0.0309 & 0.0876 \\ -0.0309 & 0.0739 & 0.0159 \\ 0.0876 & 0.0159 & 0.2762 \end{bmatrix}. \tag{80}$$

When we calculate the principal stresses and pressure stress of global stress tensors in (75) and (80) we find that they are identical. This is an important result and demonstrates that there is the same stress state before and after the rigid body rotation. Though the individual components of the stress tensor are different in (75) and (80) this is only because rigid body rotation has changed the orientation of the stress components w.r.t. the global coordinate basis.

To calculate the stress when a local coordinate frame is used we first perform a polar decomposition of $\boldsymbol{F}_2$ from which we determine the rotation matrix $\boldsymbol{R}_2$. The local deformation gradient in State 2 may then be calculated using a change of basis,

$$\boldsymbol{F}_2^{al} = \boldsymbol{R}_2^T \cdot \boldsymbol{F}_2 \cdot \boldsymbol{R}_2 \tag{81}$$

Following the same procedure for the calculation of the local stress as Worked Example #8 we calculate the local stress,

$$\boldsymbol{\sigma}_{\mathrm{MA}}^{al} = \begin{bmatrix} 0.2162 & 0.0488 & 0.0792 \\ 0.0488 & 0.0779 & 0.0409 \\ 0.0755 & 0.0409 & 0.2708 \end{bmatrix} \tag{82}$$

This stress tensor is identical to (76) demonstrating that when a local coordinate basis is used, the stress tensor co-rotates with a rigid body rotation.

The co-rotational stress in State 2 is calculated by using the right stretch tensor $\boldsymbol{U}_2$, determined from a polar decomposition of $\boldsymbol{F}_2$, in place of the deformation gradient in (69). This leads to the calculation of the co-rotational stress tensor and is identical to (82).

Figure 8 shows the stress component σ_{22} computed when a local material orientation is implemented and the local UMAT is used (Figure 8C and D). As you can see the stress does not change with rigid body rotation and σ_{22} is as per (76) and (82). This is the expected, correct result. On the other hand, when the global UMAT is used, as the body rotates from Figure 8E to F the stress changes. This is incorrect and a clear indication that the UMAT is not frame invariant.

- The Matlab script `Worked_example_9.m` demonstrates the calculation of the global, local, and co-rotational stress tensors outlined above.
- The global stress tensor is calculated by the Abaqus/Standard input file `WE9_global.inp` together with the UMAT file `umat_MA_global.for`.
- The local stress tensor is calculated by the Abaqus/Standard input file `WE9_local.inp` together with the UMAT file `umat_MA_local.for`.

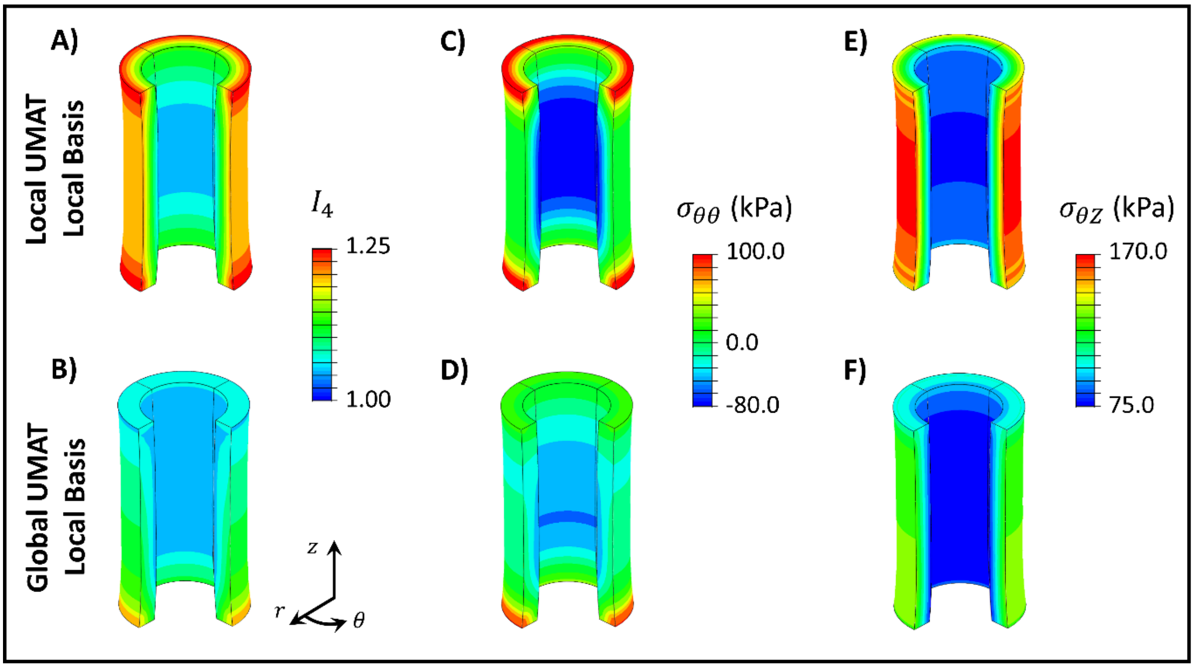

Figure 9 Torque of an anisotropic hyperelastic tube. Anisotropic invariant I_4 when **A)** the correct, local UMAT is used, and **B)** when a global UMAT is used incorrectly. Likewise, the circumferential stress $\sigma_{\theta\theta}$ **C)** and **D)**, and shear stress $\sigma_{\theta Z}$ **E)** and **F)**, are calculated using the local and global UMATs respectively.

5 Case studies

The two case studies presented in this example show the consequences of incorrectly implementing a local coordinate system for a fibre reinforced hyperelastic constitutive model.

These examples have been run using Abaqus/Standard 2017 and the global and local UMATs referred to in Section 4.6 and 4.7. The simulation files required to run these examples are included with the accompanying codes in the folder Case Studies.

5.1 Torque and axial stretch of a tube

Consider a tube whose inner radius is 2 mm, outer radius is 3 mm, and whose length is 10 mm. One end of the tube is fixed for all degrees of freedom. A torque is applied to the tube by rotating the opposite end by 1 radian, and an axial stretch by displacing this end by 0.5 mm. The fibre reinforced constitutive model given in (69) is implemented the represent the material of the tube, with parameters $C_{10} = 0.2$ MPa, $D = 2.0$ MPa, $k_1 = 0.2$ MPa, $k_2 = 2.0$. Two families of fibres are used at $\pm 30°$ to the circumferential direction, using a local cylindrical coordinate system to define these directions. This problem is simulated using FE analysis using both the global and local UMATs presented in Section 4.6.

Results for this simulation are given in Figure 9 when both the local and global UMATs. Figure 9A) and B) show the fibre invariant I_4 when the local and global UMATs are used respectively. In a similar fashion we show the circumferential stress $\sigma_{\theta\theta}$ C) and D), and the shear stress $\sigma_{\theta Z}$ E) and F).

In the cases where there is the local UMAT is used, we see that there is a symmetric pattern in each of the contours as expected. However, when the global UMAT is used with a local coordinate system, we see that this not the case. The contours on the top half of the tube are different to those on the bottom. This is because there has been large rotation that the global UMAT does not account for, as we go axially from bottom to top, the rotation becomes larger, and the error is higher.

5.2 Closing an artery segment to create residual stress

It is widely understood that there is a residual stress in arteries in their zero-pressure configuration. One method to measure this experimentally is to cut arteries and measure their opening angle (Chuong and Fung, 1986). Conversely, to recreate the residual stress in a FE simulation the opened geometry is restored to the closed geometry, see Figure 10A).

To define fibre directions, it is useful to define a local, concentric basis system based on polar coordinates. Two families of fibres are defined at $\pm 45°$ to the circumferential direction, and the constitutive model given in Section 5.1 is implemented again here.

When the artery is closed the stress and strain in the artery wall should also be concentric. Figure 10B) shows the circumferential stress $\sigma_{\theta\theta}$ when the local UMAT is used to compute the stress; as expected we calculate a concentric circumferential stress contour. On the other hand, Figure 10C) shows the circumferential stress $\sigma_{\theta\theta}$ when the global UMAT is used to compute the stress. In this case an *eccentric* stress contour is calculated. This result is incorrect, and it is useful to note that the more rotation an element undergoes, the larger the error in the stress. This is because the global UMAT fails to correctly account for the deformation of the fibre w.r.t. the local coordinate system.

This example again highlights the importance of including rotations when a local coordinate basis is used in conjunction with a fibre vector based UMAT.

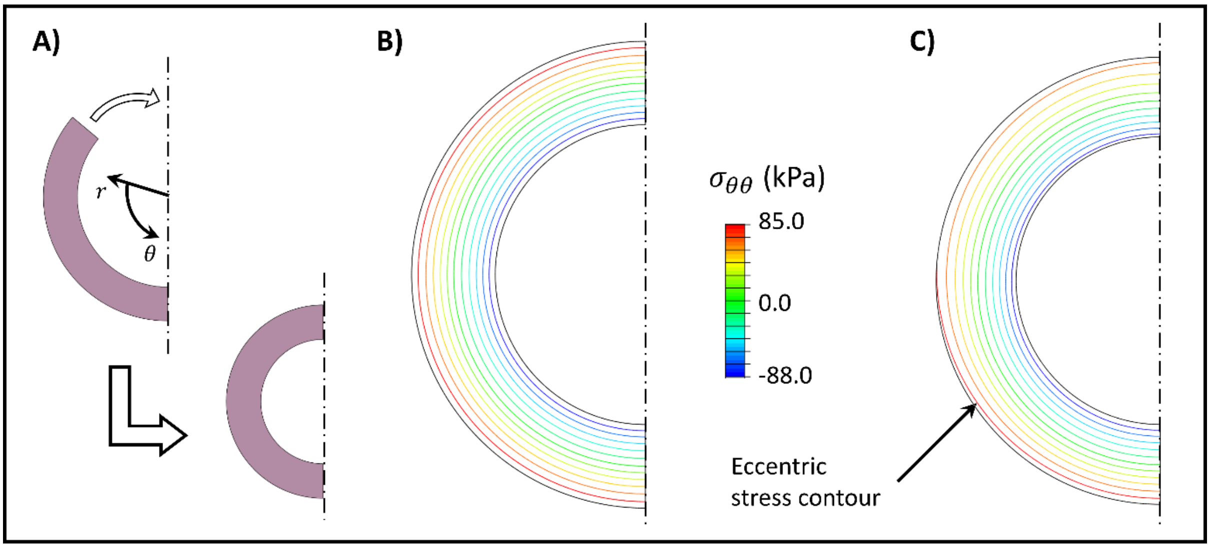

Figure 10 **A)** Schematic of the closing of an artery segment to create a residual stress in the artery wall. **B)** Contour plot showing concentric isolines of the resulting circumferential stress $\sigma_{\theta\theta}$ when the *local* UMAT is used. **C)** Contour plot showing isolines of circumferential stress $\sigma_{\theta\theta}$ when the *global* UMAT is used. Note that these are eccentric w.r.t. the geometry.

6 Discussion and Conclusions

In this tutorial paper we have discussed the form of the deformation gradient when either a global or co-rotational local basis system is used to describe the deformation. Key points arising from this paper are summarised as follows:

1. There are important differences in the way in which the local deformation gradient is calculated depending on whether a structural element (e.g. a shell or membrane element) or a continuum element is used in Abaqus. (i) A structural element implements what we term the 'Classical' definition of the local deformation gradient, i.e. where $\boldsymbol{F}' = \boldsymbol{U}$. (ii) A continuum element by default uses a global coordinate system with a global deformation gradient $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$. (iii) If a local orientation is specified for a continuum element a different form of the deformation gradient is provided. We refer to this form as the *Abaqus local* deformation gradient, which is given as $\boldsymbol{F}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R}$. The consequences of the construction of the *Abaqus local* deformation gradient are discussed in Sections 2.2 and 2.3.

2. This important difference has consequences for the interpretation of the local deformation tensors, such as the Cauchy-Green tensors, depending on whether a continuum or structural element is used. In particular, one should be aware that the eigenvectors of these tensors may not those expected (see Appendix A1).

3. When writing a user-defined material subroutine (UMAT/VUMAT) to compute the stress from a given deformation gradient, one must ensure that the Cauchy stress is returned in the current configuration basis system, be that global or local. A summary is provided in Table 1.

4. The construction of the *Abaqus local* deformation gradient for continuum elements with a local basis system has important consequences for the calculation of fibre vectors in the current configuration for anisotropic hyperelastic models. The fibre vector in the reference configuration must have its basis changed from $\boldsymbol{E}_i$ to $\boldsymbol{e}_i$ leading to Equation (58) where $\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{U} \cdot \boldsymbol{A}_{\boldsymbol{E}_i} = \boldsymbol{F}^{al} \cdot \boldsymbol{R}^T \cdot \boldsymbol{A}_{\boldsymbol{E}_i}$.

5. When very large deformations are accompanied by very large rotations, a slight numerical error in the *Abaqus local* deformation gradient is observed (Section 2.4.1). $\boldsymbol{F}^{al} = \boldsymbol{R}^T \cdot \boldsymbol{F} \cdot \boldsymbol{R}$. However, no such numerical error is observed in the log strain tensor. Such slight numerical errors are not observed for cases of large deformation with small rotations, or for cases of small deformations with large rotations.

An incomplete understanding of the constriction of the global ($\boldsymbol{F}$), classical local ($\boldsymbol{F}'$), and *Abaqus local* ($\boldsymbol{F}^{al}$) deformation gradient when writing a UMAT/VUMAT may lead to insidious errors that will not be detectable through uniaxial or biaxial verification test. Test cases that apply material deformation in conjunction with rigid body rotation must be performed to ensure that the deformation gradient is correctly interpreted.

It is essential for the progress of the field of computational mechanics that user-defined materials are rigorously verified and validated before their emergent results are published. The authors hope that this paper will provide the reader with a good guide to correctly implementing user defined material subroutines with local orientation and finite deformations.

	Continuum Elements				Structural Elements	
	Abaqus/Standard		Abaqus/Explicit[#]			
`*orientation` used?	No	Yes	No	Yes	No	Yes
Deformation tensor (input)	$\boldsymbol{F}$	$\boldsymbol{F}^{al}$	$\boldsymbol{U}_{\boldsymbol{G}_i}$	$\boldsymbol{U}_{\boldsymbol{E}_i}$	$\boldsymbol{F}'$	$\boldsymbol{F}'$
Fibre vector in current configuration	$\boldsymbol{a}_{\boldsymbol{G}_i} = \boldsymbol{F} \cdot \boldsymbol{A}_{\boldsymbol{G}_i}$	$\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}^{al} \cdot \boldsymbol{R}^{\mathrm{T}} \cdot \boldsymbol{A}_{\boldsymbol{E}_i}$	$\boldsymbol{a}^{\mathrm{cr}} = \boldsymbol{U}_{\boldsymbol{G}_i}\boldsymbol{A}_{\boldsymbol{G}_i}$	$\boldsymbol{a}^{\mathrm{cr}} = \boldsymbol{U}_{\boldsymbol{E}_i}\boldsymbol{A}_{\boldsymbol{E}_i}$	$\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}'\boldsymbol{A}_{\boldsymbol{E}_i}$	$\boldsymbol{a}_{\boldsymbol{e}_i} = \boldsymbol{F}'\boldsymbol{A}_{\boldsymbol{E}_i}$
Cauchy stress tensor (output)	$\boldsymbol{\sigma}_{\boldsymbol{G}_i}$	$\boldsymbol{\sigma}_{\boldsymbol{e}_i}$	$\boldsymbol{\sigma}^{\mathrm{cr}*}$	$\boldsymbol{\sigma}^{\mathrm{cr}}$	$\boldsymbol{\sigma}_{\boldsymbol{e}_i}$	$\boldsymbol{\sigma}_{\boldsymbol{e}_i}$

Table 1 Guide to the deformation inputs and expected stress outputs for a given coordinate basis when a user-defined material is used in either Abaqus/Standard (UMAT) or Abaqus/Explicit (VUMAT). [#]Both the deformation gradient and the stretch tensor are inputs in a VUMAT; the Abaqus manual recommends the use of the stretch tensor as this will result in the correct corotational stress being computed. *The Fortran subroutine must return the co-rotated stress, however Abaqus will internally rotate the stress to the global basis

Appendices

A.1 Relating $\boldsymbol{F}^E$ to $\boldsymbol{F}'$

$$\boldsymbol{F} = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} \left(\boldsymbol{e}_i \otimes \boldsymbol{E}_j\right) = \sum_{i,j,k=1}^{3} \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}} \theta_{ki} \boldsymbol{E}_k \otimes \boldsymbol{E}_j = \sum_{i,j=1}^{3} \frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}} \left(\boldsymbol{E}_i \otimes \boldsymbol{E}_j\right) \tag{A1.1}$$

where the components of the local deformation gradient in the $\boldsymbol{e}_i \otimes \boldsymbol{E}_j$ basis system are $F'_{ij} = \frac{\partial x_i^{\boldsymbol{e}}}{\partial X_j^{\boldsymbol{E}}}$ and the components of the global deformation gradient in the $\boldsymbol{E}_i \otimes \boldsymbol{E}_j$ basis system are $F^E_{ij} = \frac{\partial x_i^{\boldsymbol{E}}}{\partial X_j^{\boldsymbol{E}}}$

Expanding the summation over *i*, *j* and *k* for the third expression in equation (A1.1) above gives,

$$\begin{aligned}
&\sum_{i,j,k=1}^{3} F'_{ij} \theta_{ki} \boldsymbol{E}_k \otimes \boldsymbol{E}_j = \\
&F'_{11}(\theta_{11}\boldsymbol{E}_1 \otimes \boldsymbol{E}_1 + \theta_{21}\boldsymbol{E}_2 \otimes \boldsymbol{E}_1 + \theta_{31}\boldsymbol{E}_3 \otimes \boldsymbol{E}_1) \\
&+F'_{12}(\theta_{11}\boldsymbol{E}_1 \otimes \boldsymbol{E}_2 + \theta_{21}\boldsymbol{E}_2 \otimes \boldsymbol{E}_2 + \theta_{31}\boldsymbol{E}_3 \otimes \boldsymbol{E}_2) \\
&+F'_{13}(\theta_{11}\boldsymbol{E}_1 \otimes \boldsymbol{E}_3 + \theta_{21}\boldsymbol{E}_2 \otimes \boldsymbol{E}_3 + \theta_{31}\boldsymbol{E}_3 \otimes \boldsymbol{E}_3) \\
&+F'_{21}(\theta_{12}\boldsymbol{E}_1 \otimes \boldsymbol{E}_1 + \theta_{22}\boldsymbol{E}_2 \otimes \boldsymbol{E}_1 + \theta_{32}\boldsymbol{E}_3 \otimes \boldsymbol{E}_1) \\
&+F'_{22}(\theta_{12}\boldsymbol{E}_1 \otimes \boldsymbol{E}_2 + \theta_{22}\boldsymbol{E}_2 \otimes \boldsymbol{E}_2 + \theta_{32}\boldsymbol{E}_3 \otimes \boldsymbol{E}_2) \\
&+F'_{23}(\theta_{12}\boldsymbol{E}_1 \otimes \boldsymbol{E}_3 + \theta_{22}\boldsymbol{E}_2 \otimes \boldsymbol{E}_3 + \theta_{32}\boldsymbol{E}_3 \otimes \boldsymbol{E}_3) \\
&+F'_{31}(\theta_{13}\boldsymbol{E}_1 \otimes \boldsymbol{E}_1 + \theta_{23}\boldsymbol{E}_2 \otimes \boldsymbol{E}_1 + \theta_{33}\boldsymbol{E}_3 \otimes \boldsymbol{E}_1) \\
&+F'_{32}(\theta_{13}\boldsymbol{E}_1 \otimes \boldsymbol{E}_2 + \theta_{23}\boldsymbol{E}_2 \otimes \boldsymbol{E}_2 + \theta_{33}\boldsymbol{E}_3 \otimes \boldsymbol{E}_2) \\
&+F'_{33}(\theta_{13}\boldsymbol{E}_1 \otimes \boldsymbol{E}_3 + \theta_{23}\boldsymbol{E}_2 \otimes \boldsymbol{E}_3 + \theta_{33}\boldsymbol{E}_3 \otimes \boldsymbol{E}_3)
\end{aligned} \tag{A1.2}$$

Expanding the summation over *i* and *j* for the fourth expression in equation (A1.1) above gives,

$$\begin{aligned}
&\sum_{i,j=1}^{3} F^E_{ij} \left(\boldsymbol{E}_i \otimes \boldsymbol{E}_j\right) = \\
&F^E_{11}\boldsymbol{E}_1 \otimes \boldsymbol{E}_1 + F^E_{21}\boldsymbol{E}_2 \otimes \boldsymbol{E}_1 + F^E_{31}\boldsymbol{E}_3 \otimes \boldsymbol{E}_1 \\
&+F^E_{12}\boldsymbol{E}_1 \otimes \boldsymbol{E}_2 + F^E_{22}\boldsymbol{E}_2 \otimes \boldsymbol{E}_2 + F^E_{32}\boldsymbol{E}_3 \otimes \boldsymbol{E}_2 \\
&+F^E_{13}\boldsymbol{E}_1 \otimes \boldsymbol{E}_3 + F^E_{23}\boldsymbol{E}_2 \otimes \boldsymbol{E}_3 + F^E_{33}\boldsymbol{E}_3 \otimes \boldsymbol{E}_3
\end{aligned} \tag{A1.3}$$

Equating the terms in (A1.3) and (A1.2) which have the same dyadic product in common, and writing in matrix form we get,

$$\begin{bmatrix} F_{11}^E & F_{12}^E & F_{13}^E \\ F_{21}^E & F_{22}^E & F_{23}^E \\ F_{31}^E & F_{32}^E & F_{33}^E \end{bmatrix} =$$
$$\begin{bmatrix} \theta_{11}F'_{11} + \theta_{12}F'_{21} + \theta_{13}F'_{31} & \theta_{11}F'_{12} + \theta_{12}F'_{22} + \theta_{13}F'_{32} & \theta_{11}F'_{13} + \theta_{12}F'_{23} + \theta_{13}F'_{33} \\ \theta_{21}F'_{11} + \theta_{22}F'_{21} + \theta_{23}F'_{31} & \theta_{21}F'_{12} + \theta_{22}F'_{22} + \theta_{23}F'_{32} & \theta_{21}F'_{13} + \theta_{22}F'_{23} + \theta_{23}F'_{33} \\ \theta_{31}F'_{11} + \theta_{32}F'_{21} + \theta_{33}F'_{31} & \theta_{31}F'_{12} + \theta_{32}F'_{22} + \theta_{33}F'_{32} & \theta_{31}F'_{13} + \theta_{32}F'_{23} + \theta_{33}F'_{33} \end{bmatrix} \tag{A1.4}$$

Clearly, we can write,

$$\boldsymbol{F}^E = \boldsymbol{\theta} \cdot \boldsymbol{F}' \tag{A1.5}$$

A.2 Consequences for use of utility subroutine SPRIND

The difference between the Classical and Abaqus definition of the local deformation gradient has important implications for the use of the inbuilt utility subroutine `sprind` in a UMAT. This subroutine is used to determine the principal directions (eigenvectors) of stress, strain, and deformation tensors. If a global basis system is used, $\boldsymbol{C}$ does not contain any information on rigid body rotation of the material (see (4)) and therefore the principal directions are simply the reference basis vectors, i.e. $\boldsymbol{I}$. On the other hand, $\boldsymbol{B}$ contains information on the material rigid body rotation (see (6)) and therefore the use of $\boldsymbol{B}$ in the `sprind` statement returns the principal strain directions w.r.t. the global basis system. This outcome is expected from the Classical continuum mechanics framework.

In contrast, when `*orientation` is used, the construction of $\boldsymbol{C}^{al}$ from the local deformation gradient given in (27), with its reversed order of $\boldsymbol{R}$ and $\boldsymbol{U}$, results in a quantity that now does contain information on material rotation, and the use of $\boldsymbol{C}^{al}$ in `sprind` computes the principal directions w.r.t. the global coordinate system. The opposite is now the case for the $\boldsymbol{B}^{al}$ matrix which does not contain rotational information (see (25)) and cannot now be used to determine principal material orientations w.r.t. the global directions.

A.3 Table of Accompanying Codes

Filename	**Description**
Worked_example_1	Calculation of 2D deformation gradients looking in particular at the difference between structural elements, which calculate the local deformation gradient using the Classical definition, and continuum elements, which use a different transformation as outlined in Section 2.3
Worked_example_2	Looking at the difference in the deformation gradient between using a global and local coordinate system.

Worked_example_3	Same as above, except that the local coordinate system is offset by 20 degrees about the $\boldsymbol{G}_3$-axis in the reference configuration. i.e. $\boldsymbol{E}_i \neq \boldsymbol{G}_i$.
Worked_example_4	Calculating the neo-Hookean stress for the global and local coordinate systems, as per Worked_example_1
Worked_example_5	Calculating the neo-Hookean stress for the global and local coordinate systems, as per Worked_example_2
Worked_example_6	Calculating the fibre orientation vectors and structural tensor when a local or global coordinate scheme is used
Worked_example_7	Same as above, except that the local coordinate system is offset by 20 degrees from the x-axis in the reference configuration. i.e. $\boldsymbol{E}_i \neq \boldsymbol{G}_i$.

Worked_example_8	Calculate the stress for the MA hyperelastic model in both the local and global coordinate schemes.
	`abaqus j=WE8_global user=umat_MA_global.for`
	`abaqus j=WE8_local user=umat_MA_local.for`

Worked_example_9	Same as 7, except perform second step which is a rigid body rotation. Show that when a local scheme is used that there is no change in the stress upon this rigid rotation.
	`abaqus j=WE9_global user=umat_MA_global.for`
	`abaqus j=WE9_local user=umat_MA_local.for`

Case Study 1	Torque and stretch of a tube.
	`abaqus j=localTorque inp=torque_stretch_cylinder.inp user=umat_MA_local.for`
	`abaqus j=globalTorque inp=torque_stretch_cylinder.inp user=umat_MA_global.for`

Case Study 2	Creating a residual stress in an artery segment.
	`abaqus j=localResidual inp=residualStress.inp user=umat_MA_local.for`
	`abaqus j=globalResidual inp=residualStress.inp user=umat_MA_global.for`

A.4 Outputting the deformation gradient

Abaqus does not write out the deformation gradient by default, and only outputs it when hyperelastic and user-defined materials are used. To output the deformation gradient the keyword options below must be added to the Abaqus .inp file. For example in Worked Example #2, file `WE1_local.inp`, line 118 has:

```
*EL PRINT
DG
```

This outputs the deformation gradient in each element, at each integration point into the resulting .dat file for the simulation.

The Fortran code below will print out the matrix `tens` of size $m \times n$ to the .dat file when called from a (V)UMAT.

```
subroutine kprinter(tens, m, n)

INCLUDE 'ABA_PARAM.INC'

intent(in):: tens, m, n

dimension tens(m,n)

  write(6,*)
  do i = 1,m
  do j = 1,n
      write(6,'(e19.9)',advance='no'),tens(i,j)
  end do
  write(6,*)
  end do
  write(6,*)
return
end subroutine kprinter
```

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