Contravariant tensor algebra for anisotropic hyperelasticity

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Abstract. Analysis of tensors in oblique Cartesian coordinate systems always requires the definition of a set of orthogonal covariant basis vectors called the Reciprocal basis. This increases the complexity of the analysis and hence makes the method cumbersome. In this work a novel method is presented to effectively carry out the various transformations of tensors to and between oblique coordinate system/s without the need to create the covariant reciprocal basis. This will simplify the procedure of transformations involving problems where tensors are required to be defined in the oblique coordinate system. This work also demonstrates how the analysis of contravariant tensors can be applied to hyperelasticity. Continuum material and damage models can integrate this approach to model anisotropy and non-linearity using a much simpler approach. The accuracy of the models was illustrated by matching the predictions to experimental results. A finite element analysis of material and damage model based on contravariant tensors was also carried out on a simple geometry with a re-entrant corner.

Keywords: Contravariant Tensor, Anisotropy, Hyperelasticity

1. Introduction
In developing anisotropic continuum models it is essential to describe the field variables in the fibre directions. Most phenomenological models [1–3] include the strain in fibre directions in the strain energy density function which improves a material models accuracy in predicting non-linearity and anisotropy. The accepted procedure is to include the fourth invariant \( I_4 \) of the right Cauchy Green tensor to include fibre stretches. Recent works [4] have also included higher invariants to include the cross linking effects of fibres. Even modelling of continuum damage is a topic of great interest as there are various ways to include different field variables that contribute to damage. The invariant \( I_4 \) has also found application in including the shear effects in a damage model for brain tissue [5]. Continuum damage model based on octahedral shear stress can be applied in the analysis of components of the fuselage [6]. Progressive damage models based on fracture energy can be applied to analyse the crashworthiness of a composite beam [7]. Strain gradient based models with independently evolving damage variables can be very thermodynamically consistent [8]. In brittle materials damage can be assumed to evolve with effective strains [9]. Stress based anisotropic damage can also predict progressive failure of massive structures [10]. A combination of continuum damage and cohesive zone models was shown to successfully predict damage and fracture in asphalt [11]. A von Mises stress based continuum damage model could predict fatigue in sintered metals [12]. A blend of continuum damage and fracture mechanics could be shown to be effective for predicting damage in composites [13].
In a recent work [14] a different approach to use oblique contravariant tensors derived from transforming the right Cauchy Green tensor in a three dimensional oblique space was discussed. The model is capable of including fibre strains using a single invariant also for a three dimensional fibre orientation. Popular approaches to analyse tensors in oblique coordinate systems require the definition of a covariant Reciprocal basis [15, 16]. In this work a simpler method is proposed in section 2, to arrive at the tensor transformed from Cartesian space to oblique space without invoking the reciprocal basis. A simple numerical example is also demonstrated to accentuate the efficiency of the approach. The application of this approach is demonstrated in continuum mechanics in section 3 with application to material modelling (section 3.1) and continuum damage modelling (section 3.3). Validity of the models was established in section 4 with application in a finite element scheme.

2. The oblique coordinate system

Any physical phenomenon occurring in space and time requires the use of coordinate systems to describe it. The phenomenon can be as simple as the displacement of an object or as complex as the curvature of the fabric of the universe. The most popular system coordinate system is the rectangular Cartesian coordinate system which uses orthonormal basis vectors. However, sometimes it may be compelled to choose a different coordinate system to describe a phenomenon. An example of such would be the oblique Cartesian coordinate system. Such a system may have non normalized but certainly non orthogonal basis vectors.

Let us refer to Figure 1 where \( \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3 \) represents a three dimensional space with a set of right handed orthonormal basis vectors, meeting at origin \( O \), and forming a Cartesian space \((\mathbf{X}_3)\). Let \( \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \) represent a set of non orthogonal basis vectors also meeting at origin \( O \) thereby forming a three dimensional oblique space \((\mathbf{E}_3)\). \( \mathbf{X}_3 \) and \( \mathbf{E}_3 \) thus contain a a set of covariant and contravariant basis respectively.

![Figure 1. Rectangular and Oblique Coordinate Systems](image)

Let there be a point \( A \) in the three dimensional space bearing \( \mathbf{OA} \) as its position vector. The vector \( \mathbf{OA} \) can be represented in terms of the basis vectors in \((\mathbf{X}_3)\) as well as \((\mathbf{E}_3)\) as

\[
\mathbf{OA} = v_i \mathbf{e}_i = u_j \mathbf{X}_j
\]

where \( v_i \) and \( u_j \) represents the components of \( \mathbf{OA} \) in \((\mathbf{E}_3)\) and \((\mathbf{X}_3)\) respectively and \( i, j = 1, 2, 3 \).

The task now is determine the components of the vector \( \mathbf{OA} \) when defined in an oblique coordinate system whose basis vectors are known. As it turns out that the traditional approach is a bit cumbersome and requires the definition of a different three dimensional space possessing set of orthogonal basis vectors that bear a profound relationship with the oblique basis vectors. Such a set of basis vectors is generally called as the Reciprocal Basis [16].
2.1. Reciprocal Basis

Since the basis vectors in \((\mathbb{E}^3)\) are non orthogonal to each other, therefore

\[
e^i \cdot e^j \neq \delta_{ij}
\]

where \(\delta_{ij}\) represents the Kronecker Delta. Due to this property there arises certain complexities in analysing a tensor in such an oblique space which is easily taken care of when dealing with orthonormal basis.

Therefore the need arises for the use of a set of right handed basis vectors \(e_k\) where \(k = 1, 2, 3\), which are related to the basis vectors in system \((\mathbb{E}^3)\) in such a manner that \([15]\)

\[
e^i \cdot e_j = \delta_{ij}
\]

which essentially signifies that \(e_k\) is orthogonal to the plane containing \(e^i\) and \(e^j\) (where \(i \neq j \neq k\)). Such a set of basis vectors is called the Reciprocal basis \([16]\).

Let \(n\) be a scalar value. Therefore from equation (3) it can be stated

\[
e_k = n (e^i \times e^j)
\]

Using equation (4) in equation (3) it can be deduced

\[
n = \frac{1}{e^k \cdot (e^i \times e^j)}
\]

and therefore it can finally stated

\[
e_k = \frac{e^i \times e^j}{e^k \cdot (e^i \times e^j)}
\]

Therefore it is possible to define the set of covariant orthogonal reciprocal basis vectors \(e_i\) from the set of contravariant oblique basis vectors \(e^j\). These set of basis vectors are significant in determining the components of a vector when defined in an oblique space \(\mathbb{E}^3\). It is known that in order to transform any set of vectors to another set of vectors the use of a second order tensor is required. The second order transformation tensor acts as a mapping function between \(\mathbb{X}_3\) and \(\mathbb{E}^3\).

2.2. Second Order Oblique Transformation Tensor

If the scalar product of equation (1) with \(e_k\) is taken and used in equation (3) it can be arrived that

\[
v_i = (e_i \cdot X_j)u_j
\]

The second order tensor \(\alpha\) with components \(\alpha^i_j\) is defined as \([16]\)

\[
\alpha^i_j (e^i \otimes X_j) = [e_i \cdot X_j](e^i \otimes X_j)
\]

So equation 7 can be written as

\[
v_i = \alpha^i_j u_j
\]

Thus \(\alpha\) is the second order oblique transformation tensor that converts the definition of a vector in \(\mathbb{X}_3\) to its corresponding definition in \(\mathbb{E}^3\). The product \(\otimes\) is the dyadic product, also popularly called the tensor product \([17]\).
2.3. Transformation of Basis Vectors
The non-orthogonal basis vectors $e^i$ in $\mathbb{E}^3$ can be expressed in terms of the orthonormal basis $x_j$ in $\mathbb{X}_3$ and the transformation can be defined using a second order tensor $\mathcal{M}$ with components $\mathcal{M}^i_j$ as

$$e^i = \mathcal{M}^i_j x_j$$

(10)

Taking scalar product with $x_k$ on both sides of equation (10) it is arrived at as

$$\mathcal{M}^i_j = (e^i \cdot x_j)$$

(11)

It is to be noted here that the tensor $\mathcal{M}^i_j$ is a tensor that helps to express the contravariant basis vectors $e^i$ in terms of the covariant basis vectors $x_j$.

2.4. Proposition
The basis transformation tensor $\mathcal{M}^i_j$ can efficiently arrive at $\alpha^i_j$ without the need to describe the reciprocal basis $e_i$.

Proof:
Taking scalar product of equation 1 with $x_k$ and using equation 11 it can be shown

$$u_j = v_i \mathcal{M}^i_j$$

(12)

Using equation 9 in equation 12 and after some algebraic simplifications, the following relation is achieved

$$\alpha^k_i \mathcal{M}^i_j = \delta_{ij}$$

(13)

Equation 13 helps us to arrive at the second order transformation tensor $\alpha^i_j$ without the need for using the extra cumbersome step of determining the reciprocal basis vectors $e_i$. Almost in all cases when the oblique basis are defined, they are defined with respect to the Cartesian orthogonal basis. So it is pretty easy to determine the tensor $\mathcal{M}^i_j$ and hence arrive at $\alpha^i_j$.

2.5. Fourth order transformation tensors
A second order tensor $A_{pq}$, described in $\mathbb{X}_3$ will have its corresponding description $B_{ij}$ in ($\mathbb{E}^3$) and the transformation will be guided by a fourth order transformation $\mathbf{\beta}$ such that

$$B_{ij} = \beta^i_{kl} A_{kl}$$

(14)

The components $\beta^i_{kl}$ can be determined from [16] as

$$\beta^i_{kl}(e^i \otimes e^j \otimes x_k \otimes x_l) = (e_i \cdot x_j)| (e^i \otimes e^j \otimes x_k \otimes x_l) = \alpha^i_k \alpha^j_l (e^i \otimes e^j \otimes x_k \otimes x_l)$$

(15)

Again from equation 13 it can be written

$$\beta^i_{kl} = \mathcal{M}^i_k \mathcal{M}^i_l$$

(16)
2.6. Transformation between oblique coordinate systems

Let $e^i$ and $e^{*j}$ be two sets of oblique basis. Let $v_i$ and $v^{*}_j$ be the components of a vector in the two oblique coordinates respectively. Thus

$$v_i e^i = v^{*}_j e^{*j}$$

Taking scalar product of equation 17 with $X_k$ and using equation 11 it can be written after simplifications

$$v_i = [M^{*j}_i M^{-1}_i]T v^{*}_j$$

(18)

where $M^{*j}_i = (e^{*i} \cdot X_j)$. Thus even during transformation of quantities between two different oblique coordinates, the tensor defined in equation 11 can be used, without defining the reciprocal basis vectors in both the oblique systems.

2.7. Numerical example to illustrate the proposition

To demonstrate the effectiveness of the method let us look at an example. Consider an arbitrary set of oblique basis as

$$e^1 = X_1 - X_2 + X_3$$
$$e^2 = X_2 - X_3$$
$$e^3 = X_1 + X_2$$

Two different methods are now implemented, first the traditional approach and then the novel proposed approach, to determine the transformation tensor $\alpha^i_j$ and test the validity of the approach.

**Method 1**

From equation 6 the corresponding set of reciprocal basis are determined as

$$e_1 = X_1 - X_2 - X_3$$
$$e_2 = X_1 - X_2 - 2X_3$$
$$e_3 = X_2 + X_3$$

Using the reciprocal basis $e_i$, the tensor $\alpha^i_j$ from equation 8 can be arrived at as

$$\alpha = \begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & -2 \\ 0 & 1 & 1 \end{bmatrix}$$

**Method 2**

Here the validity of the proposed method is tested. From equation 11 the tensor $M^i_j$ is determined as

$$M = \begin{bmatrix} 1 & -1 & 1 \\ 0 & 1 & -1 \\ 1 & 1 & 0 \end{bmatrix}$$

And hence

$$M^{-T} = \begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & -2 \\ 0 & 1 & 1 \end{bmatrix}$$
3. Contravariant tensors in continuum models

Hyperelastic material models are continuum mechanics based mathematical functions that describe the relationship between state variables of displacements and stresses. In hyperelasticity the deformation is described using the deformation gradient tensor

\[ F_{ij} = \frac{\partial x_i}{\partial X_j} \]  

where \( x_i \) denotes the spatial/deformed/Eulerian coordinates and \( X_J \) denotes the material/undeformed/ Lagrangian coordinates. In this work material indices are denoted using capital and spatial indices using small alphabets respectively. Two strain definitions are available in literature \[17–19\] as

\[ C_{IJ} = F_{iI}F_{iJ} \quad b_{ij} = F_{iI}F_{jI} \]  

where \( C_{IJ} \) is the second order material right Cauchy Green tensor and \( b_{ij} \) is the spatial left Cauchy green tensor. Since hyperelastic materials are path independent, they are described using a scalar strain energy density function (\( \Psi \)) such that

\[ \Psi = \Psi(C) \]  

The strain energy function can be additively split into volumetric and isochoric components and the isochoric component too can be further split into isotropic and anisotropic components as

\[ \Psi = \Psi_{\text{vol}}(J) + \Psi_{\text{isoch}}(\bar{C}_{IJ}) \quad \Psi_{\text{isoch}} = \Psi_{\text{iso}} + \Psi_{\text{aniso}} \]  

Where \( J = \det(F_{ij}) \) is the Jacobian of the deformation gradient and \( \bar{C}_{IJ} = J^{-2/3}C_{IJ} \) is the isochoric component of the right Cauchy Green tensor.

### 3.1. Anisotropic hyperelasticity

Soft tissues can be idealized as a composite with a ground matrix with fibres embedded. The ground matrix is called the Elastin and embedded in the matrix are Collagen fibres. The tissues behave linearly at lower loads where the matrix takes up the majority of the loads and the fibres stay crimped. As the imposed loads increase, the fibres start unfolding and start taking part in the load bearing process. At this stage anisotropy and non linearity is induced in the tissue.

Thus in order to include the anisotropic effects in \( \Psi_{\text{aniso}} \), it is necessary to include fibre strains. From various literature \([1, 4, 21]\) it can be stated that the histological nature of the collagen fibres is such that , the seemingly random orientation of the fibres, can be idealized into two statistically mean orientations (Refer Fig. 2 (a)). These mean orientations are oblique to the principal loading directions. Figure 2 (b) is a schematic illustration of an arterial tissue sample incised from an arterial layer to be tested for extension and shear tests.

Thus it becomes very spontaneous to define a three dimensional contravariant space such that the basis vectors \( e^1 \) and \( e^2 \) are parallel to the mean fibre orientations making angles \(-\theta_1\) and \( \theta_2 \) w.r.t to the principal loading directions \( X_1 \) and \( X_2 \) respectively. The third basis vector \( e^3 \) is along \( X_3 \) which is normal to the plane of the tissue (Refer Fig. 2). A two point tensor \( \bar{C}^{*IJ} \) can thus be arrived at such that

\[ \bar{C}^{*IJ} = \beta^{IJ}_{KL} \bar{C}_{KL} \]  

The fourth order tensor \( \beta^{IJ}_{KL} \) can be arrived from equation 15 using \( \alpha^{I}_{J} \) which can further be determined from equation 13 by defining \( \mathcal{M}^{I}_{J} \) such as

\[ \mathcal{M} = \begin{bmatrix} \cos \theta_1 & -\sin \theta_1 & 0 \\ \cos \theta_2 & \sin \theta_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]
The principal invariants of $C^{*IJ}$ can thus be arrived at as

$$\bar{I}_1^* = \bar{C}^{*IJ} \delta_{IJ}, \quad \bar{I}_2^* = 0.5 \left[ (\bar{I}_1^*)^2 - \bar{C}^{*IJ} \bar{C}^{*IJ} \right], \quad \bar{I}_3^* = \det(\bar{C}^{*IJ}).$$

where $\delta_{IJ}$ is the Kronecker Delta.

An anisotropic function was proposed in [14] using the first invariant $\bar{I}_1^*$, which contains the sum of the squares of stretches in the fibre directions, such that

$$\Psi_{\text{aniso}} = \frac{\omega_1}{\omega_2} \left[ e^{\omega_2|\bar{I}_1^*/\gamma - 1|^2} - 1 \right]$$

where $\omega_1, \omega_2 > 0$ were the stress like and dimensionless material parameters respectively and the scalar dimensionless parameter $\gamma$ is the value of $\bar{I}_1^*$ when $C_{IJ} = \delta_{IJ}$. Assuming a neo-Hookean form for the isotropic function the total strain energy density function can thus be arrived at as

$$\Psi = 0.5\kappa [J - 1]^2 + \frac{\mu}{2} [\bar{I}_1 - 3] + \frac{\omega_1}{\omega_2} \left[ e^{\omega_2|\bar{I}_1^*/\gamma - 1|^2} - 1 \right]$$

Here $\kappa$ is the bulk modulus and $\mu > 0$ is the neo-Hookean constant equivalent to the shear modulus.

The second Piola Kirchhoff stress ($S_{IJ} = 2 \left[ \partial\Psi / \partial\bar{C}_{IJ} \right]$) can thus be arrived at as

$$S_{IJ} = -pJC_{IJ}^{-1} + 2J^{-2/3}P_{IJKL} \frac{\partial\Psi_{\text{isoch}}}{\partial\bar{C}_{KL}}$$

wherein $P_{IJKL}$ is the projection tensor from literature [22] and $p$ is a Lagrangian multiplier.

### 3.2. Modeling continuum damage

Damage occurs when there is a loss of stiffness in the material. Soft tissues can experience damage either due to the cyclic and repeated nature of the physiological loads they are exposed to or due to supra physiological loads. In either way modelling damage involves definition of a damage parameter $D_\epsilon \in [0, 1]$ such that

$$D_\epsilon = \begin{cases} 0 & \text{no damage} \\ 1 & \text{complete mechanical failure} \end{cases}$$
Since damage can occur at both matrix and fibre, parameter $D$ the index $\iota$ can vary between $\iota \in [\text{iso, aniso}]$ such that $D_{\text{iso}}$ is the damage in the isotropic matrix and $D_{\text{aniso}}$ is the damage in the fibres. Ignoring the volumetric contribution towards damage [23], the damaged function of strain energy density ($\Psi^{d}$) can be written as

$$\Psi^{d} = \Psi^{v} + (1 - D_{\text{iso}})\Psi^{\iota_{\text{iso}}} + (1 - D_{\text{aniso}})\Psi^{\iota_{\text{aniso}}}$$ (30)

From the temperature weighted entropy equation, the internal rate of dissipation of energy $D_{\text{int}}$ can be determined as

$$D_{\text{int}} = \sum_{\iota=\text{iso, aniso}} q_{\iota} \dot{D}_{\iota} \geq 0$$ (31)

Here $q_{\iota}$ is a scalar quantity that governs the evolution of damage and is the thermodynamic force conjugate to $D_{\iota}$ which can be expressed mathematically as

$$q_{\iota_{\text{iso}}} = -\frac{\partial \Psi^{\iota_{\text{iso}}}}{\partial D_{\iota_{\text{iso}}}} = \Psi^{u_{\text{iso}}}; \quad q_{\iota_{\text{aniso}}} = -\frac{\partial \Psi^{\iota_{\text{aniso}}}}{\partial D_{\iota_{\text{aniso}}}} = \Psi^{u_{\text{aniso}}}$$ (32)

The damaged second Piola Kirchhoff stress can be determined as

$$S_{IJ}^{d} = -p J C_{IJ}^{-1} + (1 - D_{\text{iso}}) \frac{\partial \Psi^{\iota_{\text{iso}}}}{\partial C_{IJ}} + (1 - D_{\text{aniso}}) \frac{\partial \Psi^{\iota_{\text{aniso}}}}{\partial C_{IJ}}$$ (33)

### 3.3. Definition of damage functions

The damage functions need to be decaying functions of internal parameters that can capture the damage evolution. The internal variable for isotropic damage can be taken from literature [24] as the equivalent stretch ($\lambda_{eq} = \sqrt{C_{IJ} C_{IJ}}$). An exponentially decaying function may be adopted as

$$1 - D_{\text{iso}} = e^{a_{m}(\lambda_{eq}^d - \lambda_{eq})}$$ (34)

where $a_{m} > 0$ is a material constant associated with the damage of the matrix and $\lambda_{eq}^d \geq 1$ dictates the onset of damage in the matrix.

For the anisotropic damage a decaying function that takes into account both the damage of the fibres due to extension and damage in the fibre-matrix interface can be adopted such that

$$1 - D_{\text{aniso}} = \left[ e^{a_{f}(I_{1}^{d} - I_{1}^{d})} \right]$$ (35)

Where $I_{1}^{d}$ is the invariant from equation 25 parametrizing the fibre stretches. The material constants $a_{f} > 0$ is associated with fibre damage. The constant $I_{1}^{d} \geq 1$ dictates the onset of damage in the fibre.

### 4. Applications

The approach of using the contravariant tensors for both modelling the material response as well as prediction of damage evolution can be validated with experimental data. The material model discussed in section 3.1 along with the continuum damage model discussed in section 3.3 was fitted to the experimental data of the extension of rat tail tendon fibre from literature [25] also used recently in [20].

Table 1 shows the material parameters obtained for the material model and damage model respectively. The damage in isotropic matrix was assumed to initiate when the stretch in the tissue reaches $\lambda = 1.05$. The fibre-matrix interface damage was assumed to occur when the extension vs stress curve enters into a linear phase ie $\lambda \approx 1.06$ and loss of fibre stiffness was
Figure 3. Stretch ($\lambda$) vs first Piola Kirchoff stress ($P$) under uniaxial extension. The '×' markers represent the experimental data of rat tail tendon fibre from [25] and the smooth line represents the prediction of the model.

Table 1. Summary of material parameters

| Model Type       | Parameters                        |
|------------------|-----------------------------------|
| Material Model   | $\mu = 10$ MPa                    |
|                  | $\omega_1 = 68.1$ MPa            |
|                  | $\omega_2 = 8.2$                  |
|                  | $\theta = 75^\circ$              |
| Damage Model     | $a_m = 1.2$                       |
|                  | $a_f = 0.95$                      |

assumed at a higher stretch value of $\lambda \approx 1.11$. were also executed in a finite element scheme to illustrate the robustness of the approaches.

Figure 3 illustrates the prediction of the model with respect to the observed data [25, 26]. As can be seen that the approach of using contravariant tensors into continuum models give an accurate prediction under lower as well as high stretch values.

A finite element application of the model was carried out for a 'L' shaped geometry. The geometry was fixed at one of the legs, to constrain rigid body motion, and a vertical displacement was applied at the other end (Refer Fig. 4) so as to open the re-entrant corner. The geometry was meshed using three noded constant strain triangles. In the Figure 5 both the isotropic as well as the anisotropic damage evolution can be seen. The contour plots reveal a higher damage prediction at the re-entrant corner.
Figure 4. A schematic representation of the 'L' shaped geometry

Figure 5. Evolution of (a) $D_{iso}$ and (b) $D_{aniso}$ for a 'L' shaped geometry illustrating high damage prediction at re-entrant corner

5. Conclusion
This work integrates and summarizes the application of contravariant tensors in continuum mechanics. Firstly the framework of the oblique coordinate system was introduced and a new approach was proposed to transform tensors which reduced a cumbersome step used in traditional approaches. Then it was demonstrated how contravariant tensors are applicable in material modelling as well as damage modelling. The models arrived at from contravariant tensor analysis was fitted to experimental data and validated with the observations. The models were also executed in a finite element scheme to illustrate the robustness of the approaches.

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