A Characteristic-Based Constitutive Law for Dispersed Fibers

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Biological tissues are typically constituted of dispersed fibers. Modeling the constitutive laws of such tissues remains a challenge. Direct integration over all fibers is considered to be accurate but requires very expensive numerical integration. A general structure tensor (GST) model was previously developed to bypass this costly numerical integration step, but there are concerns about the model's accuracy. Here we estimate the approximation error of the GST model. We further reveal that the GST model ignores strain energy induced by shearing motions. Subsequently, we propose a new characteristic-based constitutive law to better approximate the direct integration model. The new model is very cost-effective and closely approximates the "true" strain energy as calculated by the direct integration when stress-strain nonlinearity or fiber dispersion angle is small. [DOI: 10.1115/1.4033517]

1 Introduction

Mechanical forces play very important roles in the normal growth of soft tissues as well as their mal-development under diseased conditions. There are many ongoing research efforts to improve our understanding of soft tissue mechanics, including mechanics of hearts [1–3], blood vessels [4–7], skeletal muscles [8], and brain tissues [9], among many others. A cornerstone for biomechanical analysis of soft tissues is a suitable constitutive law that can accurately describe their nonlinear stress-strain relationship [10].

In recent years, there is a trend to move away from the phenomenological constitutive models toward microstructure based models [11]. These models generally assume one or more families of fibers are embedded in an isotropic noncollagenous ground matrix and the overall material properties are determined by contributions from all distributed fibers. The strong directional properties of these fibers lead to the anisotropic material property observed in macroscale stretching experiments. Such microstructure-based models allow experimentally observed fiber orientation data to be incorporated directly into the constitutive law [12]. Moreover, the microstructure-based models provide better numerical stability than the phenomenological ones [13].

One canonical feature of fibrous tissues is that fibers are not well aligned but disperse about a preferred axis. To best account for the mechanical effect of the fibers, it is necessary to take a statistical approach, as pioneered by Lanir [14]. Under this approach, the fiber distribution is described by a continuous probability distribution function. The total strain energy and stresses are then calculated by taking a statistical summation over all fibers.

Currently, there are two strategies to implement the distributed fiber material model. The first strategy is to directly integrate over all fiber orientations. Since there are no further assumptions introduced, this approach is considered to be the most accurate, i.e., the "gold standard" [15]. The disadvantage is that the direct integration is very complicated and requires very expensive numerical approximation to evaluate its values [16]. The second strategy is to use the so-called GST, where the statistical summation of the fiber family is approximated by invariants of a GST [17,18]. This approach is very cost-effective and also very easy to implement. It, however, has been recognized to significantly underpredict the stress when comparing with the "gold standard" [15].

In this study, we first sought to estimate the order of approximation of the GST model. We then propose a new constitutive law to reduce the approximation error from the GST model.

2 Methods

Throughout this paper, we focused on a single family of dispersed fibers. Without losing generality, we assumed this fiber family's mean orientation was aligned along the x axis (Fig. 1). Dispersed fibers that are not aligned in this fashion could be converted to such an orientation through a coordinate system transformation. Following Gasser et al. [18], we assumed the fiber family has a π -periodic von-Mises distribution, which is described by the following density function $\rho(\Theta)$

Fig. 1 Fiber direction vector e_f defined by two Eulerian angles Θ and Φ

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$$\rho(\Theta) = 4\sqrt{\frac{b}{2\pi}} \frac{e^{b\cos(2\Theta)+b}}{\text{erfi}(\sqrt{2b})} \quad (1)$$

where $\text{erfi}(x) = -i\text{erf}(ix)$ is the modified error function. The density function describes the normalized number of fibers within the orientation range of $[(\Theta, \Theta + \Delta\Theta), (\Phi, \Phi + \Delta\Phi)]$, where Θ and Φ are the Eulerian angles describing the direction of fiber orientation (Fig. 2), and has the following property:

$$\frac{1}{4\pi} \int_{\Omega} \rho(\Theta) d\omega = 1 \quad (2)$$

where $d\omega = \sin(\Theta)d\Theta d\Phi$ and $\Omega(\Theta, \Phi) = \Omega(\Theta \in [0, \pi], \Phi \in [0, 2\pi])$. Figure 2 shows the relationship between b and fiber dispersion angle.

The normal vector for a fiber oriented at (Θ, Φ) under the reference configuration is

$$\mathbf{e}_f = \cos(\Theta)\mathbf{e}_1 + \sin(\Theta)\cos(\Phi)\mathbf{e}_2 + \sin(\Theta)\sin(\Phi)\mathbf{e}_3 \quad (3)$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are the orthogonal basis of the Cartesian coordinate system (Fig. 1). We assumed the microstructure undergoes affine deformation, i.e., the microscale motion follows exactly the macroscale motion. Under such an assumption, the stretch ratio, λ_f for a fiber oriented at (Θ, Φ) subjected to a deformation gradient field of $\mathbf{F}$ is

$$\lambda_f^2(\Theta, \Phi) = \mathbf{e}_f \otimes \mathbf{e}_f : \mathbf{C} \quad (4)$$

Here $\mathbf{C}$ is the right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F}$.

We assumed the strain energy for each individual fiber is

$$w(C) = \frac{k_1}{2k_2} \left[e^{k_2(\lambda_f^2 - 1)^2} - 1 \right] \quad (5)$$

Integrating the above equation over the whole fiber family, we obtained the total strain energy [14]

$$\begin{aligned} W &= \frac{1}{4\pi} \int_{\Omega} \rho(\Theta) w(\mathbf{C}) d\omega \\ &= \frac{1}{4\pi} \frac{k_1}{2k_2} \int_{\Omega} \rho(\Theta) \left(e^{k_2(\lambda_f^2 - 1)^2} - 1 \right) d\omega \end{aligned} \quad (6)$$

The above integration does not have a closed-form solution and can only be evaluated through numerical integration.

Fig. 2 Relationship between fiber dispersion angle and b

2.1 The GST Model. In order to overcome the challenges associated with integrating Eq. (6), Freed et al. [17] and Gasser et al. [18] introduced a GST as

$$\mathbf{H} = \frac{1}{4\pi} \int_{\Omega} \rho \mathbf{e}_f \otimes \mathbf{e}_f d\omega \quad (7)$$

An invariant of this GST is defined as

$$E_i = \mathbf{H} : \mathbf{C} - 1 \quad (8)$$

The invariant E_i is essentially a weighted average of the fiber stretching factor $(\lambda_f^2 - 1)$ over the whole fiber family, as $E_i = (1/4\pi) \int_{\Omega} \rho(\lambda_f^2 - 1) d\omega$.

Gasser et al. [18] proposed to approximate the total strain energy of a dispersed fiber family as

$$W_{\text{GST}} = \frac{k_1}{2k_2} \left[e^{k_2(E_i)^2} - 1 \right] \quad (9)$$

Remark 1. Equation (9) is an $O(k_2(\lambda_f^2 - 1)^2)$ approximation of Eq. (6). The Taylor expansion of Eq. (6) is

$$W = \frac{k_1}{2k_2} \frac{1}{4\pi} \int_{\Omega} \rho \left[\sum_{n=1}^{\infty} \frac{\left(k_2 (\lambda_f^2 - 1)^2 \right)^n}{n!} \right] d\omega \quad (10)$$

Similarly, Eq. (9) can be expressed as

$$W_{\text{GST}} = \frac{k_1}{2k_2} \left[\sum_{n=1}^{\infty} \frac{1}{n!} \left(k_2 \left(\frac{1}{4\pi} \int_{\Omega} \rho (\lambda_f^2 - 1) d\omega \right)^2 \right)^n \right] \quad (11)$$

Note the Taylor expansion in Eqs. (10) and (11) is the full Taylor expansion and is thus identical to Eq. (6) and (9). Using the Schwarz's inequality, we could show that Eq. (11) approximates Eq. (10) as follows (see the Appendix)

$$W_{\text{GST}} = W - \frac{k_1}{2k_2} \int_{\Omega} \left\{ \rho k_2 \left[(\lambda_f^2 - 1) - \frac{\int_{\Omega} \rho (\lambda_f^2 - 1) d\omega}{4\pi} \right]^2 + \dots \right\} d\omega$$

where $\dots$ represents higher order terms.

Remark 2. Equation (9) underpredicts the strain energy caused by shearing motion.

To demonstrate this, consider the following (compressible) deformation gradient

$$\mathbf{F} = \begin{pmatrix} 1 & \gamma & 0 \\ 0 & \sqrt{1-\gamma^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The right Cauchy-Green tensor for such a deformation field is

$$\mathbf{C} = \begin{pmatrix} 1 & \gamma & 0 \\ \gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Applying the above deformation field on the specific dispersed fiber family considered in this study (i.e., whose mean fiber direction aligns along the direction $(1, 0, 0)$) would always lead to $E_i = 0$. Based on the GST model (Eq. (9)), the strain energy after such a deformation would always be zero for the dispersed fiber family considered here. Meanwhile, if we take a microscopic view of the dispersed fibers, many of the off-diagonal fibers would be stretched under the above deformation. The strain energy as

calculated by the direction integration approach would certainly be nonzero.

Note that the compressible deformation field was chosen here for its ease in demonstrating the strain energy underprediction phenomenon. The underprediction would also occur under an incompressible deformation. As seen in Eq. (8), the GST invariant E_i is linked to the Cauchy–Green tensor C as $E_i = H : C - 1$. For any axial-symmetric fiber families that are aligned along the major axes, the off-diagonal terms of the GST H are always zero. Therefore, all off-diagonal terms of the second Piola–Kirchhoff stress tensor of the original GST model are always zero for such fibers. Under the original GST model, adding an off-diagonal disturbance to C would cause zero change of the strain energy value for such dispersed fiber families. This is inconsistent with the microscopic view of the dispersed fibers, as this disturbance would certainly lead to extra deformation for some individual fibers (certain fibers are stretched while others are compressed) thus leading to change of strain energy. Although the discussion here focuses on fiber families aligned along the major axes, any arbitrarily aligned fibers can be made so by a coordinate transformation; therefore, the discussion here is applicable to any axial-symmetrically dispersed fiber families after such a transformation.

2.2 A Characteristic Invariant. As seen in Eq. (10), each term on the right-hand side of the Taylor expansion of the direct integration is a function of $(\lambda_f^2 - 1)^2$. We hereby introduced a characteristic invariant as

$$\Lambda_i^2 = \frac{1}{4\pi} \int_{\Omega} \rho(\Theta) (\lambda_f^2 - 1)^2 d\omega \quad (12)$$

We proposed to use the following strain energy function to approximate Eq. (6):

$$W_{CH} = \frac{k_1}{2k_2} [e^{k_2 \Lambda_i^2} - 1] \quad (13)$$

Remark 3. Equation (13) is an $O([k_2(\lambda_f^2 - 1)^2]^2)$ approximation to Eq. (6).

The Taylor expansion of Eq. (13) is

$$\begin{aligned} W_{CH} &= \frac{k_1}{2k_2} \left[\sum_{n=1}^{\infty} \frac{(k_2 \Lambda_i^2)^n}{n!} \right] \\ &= \frac{k_1}{2k_2} \left[\frac{1}{4\pi} \int_{\Omega} \rho k_2 (\lambda_f^2 - 1)^2 d\omega \right. \\ &\quad \left. + \frac{1}{2} \left(\frac{1}{4\pi} \int_{\Omega} \rho (k_2 (\lambda_f^2 - 1)^2)^2 d\omega \right)^2 + \dots \right] \quad (14) \end{aligned}$$

In a similar way as Eq. (11), we can show that

$$\begin{aligned} W_{CH} &= W - \frac{k_1}{2k_2} \frac{1}{32\pi^2} \int_{\Omega} \rho k_2^2 \left[(\lambda_f^2 - 1)^2 - \frac{\int_{\Omega} \rho (\lambda_f^2 - 1)^2 d\omega}{4\pi} \right]^2 \\ &\quad \times d\omega - \dots \quad (15) \end{aligned}$$

It is easy to see the following three parameters would strongly affect the quality of the approximation: (1) ρ , (2) k_2 , and (3) strain. Equation (13) would be a good approximation of Eq. (6) for cases where the fibers have a small dispersion angle, small k_2 values, or undergo small deformation. We demonstrate these properties in Sec. 3.

Remark 4. Based on the Schwarz inequality and the Holder's inequality [19], it can be shown that

$$W \geq W_{CH} \geq W_{GST} \quad (16)$$

The equality only holds when $C = 0$. The above equation indicates that the characteristic model approximates the true strain energy better than the GST model (the issue of zero-loading under compression is discussed in Sec. 4.4)

2.3 Implementation of the Characteristic Invariant. At first glance, the integral in Eq. (12) is as complicated as that of the direct integration approach. We could, however, take advantage of fact that the fiber distribution function is independent of the Eulerian angle Φ ; therefore, Eq. (12) could be rearranged into

$$\Lambda_i^2 = \frac{1}{4\pi} \int_{\Theta=0}^{\pi} \rho(\Theta) \left(\int_{\Phi=0}^{2\pi} (\lambda_f^2 - 1)^2 d\Phi \right) \sin(\Theta) d\Theta \quad (17)$$

The inner integral over Φ involves trigonometric function only and has closed form solutions. We used the open source mathematics software SAGE [20] to calculate this integration.

$$\begin{aligned} \int_{\Phi=0}^{2\pi} (\lambda_f^2 - 1)^2 d\Phi &= 4\pi \left(M_1 \cos(\Theta)^4 + M_2 \sin(\Theta)^4 + M_3 \cos(\Theta)^2 \right. \\ &\quad \left. \times \sin(\Theta)^2 + M_4 \cos(\Theta)^2 + M_5 \sin(\Theta)^2 + \frac{1}{2} \right) \quad (18) \end{aligned}$$

where M_i for $i = 1 \dots 5$ are

$$\begin{aligned} M_1 &= \frac{1}{2} C_{11}^2 \\ M_2 &= \frac{3}{16} C_{22}^2 + \frac{1}{8} (C_{23}^2 + C_{32}^2) + \frac{1}{8} C_{22} C_{33} + \frac{3}{16} C_{33}^2 \\ M_3 &= \frac{1}{2} (C_{12}^2 + C_{21}^2 + C_{13}^2 + C_{31}^2 + C_{11} C_{22} + C_{11} C_{33}) \\ M_4 &= -C_{11} \\ M_5 &= -\frac{1}{2} C_{22} - \frac{1}{2} C_{33} \quad (19) \end{aligned}$$

where C_{ij} , $i, j = 1, 3$ are the components of the right Cauchy–Green tensor C . Plugging these into Eq. (12) leads to

$$\Lambda_i^2 = M_1 \kappa_1(b) + M_2 \kappa_2(b) + M_3 \kappa_3(b) + M_4 \kappa(b) + M_5 \kappa(b) + 1 \quad (20)$$

where

$$\begin{aligned} \kappa_1(b) &= \int_{\Theta=0}^{\pi} \rho \cos(\Theta)^4 \sin(\Theta) d\Theta \\ \kappa_2(b) &= \int_{\Theta=0}^{\pi} \rho \sin(\Theta)^5 d\Theta \\ \kappa_3(b) &= \int_{\Theta=0}^{\pi} \rho \cos(\Theta)^2 \sin(\Theta)^3 d\Theta \\ \kappa_4(b) &= \int_{\Theta=0}^{\pi} \rho \cos(\Theta)^2 \sin(\Theta) d\Theta \\ \kappa_5(b) &= \int_{\Theta=0}^{\pi} \rho \sin(\Theta)^3 d\Theta \quad (21) \end{aligned}$$

The quantities κ_i for $i = 1 \dots 5$ have to be evaluated through numerical approximation. However, these quantities only need to be evaluated once for a given b value and can be precalculated for finite-element analysis, thereby drastically reducing the computational cost. Figure 3 shows the relationship between κ and b .

2.4 Second Piola–Kirchhoff Stress. The second Piola–Kirchhoff stress is calculated as

Fig. 3 Relationship between κ_i , ($i = 1, 5$), and b

$$\mathbf{S} = 2 \frac{\partial W_{CH}}{\partial \mathbf{C}} = k_1 [e^{k_2 \Lambda_f^2}] \frac{\partial (\Lambda_f^2)}{\partial \mathbf{C}} = k_1 [e^{k_2 \Lambda_f^2}] \mathbf{L} \quad (22)$$

Inserting Eq. (20) into $\mathbf{L} = (\partial(\Lambda_f^2)/\partial \mathbf{C})$, we obtain

$$\mathbf{L} = \frac{\partial (\Lambda_f^2)}{\partial \mathbf{C}} = \frac{\partial (M_1 \kappa_1 + M_2 \kappa_2 + M_3 \kappa_3 + M_4 \kappa_4 + M_5 \kappa_5)}{\partial \mathbf{C}} \quad (23)$$

The six unique terms of the matrix $\mathbf{L}$ are

$$\begin{aligned} L_{11} &= C_{11} \kappa_1 + \frac{1}{2} (C_{22} + C_{33}) \kappa_3 - \kappa_4 \\ L_{12} &= C_{12} \kappa_3 \\ L_{13} &= C_{13} \kappa_3 \\ L_{22} &= \frac{1}{8} (3C_{22} + C_{33}) \kappa_2 + \frac{1}{2} C_{11} \kappa_3 - \frac{1}{2} \kappa_5 \\ L_{23} &= \frac{1}{4} C_{23} \kappa_2 \\ L_{33} &= \frac{1}{8} (C_{22} + 3C_{33}) \kappa_2 + \frac{1}{2} C_{11} \kappa_3 - \frac{1}{2} \kappa_5 \end{aligned} \quad (24)$$

3 Results

We compared the strain energy as calculated by the three different models in Eqs. (6), (9), and (13). We applied a deformation gradient field $\mathbf{F} = \mathbf{F}_1 * \mathbf{F}_2$ to a dispersed fiber family, where

$$\mathbf{F}_1 = \begin{pmatrix} 1 & \gamma & 0 \\ 0 & \sqrt{1-\gamma^2} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1-\gamma^2}} \end{pmatrix}$$

is a shear motion with the degree of shearing controlled by the parameter γ and

$$\mathbf{F}_2 = \begin{pmatrix} l_1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{l_1}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{l_1}} \end{pmatrix}$$

is a stretching motion governed by the principal stretching ratio l_1 . We focused our investigation on $\gamma \in [0, 0.2]$ and $l_1 \in [1, 1.2]$.

These values correspond to the typical strain range experienced by biological tissues under physiological conditions. Throughout this study, k_1 was set to be 996 kPa [18]. All computations presented in this section were carried out using SAGE [20].

Figures 4–6 shows that the strain energy calculated from these three models for $k_2 = 1, 10$, and 50, respectively. In each figure, the stretching parameter l_1 increases from the top to bottom (1.0 for the top row, 1.1 for the middle row, and 1.2 for the bottom row). The solid lines indicate strain energy calculated by the direct integration approach. As seen in these figures, the value of W_{CH} always falls in between W_{GST} and W , which agrees with Remark 4.

We define the modeling error as $\text{Err}_{GST,CH} = (W - W_{GST,CH})/W$. The error of both GST and characteristic models increases as k_2 increases (from Figs. 4 to 6) or b decreases (from column (a) to column (c) in Figs. 4–6). This observation confirms Remark 3. For all $k_2 = 1$ cases, the characteristic model recovers the true strain energy very well. The biggest approximation error is less than 5% and occurs when $b = 1$, $l_1 = 1.2$, and $\gamma = 0.2$. As the value of k_2 increases, the approximation error of both the characteristic model and the GST model increases. When $k_2 = 10$, the biggest approximation errors for the characteristic model for $b = 10, 5$, and 1 cases are 15%, 24%, and 45%, respectively. The errors for the GST model are 20%, 35%, and 85%, respectively. For $k_2 = 50$ cases, the approximation error for both the characteristic and GST models are very large, reaching ~90% when $l_1 = 1.2$. Note that the true strain energy density as calculated by the direct integration model is extraordinarily high, thus suggesting a k_2 value of 50 is likely nonphysiological. The strain energy reaches 10^5 , which corresponds to a nonphysiological stress level of several GPa, suggesting that such a k_2 value is likely nonphysiological.

4 Discussion

This study, which focused on the constitutive laws for dispersed fibers, first estimated the approximation error of the popular GST model, showing that the GST model ignores strain energy induced by shearing motion. We also proposed a new characteristic-based strain energy function to recapture the ignored shearing strain energy. Finally, we demonstrated that this new model can approximate the “true” strain energy as calculated by the direct integration approach fairly closely when k_2 values are low, fiber dispersion angle is small or the deformation is relatively small. The new model’s computational cost is significantly lower than that of the direct integration approach, but slightly higher than the GST model.

4.1 Impact of Nonlinearity Parameter k_2 on the Approximation. The quality of approximation of the new characteristic model is strongly dependent on the value of k_2 , which reflects the nonlinearity of the stress–strain response. Published k_2 values vary significantly. Many studies reported k_2 values to be smaller than about 50, for examples, from 0.48 for abdominal aortas from patients <30 years of age to 59.14 for patients >60 years of age [4]. A value of 30 approximated the behavior of the supraspinatus tendon [15]. Values of $k_2 \approx 3 - 4$ fit equibiaxial stretching data of fibroblast-populated collagen cruciforms quite well [21]. For passive myocardium, values of k_2 were reported between 7 and 16 [1]. Values of 1–6 were reported for rabbit basilar arteries and mouse carotid arteries [22]. Even smaller value, of 0.265, was reported for femoral arteries [11]. However, several reports have suggested very large values of k_2 . For example, values greater than 1500 would fit experimental measurements well [23]. Values of 68.9 ± 59.3 were reported for intact human carotid aortic walls, 109.8 ± 104 and 48.4 ± 22.8 for adventitia, and 16.5 ± 9.3 for media-intima [24]. A value of $k_2 = 524.6$ was suggested for iliac arteries [18]. The k_2 parameter in all but one of these studies [21] was fitted against the GST model. Because of the huge difference between the GST model and the direct

Fig. 4 Strain energy as calculated by direct integration (DI-solid lines), general structure tensor (GST-dash-dotted lines), and characteristic (CH-dashed lines) models for $k_2 = 1$: (a) $b = 10$, (b) $b = 5$, and (c) $b = 1$

integration model (i.e., the gold standard) for large k_2 , these very large values of k_2 need to be interpreted very carefully.

4.2 Impact of Fiber Dispersion Angle on the Approximation.

In our study, the distribution parameter b of the von-Mises PDF strongly affected the quality of approximation, with the approximation error increasing as b decreases (Figs. 4–6). The parameter b reflects the degree of fiber dispersion (Fig. 2). Fiber dispersion angle varies a lot from tissue to tissue. For example, for healthy mice heart-muscle, the fiber dispersion angle was found to be about 10 deg [25], which corresponds to a b value of about 10 (Figs. 4(a)–6(a)). For such tissues, the new characteristic model would lead to good approximation to the true strain energy assuming $k_2 \leq 10$. For coronary arteries, the fiber dispersion angle was reported to be 22.3 deg for collagen fibers of the adventitial and 5 deg for medial smooth muscle [26]. For carotid arteries, a recent confocal laser scanning microscopy study [27] of rabbit carotid arteries showed that there were multiple families of collagen and the standard deviation of their distribution is about 40 deg, corresponding to a b value of about 0.8. As suggested by Figs. 4–6, the characteristic model would simulate the smooth muscle fibers very well but lead to quite significant error for the collagen fibers. More work is certainly warranted to improve the quality of approximation for those tissues.

4.3 Relationship With Previous Models. This study is greatly inspired by the works of several others [17,18,21]. Recognizing the challenge associated with the direct integration approach, Freed et al. [17] and Gasser et al. [18] proposed using a GST to characterize the complicated interaction between macro-scale deformation and microscale fiber kinematics. Such a

strategy significantly reduces the computation cost. As shown in Figs. 4 and 5, this GST approach can provide good approximation of the true strain energy caused by simple stretching motions (i.e., the principal deformation aligns with the fiber axes) for cases where k_2 values are small. However, as noted in Remark 2 and evidenced in Figs. 4–6, the GST approach ignores the strain energy caused by shearing motion, i.e., where the principal motion direction is not aligned with the fiber axes. The characteristic model we propose recaptures part of the shearing strain energy ignored by the GST model.

The work by Raghupathy and Barocas [21] is another meticulous effort in developing a computationally inexpensive material model for dispersed fibers. They simplified the direct integration of the second Piola–Kirchhoff stress tensor of 2D planar fibrous tissues into a function of the modified Bessel function

$$I_n(z) = \frac{1}{\pi} \int_0^\pi e^{z \cos(2\theta)} \cos(2n\theta) d\theta \quad (25)$$

The numerical solution of the Bessel function is very well studied and can be calculated much faster than numerical integration of the stress tensor. Raghupathy and Barocas [21] demonstrated that the computation speed of the Bessel function approach is about 200 times faster than the numerical integration approach. Note that their model is not an approximation but a simplification to the true stress tensor. Their model can be applied to any material parameters and deformations. The main drawback of their approach, however, is that it is extremely difficult to extend it to 3D problems.

4.4 Fiber Compression. It is typically assumed that collagen fibers do not sustain compression load, based on the observation

Fig. 5 Strain energy as calculated by direct integration (DI-solid lines), general structure tensor (GST-dash-dotted lines) and characteristic (CH-dashed lines) models for $k_2 = 10$: (a) $b = 10$, (b) $b = 5$, and (c) $b = 1$

that all collagen fibers under compression would buckle. Accounting for such an effect in the current characteristic model would be very costly, as Eq. (13) needs to be reorganized as

$$\Lambda_i^2 = \frac{1}{4\pi} \int_{\Omega} H(\lambda_f - 1) \rho(\Theta) (\lambda_f^2 - 1)^2 d\omega \quad (26)$$

where $\mathbf{H}$ is a Heaviside function

$$H(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ 0, & \text{otherwise} \end{cases} \quad (27)$$

The above integral cannot be simplified using the procedure in Sec. 2.3 and can only be calculated through numerical approximations. In many biomechanics applications, the fibers are typically stretched, making this issue less significant. Moreover, the GST approach only accounts for the zero-compression loading condition under the macroscale (the strain energy is set to 0 when $E_i < 0$) but ignores this condition under the microscale level (i.e., if certain fibers are compressed but the E_i value is larger than 0, the strain energy contribution from those compressed fibers is not zero). Considering all these factors, we believe that the ignoring of fiber compression issue in the characteristic model is a compromise worth making. However, we do not suggest applying this characteristic-based model on applications with predominantly compressed tissues.

Note that in the GST approach, the issue of tissue compression is partially accounted for by defining a modified invariant of the GST as

$$\bar{E}_i = \mathbf{H}(E_i) E_i$$

and calculating the strain energy function with this modified invariant. Similarly, we could also define a modified characteristic invariant as

$$\bar{\Lambda}_i^2 = H(E_i) \Lambda_i^2$$

for strain energy calculation. It should be cautioned that the modified GST invariant equals to 0 when $E_i = 0$. This however is not the case for the modified characteristic invariant as $\Lambda_i^2 \neq 0$ for any $\mathbf{C} \neq \mathbf{I}$. The modified characteristic invariant as defined above is discontinuous near $E_i = 0$. Such a discontinuity could cause numerical instability in finite-element analysis thus requiring extra care.

4.5 Fiber Distribution Function. We were able to drastically reduce the computational cost with the characteristic model because the von-Mises fiber distribution function is independent on the Eulerian angle Φ . For such a fiber distribution, the double integral in Eq. (12) can be separated into two steps and the inner integration over Φ can be precalculated and reorganized into a closed form as in Eq. (20). Fiber distribution in actual biological tissues, however, is often very complicated and cannot be approximated by the von-Mises distribution function. For example, Gasser et al. [28] reported that the collagen fiber distribution for abdominal aortic aneurysm walls is best approximated by the Bingham distribution function, which reads

$$\rho(\Theta, \Phi) = \frac{1}{c} e^{\kappa_1 (\cos(\Theta) \cos(\Phi))^2 + \kappa_2 (\sin(\Theta) \cos(\Phi))^2} \quad (28)$$

Such distribution functions cannot be separated into a form of $f(\Theta)g(\Phi)$, which makes it impossible to apply the approach in

Fig. 6 Strain energy as calculated by direct integration (DI-solid lines), general structure tensor (GST-dash-dotted lines), and characteristic (CH-dashed lines) models for $k_2 = 50$: (a) $b = 10$, (b) $b = 5$, and (c) $b = 1$

Sec. 2.3 to simplify the characteristic invariant in Eq. (12). A different strategy than the one used in this work is needed for these more realistic fiber distributions.

4.6 The Assumption of Affine Deformation at the Micro-scale. Our study assumed that the microstructure undergoes affine deformation following the macroscale motion. Previous experimental studies, however, show that the microscale fibers re-orient when subjected to a tension field [29]. Numerical models show that the stresses predicted under the affine deformation assumption are much higher than stresses predicted under non-affine models [30]. It is impossible to use Sec. 2.3's approach to directly incorporate the microscale non-affine deformation into the strain energy calculation; a costly numerical integration of the strain energy is the only feasible way to account for the non-affine deformation. Many biological tissues, such as arterial walls, have large amount of noncollagenous tissues. For such tissues, the non-affine effect is believed to be small and can be ignored [30]. Therefore, the model we developed could be a great model for such tissues.

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Appendix: Proof of Remark 1

Let $\Psi = f + \alpha g$, where $f = \sqrt{\rho k_2}(\lambda_f^2 - 1)$, $g = \sqrt{\rho k_2}$, and $\alpha = -(\int_{\Omega} \rho k_2(\lambda_f^2 - 1)d\omega) / (\int_{\Omega} \rho k_2 d\omega)$. Since $\Psi^2 \geq 0$

$$\int_{\Omega} \Psi^2 d\omega = \int_{\Omega} f^2 d\omega + \alpha^2 \int_{\Omega} g^2 d\omega + 2\alpha \int_{\Omega} fg d\omega \geq 0 \quad (A1)$$

Now plug f , g , and α into the above equation to obtain

$$\begin{aligned} & \int_{\Omega} \rho k_2 (\lambda_f^2 - 1)^2 d\omega + \frac{1}{4\pi k_2} \left[\int_{\Omega} \rho k_2 (\lambda_f^2 - 1) d\omega \right]^2 \\ & - 2 \frac{1}{4\pi k_2} \left[\int_{\Omega} \rho k_2 (\lambda_f^2 - 1) d\omega \right]^2 \\ & = \int_{\Omega} \rho k_2 (\lambda_f^2 - 1)^2 d\omega - \frac{1}{4\pi k_2} \left[\int_{\Omega} \rho k_2 (\lambda_f^2 - 1) d\omega \right]^2 \\ & = \int_{\Omega} \rho k_2 \left[(\lambda_f^2 - 1) - \frac{\int_{\Omega} \rho (\lambda_f^2 - 1)}{4\pi} \right]^2 d\omega \geq 0 \end{aligned}$$

So, the first term on the right-hand side of Eq. (11) is related to Eq. (10) as

$$\begin{aligned} & \frac{1}{4\pi k_2} \left[\int_{\Omega} \rho k_2 (\lambda_f^2 - 1) d\omega \right]^2 = \int_{\Omega} \rho k_2 (\lambda_f^2 - 1)^2 d\omega \\ & - \int_{\Omega} \rho k_2 \left[(\lambda_f^2 - 1) - \frac{\int_{\Omega} \rho (\lambda_f^2 - 1)}{4\pi} \right]^2 d\omega \end{aligned}$$

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