Published in final edited form as:

Mech Mater. 2014 August 1; 75: 73–83. doi:10.1016/j.mechmat.2014.04.006.

Accurate Prediction of Stress in Fibers with Distributed Orientations Using Generalized High-Order Structure Tensors

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Abstract

The orientation of collagen fibers plays an important role on the mechanics of connective tissues. Connective tissues have fibers with different orientation distributions. The angular integration formulation used to model the mechanics of fibers with distributed orientation is accurate, but computationally expensive for numerical methods such as finite elements. This study presents a formulation based on pre-integrated Generalized High-Order Structure Tensors (GHOST) which greatly improves the accuracy of the predicted stress. Simplifications of the GHOST formulation for transversely-isotropic and planar fiber distributions are also presented. Additionally, the GHOST and the angular integration formulations are compared for different loading conditions, fiber orientation functions, strain energy functions and degrees of fiber non-linearity. It was found that the GHOST formulation predicted the stress of the fibers with an error lower than 10% for uniaxial and biaxial tension. Fiber non-linearity increased the error of the GHOST formulation; however, the error was reduced to negligible values by considering higher order structure tensors. The GHOST formulation produced lower errors when used with an elliptical fiber density function and a binomial strain energy function. In conclusion, the GHOST formulation is able to accurately predict the stress of fibers with distributed orientation without requiring numerous integral calculations. Consequently, the GHOST formulation may reduce the computational effort needed to analyze the mechanics of fibrous tissues with distributed orientations.

1. Introduction

Collagen fibers are one of the most important structural components in connective tissues. Connective tissues mechanical properties and functions are largely determined by the fiber orientation. For instance, collagen fibers in the Achilles tendon are oriented along the axis of the tendon since the function of the tendon is to transmit force in one direction. Fibers in most connective tissues, however, are not completely parallel, but have different distributions of fiber orientations. This variation can be represented by a distribution function which mathematically represents the fraction of fibers oriented in a given direction.

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Distribution functions are usually characterized by two parameters: the mean (average) orientation and the spread of the distribution function. The fiber-orientation distribution is a structural characteristic that has an important role on the mechanics of these tissues (Ateshian et al., 2009; Federico and Gasser, 2010; Federico and Herzog, 2008; Gasser et al., 2006; Gilbert et al., 2008; Lake et al., 2009; Pandolfi and Vasta, 2012; Szczesny et al., 2012). For instance, the tensile modulus of the supraspinatus is lower in regions with a wider distribution function (Lake et al., 2009; Szczesny et al., 2012). Similarly, several important characteristics of the mechanical behavior of articular cartilage, including the non-linearity of the Poisson's ratio, can be accurately described by a model including a distribution function (Ateshian et al., 2009).

Several formulations are used to model the mechanical behavior of fibrous tissues with distributed orientations. The Angular-Integration (AI) formulation is considered the exact method to model the mechanics of fibrous tissues with distributed orientations (Lanir, 1983). In this method, the contribution of infinitesimal fractions of fibers oriented in all directions is added (integrated) to obtain the total stress of the fibers. However, when used in numerical methods such as finite elements, it may be computationally expensive because an angular integral needs to be evaluated every time a stress component is calculated. In finite element analysis of nonlinear tissues with distributed fibers, thousands of integrals are calculated since the stress needs to be evaluated for every Gauss point of every element, at every iteration of every time step.

To overcome the problem of computational expense, a formulation based on a pre-integrated 2nd-order structure tensor (2ST) was developed (Gasser et al., 2006). The advantage of using the 2ST formulation is that, once the structure tensor is calculated, no integrations are required to calculate the stresses. However, structure tensors may lead to significant errors in the stress values for particular distribution functions and loading conditions due to averaging of the fiber stretch and fiber buckling (Cortes et al., 2010; Federico and Herzog, 2008; Pandolfi and Vasta, 2012). An extension of the 2ST formulation, where the strain energy was expanded in a Taylor series and the first two non-zero terms were used to calculate the stresses of the fibers, was recently proposed (Pandolfi and Vasta, 2012). This formulation used 2nd- and 4th-order pre-integrated structure tensors, which reduces the error with respect to the AI formulation. Although, the 4th-order structure tensor (4ST) formulation improves the accuracy of the 2ST formulation, considerable differences are still obtained compared to the AI formulation.

The objective of this study is to present a formulation based on pre-integrated structure tensors to calculate the stress of fibers with distributed orientations. The error reduction using the GHOST formulation is shown for an isotropic fiber distribution and for different degrees of fiber non-linearity. The effect of anisotropy is analyzed using an ellipsoidal orthotropic distribution. Additionally, the GHOST formulation is simplified for transversely-isotropic and planar distributions. Then, several typical fiber strain energy functions are compared to determine which produces lower errors. Finally, it is shown that the total error can be separated in two components: averaging of the fiber stretch and fiber buckling. The method presented here may potentially improve the computational efficiency and accuracy

of numerical methods used to analyze the mechanics of fibrous tissues with distributed orientations.

2. Theoretical Formulation

In this section, the AI and pre-integrated structure tensor formulations are described. The proposed GHOST formulation will be presented in section 3. Collagenous soft-tissues are frequently modeled as hyperelastic fiber-reinforced materials (Holzapfel, 2000; Spencer, 1984). The mechanical behavior of hyperelastic materials is defined by a strain energy function (Ψ) from which the relationship between the second Piola-Kirchhoff stress ($\mathbf{S}$) and right Cauchy-Green strain ($\mathbf{C}$) as well as the elasticity tensor ($\mathbf{\Xi}$) can be calculated:

$$\mathbf{S} = 2 \frac{\partial \Psi}{\partial \mathbf{C}}, \quad (1)$$

$$\mathbf{\Xi} = 4 \frac{\partial^2 \Psi}{\partial \mathbf{C} \partial \mathbf{C}}, \quad (2)$$

The strain energy function can also be divided into the addition of the isotropic (iso) and anisotropic (ani) components:

$$\Psi = \Psi_{iso} + \Psi_{ani}. \quad (3)$$

The isotropic and anisotropic components of the strain energy represent the matrix and the fibers, respectively. Similarly, the stress and elasticity tensor can also be additively divided as:

$$\mathbf{S} = \mathbf{S}_{iso} + \mathbf{S}_{ani}, \quad (4)$$

$$\mathbf{\Xi} = \mathbf{\Xi}_{iso} + \mathbf{\Xi}_{ani}. \quad (5)$$

When the fibers in the tissue are parallel, the strain energy of fibers can be expressed in terms of an invariant of the strain tensor $\mathbf{C}$:

$$\Psi_{ani} = \Psi_{ani}(I_4), \quad (6)$$

where

$$I_4 = \mathbf{a} \cdot \mathbf{C} \cdot \mathbf{a} = \mathbf{C} : \mathbf{a} \otimes \mathbf{a}, \quad (7)$$

I_4 is a pseudo-invariant of $\mathbf{C}$, $\mathbf{a}$ is a unit vector in the direction of the fibers, and $\mathbf{a} \otimes \mathbf{a}$ is a second order tensor representing the structure of the fibers.

Equations (1)-(7) describe the mechanical behavior of tissues reinforced with parallel fibers oriented in one direction. If a tissue has fibers oriented in several discrete directions, the stress of each fiber family is added to obtain the total stress. Similarly, in the case of a

continuous fiber density distribution (infinite number of fiber orientations), the total stress of the fibers is obtained by adding (integrating) the stress of infinitesimal fractions of fibers.

2.1. Angular-integration formulation

The AI formulation is the exact method to calculate the stress in fibrous tissues with distributed orientations. This formulation is valid for continuous fiber density functions and for experimentally derived (histogram) distributions. In this section, only continuous fiber density functions are considered, but the AI formulation can be easily adapted to use with histogram distributions.

Fiber-orientation distribution can be represented using a fiber density function $R(\theta, \varphi)$. This function satisfies the condition:

$$\int_0^{2\pi} \int_0^{\pi/2} R(\theta, \varphi) \sin\theta d\theta d\varphi = 1. \quad (8)$$

A distribution-weighted average in terms of the fiber density function can be defined as:

$$\langle * \rangle = \int_0^{2\pi} \int_0^{\pi/2} R(\theta, \varphi) (*) \sin\theta d\theta d\varphi. \quad (9)$$

Using this notation, the strain energy of the fibers can be expressed as:

$$\Psi_{ani} = \langle \bar{\Psi}(I_4) H(I_4 - 1) \rangle, \quad (10)$$

where H is the Heaviside function which ensures that fibers in compression do not contribute to the mechanics of the tissue, and Ψ is the strain energy of an infinitesimal fraction of fibers in the direction of a unit vector $\mathbf{a}$. I_4 follows the definition shown in Eq. (7) and the unit vector can be expressed in terms of the Euler angles as

$$\mathbf{a} = [\sin\theta \sin\varphi, \sin\theta \cos\varphi, \cos\theta]. \quad (11)$$

The stress in the fibers can be then expressed as:

$$\mathbf{S}_{ani} = \langle 2 \frac{\partial \bar{\Psi}(I_4)}{\partial I_4} \frac{\partial I_4}{\partial \mathbf{C}} H(I_4 - 1) \rangle = \langle 2 H(I_4 - 1) \frac{\partial \bar{\Psi}(I_4)}{\partial I_4} \mathbf{a} \otimes \mathbf{a} \rangle. \quad (12)$$

This formulation requires an angular integration to find each component of the stress tensor for every value of the strain tensor $\mathbf{C}$. Consequently, this formulation may be computationally expensive when used in numerical methods such as finite elements analysis. A structure tensor formulation for fibers with distributed orientations, which requires only one angular integration, was proposed by Gasser et al., (2006) and is described in the following section.

2.2. Structure Tensor Formulation

To simplify AI formulation, Gasser et al., (2006) proposed a structure tensor representing the fiber distribution:

$$\mathbf{A} = \langle \mathbf{a} \otimes \mathbf{a} \rangle, \quad (13)$$

which is the weighted average of the second order tensor $\mathbf{a} \otimes \mathbf{a}$. For a transversely isotropic distribution, the generalized structure tensor reduces to:

$$\mathbf{A} = \kappa \mathbf{I} + (1 - 3\kappa) \mathbf{a}_0 \otimes \mathbf{a}_0, \quad (14)$$

where $\mathbf{a}_0$ is the mean orientation of the fiber family and κ is defined as:

$$\kappa = \langle \sin^2 \theta \sin^2 \varphi \rangle = \pi \int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta. \quad (15)$$

Similar to eq. (7), a pseudo-invariant $\overline{I}_4$ was defined as:

$$\overline{I}_4 = \mathbf{C} : \mathbf{A} = \langle I_4 \rangle, \quad (16)$$

which can be considered the weighted average of I_4 . The following strain energy function was proposed for a family of distributed fibers:

$$\Psi_{ani} = \Psi_{ani}(\overline{I}_4) = \frac{k_1}{2k_2} \left(e^{k_2(\overline{I}_4 - 1)^2} - 1 \right). \quad (17)$$

Consequently, the stress in the fibers can be expressed as:

$$\mathbf{S}_{ani} = 2 \frac{\partial \Psi_{ani}}{\partial \mathbf{C}} = 2 \frac{\partial \Psi_{ani}}{\partial \overline{I}_4} \mathbf{A}. \quad (18)$$

The buckling condition for this formulation is that the anisotropic part of the generalized structure tensor, $(1 - 3\kappa) \mathbf{a}_0 \otimes \mathbf{a}_0$, does not contribute to $\mathbf{A}$ when $\mathbf{C} : \mathbf{a}_0 \otimes \mathbf{a}_0 < 1.0$.

Equation (18) is the expression to calculate the stress of the fiber using the 2ST formulation (Gasser et al., 2006). In this formulation, only one integral is required (Eq. 15) to calculate the pseudo-invariant $\overline{I}_4$ and the fiber stress $\mathbf{S}_{ani}$. Consequently, the reduction of computational effort is evident. However, as shown in the following section, the stress values obtained from the 2ST formulation may differ from those obtained with the AI formulation.

2.3. Differences between angular-integration and structural tensor formulations

The AI and 2ST formulations may produce different values of stress from the same strains depending of the fiber density function and the loading case (Cortes et al., 2010; Federico and Gasser, 2010; Federico and Herzog, 2008; Pandolfi and Vasta, 2012). In this section, the

causes of these differences are discussed and a method to reduce these differences proposed by Pandolfi and Vasta (2011) is presented.

The difference between the AI and the 2ST formulations has two sources. The first source is that $\bar{I}_4$ may include fibers in compression. Consider the case of isotropic fiber distribution under uniaxial tension. In this loading case a fraction of the fibers is under compression due to lateral contraction. According to Eqs. (13) and (16), those fibers are not excluded from the calculation of the structure tensor $\mathbf{A}$ or the pseudo-invariant $\bar{I}_4$. If these fibers are not excluded from the calculation, $\bar{I}_4$ is under-predicted. Consequently, the values of stress are lower compared to the AI formulation. The second source of difference is the use of weighted average of the fiber strain invariant ($\bar{I}_4$) instead of averaging the stresses in fibers (Cortes et al., 2010). Consider a loading case where all fibers are in tension. Using the average value of I_4 in the calculation of fiber stress causes errors for non-linear fibers. In general, for non-linear functions, the average of the function output is not the same as the output of the average input. This effect has been shown and discussed by Federico et al. (2008) and Pandolfi and Vasta, (2011) and can be visualized by considering the Taylor expansion of the strain energy function about $\bar{I}_4$:

$$\Psi(I_4) = \Psi(\bar{I}_4) + \frac{\partial \Psi(\bar{I}_4)}{\partial I_4} (I_4 - \bar{I}_4) + \frac{1}{2!} \frac{\partial^2 \Psi(\bar{I}_4)}{\partial I_4^2} (I_4 - \bar{I}_4)^2 + \frac{1}{3!} \frac{\partial^3 \Psi(\bar{I}_4)}{\partial I_4^3} (I_4 - \bar{I}_4)^3 + \dots \quad (19)$$

The approximation taken in the 2ST approach (Eq. 17) is equivalent to considering just the first term of the right hand side of Eq (19) and ignoring all the high order terms. The 4ST formulation included the first three terms of the right hand side of Eq (19) and resulted in a decreased error compared to the AI formulation. Notice that in both formulations (2ST and 4ST) the error depends on the derivatives of the strain energy function and the applied strain (I_4 and $\bar{I}_4$). The dependence of the error on the strain energy function and the applied strain is a disadvantage of all the formulations based on pre-integrated structure tensors, including this one. However, the approach shown below to consider more terms in Eq (19) (see section 3) will reduce the error associated with the non-linearity of strain energy function and the applied strains. The error caused by buckling of a fraction of fibers is not reduced by considering more terms of Eq. (19). However, the contribution of fiber buckling to the total error is minor (see section 3.4).

3. Generalized High-Order Structure Tensor (GHOST): formulation and results

In this section, a formulation considering any number of terms of the Taylor expansion is presented. Additionally, simplifications for special fiber distributions are also discussed. The expression of the AI formulation, without considering fiber buckling, is:

$$\Psi_{ani} \approx \langle \Psi(I_4) \rangle. \quad (20)$$

By replacing the energy function on the right-hand side of Eq (20) by a Taylor expansion about $\overline{I}_4$ we obtain:

$$\Psi_{ani} \approx \left\langle \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\overline{I}_4) (I_4 - \overline{I}_4)^n \right\rangle, \quad (21)$$

where $\Psi^{(n)}(\overline{I}_4) = \frac{\partial^n \Psi(\overline{I}_4)}{\partial \overline{I}_4^n}$. Since $\overline{I}_4$ is constant for a given angular orientation, $\Psi^{(n)}(\overline{I}_4)$ can be taken out of the integrand in Eq (9). Eq (21) can be rewritten as:

$$\Psi_{ani} \approx \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\overline{I}_4) \langle (I_4 - \overline{I}_4)^n \rangle. \quad (22)$$

The binomial raised to the n^{th} power in Eq (22) can be expanded by means of the binomial theorem or, equivalently, using Pascal's triangle as:

$$(I_4 - \overline{I}_4)^n = \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} I_4^{n-p} \overline{I}_4^p. \quad (23)$$

Substituting Eq (23) into (22), we obtain:

$$\Psi_{ani} \approx \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\overline{I}_4) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \langle I_4^{n-p} \rangle \overline{I}_4^p. \quad (24)$$

The term that contains I_4 can be approximated in the terms of the right Cauchy strain tensor $\mathbf{C}$ and the unit vector $\mathbf{a}$ (Eq. 7) as:

$$\langle I_4^n \rangle \approx \langle (\mathbf{C} : \mathbf{a} \otimes \mathbf{a})^n \rangle = \langle \mathbf{C}^n \odot^{2n} \mathbf{a}^{2n} \rangle, \quad (25)$$

where the notation $\mathbf{a}^n$ indicates the n^{th} outer product of the tensor $\mathbf{a}$ with itself. For instance, $\mathbf{a}^2 = \mathbf{a} \otimes \mathbf{a}$. The operator $\odot^n$ denotes the n^{th} -dimensional inner product of two tensors. For instance, $\mathbf{C} \odot^2 \mathbf{a}^2 = \mathbf{C} : \mathbf{a} \otimes \mathbf{a} = I_4$ or $\mathbf{C}^2 \odot^4 \mathbf{a}^4 = I_4^2$.

Substituting Eq. (25) into (24), we obtain:

$$\Psi_{ani} \approx \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\overline{I}_4) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \overline{I}_4^p \langle \mathbf{C}^{n-p} \odot^{2(n-p)} \mathbf{a}^{2(n-p)} \rangle. \quad (26)$$

Since the tensor $\mathbf{C}^{n-p}$ is not a function of the angular integration, Eq. (26) can be expressed as:

$$\Psi_{ani} \approx \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\overline{I}_4) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \overline{I}_4^p \mathbf{C}^{n-p} \odot^{2(n-p)} \mathbf{A}^{n-p}, \quad (27)$$

where $\mathbf{A}^{n-p} = \langle \mathbf{a}^{2(n-p)} \rangle$ is a GHOST of $2(n-p)$ order. Notice that $\mathbf{A}^1 = \langle \mathbf{a}^2 \rangle = \langle \mathbf{a} \otimes \mathbf{a} \rangle$ is the structure tensor proposed by Gasser et al. (2006) shown in Eq. (14). The second Piola-Kirchhoff stress can be expressed for the GHOST formulation as:

$$\mathbf{S}_{ani} = 2 \frac{\partial \Psi_{ani}}{\partial \mathbf{C}} \approx \mathbf{S}_{GHOST} = \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)}(\bar{I}_4) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \bar{I}_4^p \mathbf{C}^{n-p-1} \odot^{2(n-p)} \mathbf{A}^{n-p}. \quad (28)$$

Equation (28) represents an expression for the fiber stress in terms of $\bar{I}_4$ and the tensors $\mathbf{C}^n$ and $\mathbf{A}^n$. An important characteristic of Eq (28) is that once the GHOSTs have been calculated, no angular integrals are required to calculate the stresses. Therefore, this formulation may potentially improve the computational efficiency of numerical methods such as finite elements. For an n large enough, the error caused by averaging is negligible (See section 4). Notice that $\bar{I}_4$ was not derived with respect to $\mathbf{C}$ in Eq. (28). Although $\bar{I}_4$ is function of $\mathbf{C}$ (Eq. 16), it is considered as a constant parameter for derivation purposes, since it was used as the center of the Taylor expansion (Eq. 21). In other words, after the Taylor expansion, Ψ_{ani} is still a function of I_4 not $\bar{I}_4$. Consequently, the derivatives with respect to $\mathbf{C}$ were only applied to the term $\mathbf{C}^{n-p} \odot^{2(n-p)} \mathbf{A}^{n-p}$. This is a subtle difference compared to the 4ST formulation where $\bar{I}_4$ was also derived with respect to $\mathbf{C}$.

The number of elements of $\mathbf{A}^n$ is 3^{2n} for 3-dimensional fiber density functions. Due to the symmetry of the GHOSTs, the number of independent elements of $\mathbf{A}^n$ is $N_A = (2n+1)(n+1)$. N_A is the number of elements (i.e., integrals) needed to completely define the GHOST $\mathbf{A}^n$. For instance, a total 231 angular integrations are needed for a 10th order GHOST, which is still much lower than the number of numerical integrations required to solve a finite element model using the AI formulation. Additionally, if the fiber distribution is axis-symmetric, many of the independent elements of the GHOST are equal to zero, further reducing the number of required integrations. The number of independent elements of the tensor $\mathbf{C}^n$ is $N_C = (n+5)!/n!5!$ and the multiplicity (number of times an independent element is included in the tensor) is:

$$\mu = \frac{n!}{c_1!c_2!c_3!c_4!c_5!c_6!}, \quad (29)$$

where c_i is the number of times the i^{th} element of $\mathbf{C}$ is multiplied in the independent element of $\mathbf{C}^n$. The multiplicity of the elements of the tensor $\mathbf{C}^n$ is important to calculate the tensor operation of Eq (28).

To compare the AI and the GHOST formulations, the case of uniaxial tension of an isotropic fiber distribution with a range of applied stretch of $\lambda_a = 1.0$ -1.5 was considered. The fibers were assumed to be embedded in an incompressible isotropic matrix to simplify the calculation of lateral contraction. The error between the formulations is defined in terms of the second Piola-Kirchhoff stress as:

$$Err = \frac{s_{GHOST} - s_{AI}}{s_{AI}} \cdot 100. \quad (30)$$

Additionally, the strain energy function shown in Eq. (18) was used with base parameters $k_1 = 1.0$ MPa, and $k_2 = 1.0$ (Pandolfi and Vasta, 2012). To evaluate the effect of non-linearity the parameter k_2 was changed to 10 and 30. These values represent a range of soft and stiff tissues (Kadlowec, 2009). The fiber density function for an isotropic distribution can be expressed as:

$$R(\theta, \varphi) = \frac{1}{2\pi}. \quad (31)$$

The comparison showed that increasing the number of terms considered for the Taylor series results in a reduction of the error to values lower than 20% over the range of stretches from considered (Figure 1A). Notice that increasing the number of terms of the Taylor expansion does not remove the error completely. The remaining error is caused by fiber buckling due to the lateral contraction of the material during the uniaxial tension test (see section 3.4).

Increasing the non-linearity of the fibers (i.e., increasing the value of parameter k_2 of Eq. 17) decreases the range of stretch where the GHOST formulation has low error (Figures 1B and 1C). For k_2 equal to 10.0, the error increases rapidly after an applied stretch of 1.2; while for k_2 equal to 30.0, the error increases after a stretch of 1.1. In any case, the range of applied stretch with low values of error can be increased by increasing the number of terms of the Taylor expansion.

To evaluate the effect of anisotropy of the fiber distribution, an orthotropic ellipsoidal distribution function was considered:

$$R(\theta, \varphi) = \frac{1}{R} \left(\frac{(\cos\varphi \sin\theta)^2}{\xi_1^2} + \frac{(\sin\varphi \sin\theta)^2}{\xi_2^2} + \frac{(\cos\theta)^2}{\xi_3^2} \right)^{-\frac{1}{2}}, \quad (32)$$

where

$$\overline{R} = \int_0^{2\pi} \int_0^{\pi/2} \left(\frac{(\cos\varphi \sin\theta)^2}{\xi_1^2} + \frac{(\sin\varphi \sin\theta)^2}{\xi_2^2} + \frac{(\cos\theta)^2}{\xi_3^2} \right)^{-\frac{1}{2}} \sin\theta d\theta d\varphi. \quad (33)$$

The parameters ξ_1 , ξ_2 , and ξ_3 , which define the principal axes of the ellipsoid, were chosen as ξ^{-1} , 1, and ξ , respectively. Increasing the value of the parameter ξ results in an orthotropic distribution with one major axis ξ^2 times higher than the minor axis (Figure 2). The fibers were subjected to a biaxial stretch of $\lambda_a = 1.2$ in the directions 2 and 3. The difference between the GHOST and AI formulations was calculated for the stress in the direction 3 (Figure 3). Increasing the number of terms in the Taylor expansion makes the error to converge to a low value but the error is not eliminated completely. The remnant error is caused by fiber buckling due to the out-of-plane contraction (direction 1). The difference between formulations decreased with the anisotropy parameter ξ and with the value of n , probably due to the reduction on the fraction of fibers oriented perpendicularly to the loading plane. In the next sections, the GHOST formulation is simplified for the transversely-isotropic and planar distributed orientations.

3.1 Special case 1: GHOST formulation for tissues with transversely-isotropic distributed orientations

A case of interest is a transversely isotropic tissue. Arteries and cornea are modeled using this type of distribution (Gasser et al., 2006; Holzapfel and Ogden, 2010; Pandolfi and Holzapfel, 2008; Pierce et al., 2010). For a transversely isotropic distribution, the GHOST can be calculated as:

$$\mathbf{A}^n = \langle \mathbf{a}^{2n} \rangle = \int_0^{2\pi} \int_0^{\pi/2} R(\theta) \mathbf{a}^{2n} \sin\theta d\theta d\varphi. \quad (34)$$

A particular element of the GHOST can be expressed as:

$$A_{ijk\dots}^n = \int_0^{2\pi} \int_0^{\pi/2} R(\theta) (\sin\theta \sin\varphi)^{n_1} (\sin\theta \cos\varphi)^{n_2} (\cos\theta)^{n_3} \sin\theta d\theta d\varphi, \quad (35)$$

where n_i is the number of times the i^{th} element of $\mathbf{a}$ is multiplied within the particular component of $\mathbf{A}^n$. Therefore, $n_1 + n_2 + n_3 = 2n$. For instance, for the element $A_{1311223}$, $n_1 = 3$, $n_2 = 2$ and $n_3 = 1$. Since the fiber density function is not function of φ , Eq (34) can be expressed as:

$$A_{ijk\dots}^n = \alpha_{n_1 n_2} \int_0^{\pi/2} R(\theta) \sin^{n_1+n_2+1} \theta \cos^{n_3} \theta d\theta. \quad (36)$$

where the coefficient $\alpha_{n_1 n_2}$, for even values of n_1 and n_2 , can be expressed as:

$$\alpha_{n_1 n_2} = \int_0^{2\pi} \sin^{n_1} \varphi \cos^{n_2} \varphi d\varphi = 2\pi \frac{(n_1 - 1) \cdot (n_1 - 3) \cdot (n_1 - 5) \cdots 1 \cdot (n_2 - 1) \cdot (n_2 - 3) \cdot (n_2 - 5) \cdots 1}{(n_1 + n_2) \cdot (n_1 + n_2 - 2) \cdot (n_1 + n_2 - 4) \cdots 2} \quad (37)$$

For odd values of n_1 or n_2 , $\alpha_{n_1 n_2} = 0$. Eq. (36) can be expressed in terms of sine functions as follows:

$$A_{ijk\dots}^n = \alpha_{n_1 n_2} \int_0^{\pi/2} R(\theta) \sin^{n_1+n_2+1} \theta (1 - \sin^2 \theta)^{n_3/2} d\theta \quad (38)$$

Notice that n_3 is always an even number; therefore the fraction $n_3/2$ is always an integer value. Using the Pascal's triangle, Eq. (38) can be expressed as:

$$A_{ijk\dots}^n = \alpha_{n_1 n_2} \sum_{q=0}^{n_3/2} (-1)^q \frac{(n_3/2)!}{q!(n_3/2 - q)!} \int_0^{\pi/2} R(\theta) \sin^{2q+n_1+n_2+1} \theta d\theta. \quad (39)$$

The expression in Eq. (39) can be used to find the values of the GHOSTs for transversely isotropy fiber distributions. An important characteristic of the GHOST formulation for transversely-isotropic distributions is that few one-dimensional integrals are needed to calculate the GHOSTs. For instance, only 5 numerical integrations are needed for a 10th order GHOST. The non-zero elements of a second order GHOST are:

$$\begin{aligned}
A_{11} &= \pi \int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta = \kappa \\
A_{22} &= \pi \int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta = \kappa \\
A_{33} &= 1 - 2\pi \int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta = 1 - 2\kappa
\end{aligned} \quad (40)$$

where the definition used in Eq. (15) have been used. Eq. (40) matches the structure tensor proposed by Gasser et al. (2006). Eq. (39) also matches the fourth-order tensor proposed by Pandolfi and Vasta (2011):

$$\begin{aligned}
A_{1111} &= A_{2222} = \frac{3}{4}\pi \int_0^{\pi/2} R(\theta) \sin^5 \theta d\theta = 3\hat{\kappa} \\
A_{3333} &= 2\pi \left(\frac{1}{2\pi} - 2 \int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta + \int_0^{\pi/2} R(\theta) \sin^5 \theta d\theta \right) = 1 - 4\kappa + 8\hat{\kappa} \\
A_{1133} &= A_{2233} = \pi \left(\int_0^{\pi/2} R(\theta) \sin^3 \theta d\theta - \int_0^{\pi/2} R(\theta) \sin^5 \theta d\theta \right) = \kappa - 4\hat{\kappa} \\
A_{1122} &= \frac{1}{4}\pi \int_0^{\pi/2} R(\theta) \sin^5 \theta d\theta = \hat{\kappa}.
\end{aligned} \quad (41)$$

The error for the GHOST formulation was evaluated for two transversely-isotropic fiber density functions. The first distribution considered is an axi-symmetric version of the von Mises distribution (Gasser et al., 2006):

$$R(\theta) = 4 \sqrt{\frac{b}{2\pi}} \frac{e^{[b(\cos(2\theta)+1)]}}{\text{erfi}(\sqrt{2b})}, \quad (42)$$

where b is a concentration parameter associated with the von Mises distribution, and $\text{erfi}(x) = -i * \text{erf}(ix)$ denotes the imaginary error function with $i = \sqrt{-1}$. Although, the parameter b controls the spread of fiber orientations, a parameter κ defined by Eq. (15) is commonly used to describe the spread of the fiber distribution. A value of κ equal to 0.0 corresponds to parallel fibers, while a value of κ equal to 1/3 correspond to an isotropic distribution. The second distribution considered is an ellipsoidal distribution function where two principal axes have the same value. To represent different degrees of the spread of the distribution, the principal axes of the ellipsoid ξ_1 , ξ_2 , and ξ_3 were chosen as ξ^{-1} , ξ^{-1} , and ξ , respectively. The parameter ξ controls the spread of the distribution. For instance, $\xi = 1.0$ corresponds to an isotropic distribution, while values of ξ larger than 1.0 correspond to a transversely isotropic distribution with a major axis that is ξ^2 times larger than the minor axes. Examples of this distribution as function of the angle θ from the major axis are shown in Figure 4.

The error of the GHOST formulation was reduced to values lower 5% for the case of uniaxial tension in the direction 3, with $\lambda_a = 1.2$, and using the Gasser fiber density function with the base values of the elastic parameters of the fibers (Figure 5A). The effect of the fiber non-linearity can be observed for the Gasser distribution increasing with the non-linearity of the fibers using a value of $k_2 = 30$ (Figure 5B). It can be observed that GHOST formulation diverges around $\kappa = 0.07$. The effect of fiber non-linearity ($k_2 = 30$) for the ellipsoidal distribution is also an increase of the error, but no divergence was observed in the range of values of ξ considered in this study (Figure 5C).

3.2 Special case 2: GHOST formulation for tissues with planar distributed orientations

Collagenous tissues such as skin, pericardium, and aortic leaflets are modeled using planar fiber density functions (Alavi et al., 2013; Billiar and Sacks, 2000, 1997; Gilbert et al., 2008; Sacks, 2003; Tonge et al., 2013a, 2013b). To analyze these tissues, the angular average operator can be re-defined as:

$$\langle \cdot \rangle_{2D} = \int_0^\pi R(\theta)(\cdot) d\theta, \quad (43)$$

where $\int_0^\pi R(\theta) d\theta = 1.0$. The strain energy function can be written as:

$$\Psi_{ani} = \langle \bar{\Psi}(I_4) \rangle_{2D}. \quad (44)$$

The fiber stress shown in Eq. (12) is valid for a general 3-dimensional fiber distribution. However, it can be simplified for the case of planar fiber distributions as

$$\mathbf{S}_{ani} = \langle 2H(I_4 - 1) \frac{\partial \bar{\Psi}(I_4)}{\partial I_4} \mathbf{a} \otimes \mathbf{a} \rangle_{2D} \quad (45)$$

Although Eq. (45) has been solved for a particular choice of $R(\theta)$ and $\bar{\Psi}$ (Raghupathy and Barocas, 2009), in general, it is very difficult to obtain a closed-form solution; therefore, numerical integration is the usual alternative.

Eq. (44) can be expanded using a Taylor expansion around the average value of I_4 ($2D \ 4 = \langle I_4 \rangle_{2D}$) as:

$$\Psi_{ani} = \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)} \left(\overline{2D I_4} \right) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \overline{2D I_4}^p \langle I_4^{n-p} \rangle_{2D}. \quad (46)$$

Eq. (45) can be rewritten in terms of planar GHOSTs as:

$$\Psi_{ani} = \sum_{n=0}^{\infty} \frac{1}{n!} \Psi^{(n)} \left(\overline{2D I_4} \right) \sum_{p=0}^n (-1)^p \frac{n!}{p!(n-p)!} \overline{2D I_4}^{2D} \mathbf{C}^{n-p} \odot^{2(n-p)} \mathbf{A}^{n-p}, \quad (47)$$

where, $2D \mathbf{A}^n = \langle 2D \mathbf{a}^{2n} \rangle_{2D}$. In planar fiber distributions, the unit vector can be expressed as $\mathbf{a} = [\sin \theta, \cos \theta]$ and $2D \mathbf{C} = [C_{11} \ C_{12}; C_{12} \ C_{22}]$. A particular element of the planar GHOST can be written as

$$A_{ijk...} = \int_0^\pi R(\theta) \sin^{n_1} \theta \cos^{n_2} \theta d\theta. \quad (48)$$

The subindices in Eq. (48) take only values of 1 or 2. n_1 and n_2 have similar meaning as those in Eq. (35). Additionally, only the elements of the planar fiber distribution with even values of n_1 and n_2 are different than zero and can be rewritten as:

$$A_{ijk...} = \int_0^\pi R(\theta) \sin^{n_1} \theta (1 - \sin^2 \theta)^{n_2/2} d\theta = 2 \sum_{q=0}^{n_2/2} (-1)^q \frac{(n_2/2)!}{q!(n_2/2 - q)!} \int_0^{\pi/2} R(\theta) \sin^{n_1+2q} \theta d\theta. \quad (49)$$

Eq. (49) shows that the GHOSTs can be calculated using few one-dimensional integrals.

3.3 Comparison between strain energy functions

Since the high-order derivatives of the strain energy functions can have very large values when evaluated in the range of deformations typically found in fibrous soft tissues, the choice of the strain energy function becomes particularly important to achieve convergence of the GHOST formulation. In this section, the strain energy function presented in Eq. (17) is compared to the following exponential and binomial strain energy functions:

$$\Psi(I_4) = c_1 \left(e^{c_2(I_4-1)} - 1 \right) \quad (50)$$

$$\Psi(I_4) = d_1 (I_4 - 1)^{d_2} \quad (51)$$

Similarly to the strain energy function of Eq (17), these energy functions are defined by two parameters that are constrained to be positive. To have a fair comparison between these functions, the elastic parameters of Eqs (50) and (51) were obtained by curve-fitting the response of Eq (17) with $k_1 = 1.0$ and $k_2 = 30$, in the range of uniaxial stretch 1.0-1.2. The parameters of the strain energy functions of Eqs (50) and (51) are $c_1 = 0.0067$, $c_2 = 24.54$, $d_1 = 1.22 \times 10^6$, $d_2 = 10.01$. The differences between these formulations are negligible (Figure 6). The error of the GHOST formulation for a transversely isotropic distribution is shown for uniaxial tension in the main fiber direction (Figure 5B). The divergence observed for the strain energy function shown in Eq. (17) around $\kappa = 0.07$ is reduced by using the exponential strain energy function from Eq (50) and it is almost eliminated using the binomial strain energy function from Eq (51) (Figures 7a and 7b). This comparison suggests that subtle differences in the non-linearity of the functions are amplified for high-order derivatives causing convergence problems in the GHOST formulation. Therefore, a binomial function for the strain energy of the fibers is recommended.

So far, the angular integrals in the GHOST formulation include fibers in all directions without excluding fibers that undergo compression. Increasing the number of terms does not eliminate this source of error. Instead, the GHOST formulation converges to error values that represent the difference between the GHOST and the AI formulations due to local fiber buckling. The next section presents a comparison that suggests that the error caused by fiber buckling is minor compared to that caused by averaging of the fiber stretch.

3.4 Contribution of Averaging of the fiber stretch and Fiber Buckling to the Total Error

The error of utilizing structure tensors can be divided in two components: error caused by strain averaging of the fiber stretch, and error cause by including buckled fibers. The GHOST formulation was implemented to reduce the error caused by averaging of the fiber

stretch. This is achieved by the Taylor expansion of the strain energy around $\mathbf{C}_4$. However, in general, it is not possible to eliminate fiber buckling error for a formulation based on structure tensors. The reason for this is that the fraction of buckled fibers depends on the applied deformation. Therefore, the angular integration, used to define the structure tensor, would need to be modified for each possible loading condition.

To evaluate the contribution of the fiber buckling error to the total, unconstrained and constrained uniaxial deformations were compared. In the unconstrained case, lateral contraction was allowed and calculated assuming incompressibility. In this case, fibers oriented in the lateral direction experience buckling and contribute to the total error. For the constrained case, lateral contraction and the associated fiber buckling were prevented. An isotropic fiber distribution and an exponential strain energy function (Eq. 17) were considered. The comparison shows that, when fiber buckling is present, the GHOST formulation converges to a small error (Figure 8a). However, when fiber buckling is not present, the GHOST formulation eliminates the error completely (Figure 8b). This comparison also shows that error values are reduced from 80% to less than 10%. Other loading conditions, fiber distributions, and strain energy function showed similar error reductions (Figures 1, 3, 5a, 5c, 7b).

4. Discussion

This study presents a method to model the mechanics of distributed fibers using pre-integrated generalized high-order structure tensors (GHOST). In this formulation, the error caused by using the average value of the $\mathbf{C}$ invariant ($\mathbf{C}_4$) is minimized by considering several terms of the Taylor expansion of the energy function around $\mathbf{C}_4$. The numerical comparisons revealed several important characteristics of the GHOST formulation as follows. Although the error increased with the non-linearity of the fibers, which is true for any pre-integrated structure tensor formulation, increasing the order of the GHOST reduced the error with respect to AI formulation (Figure 1). Another important observation is that averaging is the main source of error in the structure tensor formulation. The error can be reduced to values lower than 20% just by correcting the averaging error; i.e., considering high order terms of the Taylor expansion (Figures 1, 3, 5, and 7a).

The type of equation used to describe the strain energy function plays an important role on the accuracy of the GHOST formulation. The equivalent binomial function resulted in negligible error of the stress compared to exponential functions. This is a very important result since it shows that the error of GHOST can be significantly improved with just the proper choice of strain energy function used to describe (curve-fit) the experimental mechanical behavior of the tissue. A possible explanation is that small variations of the energy function are amplified on the high-order derivatives. For instance, depending on the parameters used, the derivatives of the exponential function may have higher numerical values than the original function. This is not the case for binomial functions. Consequently, the use of polynomial energy function results in a more robust behavior of the GHOST formulation. Similarly, the use of an ellipsoidal fiber distribution resulted in a more stable convergence of the GHOST formulation. It is important to note that, although the GHOST formulation did not reduce the error to negligible values for all the cases considered in this

study, the error was always lower than the two structure tensor formulations available (2ST and 4ST).

The GHOST formulation may decrease the computational time in finite elements analysis of tissues with distributed fibers. However, there are many parameters of a finite element model that will influence the run-time difference. For instance, a finite element model with high number of elements may show a large difference since a single set of structure tensors can be calculated for elements with the same material properties. Conversely, in a model with a very low number of elements, the difference in calculation time may be less significant or could even favor the AI formulation for extreme cases. Another parameter that will influence the run-time difference is the nonlinearity of the constitutive equations, since it will increase the number of iterations required to find convergence. Therefore, further study is warranted to determine the effects of GHOST on computational efficiency.

5. Conclusion

A formulation was presented to reduce the error of previous structure tensor formulations. The method demonstrated a high accuracy for a variety of loading cases, fiber distributions, and energy functions. One of the advantages of this method is that once the tensors are calculated no additional integrals are required to evaluate the stress components. This characteristic may be useful to improve the efficiency of numerical methods, such as finite elements, used in the analysis of non-linear tissues with distributed fibers.

Acknowledgments

This study was funded by the National Institute of Arthritis and Musculoskeletal and Skin Diseases (R01AR050052).

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Highlights

- A formulation to predict stresses of fibers with orientation distribution is shown
- The proposed method is compared to the gold standard method of angular integration
- Low values of error (compared to angular integration) were obtained
- The method was simplified for special symmetries of the fiber distribution
- A method to correct for fiber buckling is included
- The proposed formulation may improve the mechanical efficiency of numerical methods

Figure 1.

Error of the GHOST formulation compared to angular integration as function of applied stretch (λ_a) for an isotropic fiber density function under uniaxial tension. The error decreased when high order terms are considered (increasing n) and increased when the non-linearity of the fibers increased (i.e., higher values of the elastic parameter k_2): A) $k_2 = 1.0$, B) $k_2 = 10.0$, C) $k_2 = 30.0$.

Figure 2.

Orthotropic fiber density function defined using an ellipsoidal function. The principal axes were assigned as $(\xi^{-1}, 1, \xi)$. ξ is an anisotropy factor with values higher than 1.0.

Figure 3.

Error of the GHOST formulation for biaxial tension ($\lambda a = 1.2$) applied to directions 2 and 3 of an orthotropic ellipsoid distribution function. The principal axes of the ellipsoid were chosen as $(\xi^{-1}, 1, \xi)$, where ξ is an anisotropy factor with values higher than 1.0.

Figure 4.

Transversely isotropic fiber density function defined using ellipsoidal function. The principal axes of the ellipsoid are chosen as $(\xi^{-1}, \xi^{-1}, \xi)$, where ξ is an anisotropy factor with values higher than 1.0. The average fiber orientation was chosen as $\theta = 0^\circ$ and the spread of the distribution was controlled by the anisotropy factor ξ .

Figure 5.

Error of the GHOST formulation for uniaxial tension ($\lambda a = 1.2$) applied in the main fiber orientation of a transversely isotropic distributions: A) Gasser fiber density function with base parameter for the fiber strain energy function $k_1 = k_2 = 1.0$. B) Gasser fiber density function with increased non-linearity for the fiber strain energy function $k_1 = 1.0$, $k_2 = 30.0$. The GHOST formulation seem to diverge for $\kappa = 0.07$. C) Ellipsoidal distribution with increased non-linearity for the fiber strain energy function $k_1 = 1.0$, $k_2 = 30.0$. Notice that no divergence was observed for the range of values considered for the anisotropy factor ξ .

Figure 6.

Comparison strain energy functions (Eqs. 17, 49 and 50). The binomial and exponential strain energy functions were fitted to the energy function proposed by Holzapfel et al. (2000) (Eq 17) with parameters $k_1 = 1.0$ and $k_2 = 30.0$.

Figure 7.

Comparison of the error of the GHOST formulation for strain energy functions equivalent to that of Eq. (17) with fiber parameters $k_1 = 1.0$ and $k_2 = 30.0$. A) exponential energy function (Eq. 49), B) binomial (Eq. 50) energy function.

Figure 8.

The GHOST formulation eliminates the error associated with averaging of the fiber stretch, but the buckling error is not corrected. This is verified by comparing two cases of uniaxial tension where: A) the lateral contraction and fiber buckling are allowed in the lateral direction, B) the lateral contraction and fiber buckling are constrained.