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Accurate prediction of stress in fibers with distributed orientations using generalized high-order structure tensors

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A R T I C L E I N F O

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A B S T R A C T

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. 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

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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 non-linear 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 fiber 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 their effect on the formulation error. 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 (Ξ) can be calculated:

$$\mathbf{S} = 2\frac{\partial \Psi}{\partial \mathbf{C}} \tag{1}$$

$$\Xi = 4\frac{\partial^2 \Psi}{\partial \mathbf{C}\partial \mathbf{C}} \tag{2}$$

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

$$\Psi = \Psi_{\text{iso}} + \Psi_{\text{ani}} \tag{3}$$

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:

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{ani}} \tag{4}$$

$$\Xi = \Xi_{\text{iso}} + \Xi_{\text{ani}} \tag{5}$$

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 $\mathbf{C}$:

$$\Psi_{\text{ani}} = \Psi_{\text{ani}}(I_4) \tag{6}$$

where

$$I_4 = \mathbf{a}\cdot\mathbf{C}\cdot\mathbf{a} = \mathbf{C} : \mathbf{a}\otimes\mathbf{a} \tag{7}$$

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.

Eqs. (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:

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