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Gauss-Kronrod-Trapezoidal Integration Scheme for Modeling Biological Tissues with Continuous Fiber Distributions

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Abstract

Fibrous biological tissues may be modeled using a continuous fiber distribution (CFD) to capture tension-compression nonlinearity, anisotropic fiber distributions, and load-induced anisotropy. The CFD framework requires spherical integration of weighted individual fiber responses, with fibers contributing to the stress response only when they are in tension. The common method for performing this integration employs the discretization of the unit sphere into a polyhedron with nearly uniform triangular faces (finite element integration or FEI scheme). Although FEI has proven to be more accurate and efficient than integration using spherical coordinates, it presents three major drawbacks: First, the number of elements on the unit sphere needed to achieve satisfactory accuracy becomes a significant computational cost in a finite element analysis. Second, fibers may not be in tension in some regions on the unit sphere, where the integration becomes a waste. Third, if tensed fiber bundles span a small region compared to the area of the elements on the sphere, a significant discretization error arises. This study presents an integration scheme specialized to the CFD framework, which significantly mitigates the first drawback of the FEI scheme, while eliminating the second and third completely. Here, integration is performed only over the regions of the unit sphere where fibers are in tension. Gauss-Kronrod quadrature is used across latitudes and the trapezoidal scheme across longitudes. Over a wide range of strain states, fiber material properties, and fiber angular distributions, results demonstrate that this new scheme always outperforms FEI, sometimes by orders of magnitude in the number of computational steps and relative accuracy of the stress calculation.

Keywords

Soft tissue mechanics; Fibrous tissues; Fiber density distribution; Integration on the sphere; Finite element analysis

1. Introduction

Starting with the studies of Lanir (Lanir 1979, 1983), fibrous biological tissues have increasingly been modeled using a continuous fiber distribution (CFD) to better capture tension-compression nonlinearity, anisotropic fiber distributions, and load-induced anisotropy. In Lanir's original work, flat collagenous tissues such as skin, mesentery, and

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pericardium were modeled such that individual fibers were described by Hooke's law, and the overall tissue response was evaluated from the weighted sum of individual fiber responses along all spatial directions, with the weight factor given by the fiber density along those directions.

Since then, many other tissues have been modeled successfully via the CFD framework, including the stress-stretch response of tendons and ligaments (Hurschler, Loitz-Ramage and Vanderby 1997), the planar biaxial stress-strain relationship in the aortic valve cusp (Billiar and Sacks 2000), the mechanical behavior of arterial layers with dispersion of the collagen fibers (Gasser, Ogden and Holzapfel 2006), and the mechanical response of the solid matrix of articular cartilage (Ateshian, Rajan, et al. 2009). Furthermore, several studies have shown that CFD captures the experimental response of fibrous tissues effectively. For example, Sacks and Sun (2003) demonstrated that CFD can reproduce biaxial in-plane responses accurately for various biological tissues, while providing insight into the structure and mechanics of tissue components. Gasser, Ogden and Holzapfel (2006) represented CFD as a generalized structure tensor that describes the dispersion of collagen fibers within the arterial adventitia layer and showed that CFD has a significant effect on the tissue's mechanical response. Ateshian, Rajan, et al. (2009) showed that CFD is able to predict a number of experimental responses of articular cartilage which had previously not been modeled successfully, such as the incremental Poisson's ratio from compression to tension, the alteration in tensile response following digestion of the proteoglycan ground matrix, and the complex uniaxial response to increasing strains in varying bath salt concentrations.

The CFD framework can be expressed as a spherical integration of weighted individual fiber responses. Using the notation of our prior study (Ateshian 2007), the overall tissue response is described by the total strain energy density $W(\mathbf{E})$ as a function of the Lagrangian strain tensor $\mathbf{E}$. Each fiber is assumed hyperelastic, with its response described by the strain energy function $\Psi(E_n)$, where E_n is the normal strain along the fiber direction. $W(\mathbf{E})$ is obtained from the integration of $\Psi(E_n)$ over the unit sphere, weighted by a fiber density distribution $R(\mathbf{n}^0)$ which varies with the fiber direction $\mathbf{n}^0$ in the reference configuration, and a Heaviside step function $H(E_n)$ to ensure that only fibers in tension contribute to the integration,

$$W(\mathbf{E}) = \int_0^{2\pi} \int_0^\pi R(\mathbf{n}^0) \Psi(E_n) H(E_n) \sin\phi \, d\phi d\theta. \quad (1)$$

The total stress and elasticity tensors can be obtained accordingly, as described previously (Ateshian 2007). This formulation is generally employed for compressible materials, as typically required when modeling the porous solid matrix of a hydrated biological tissue such as articular cartilage, where pore volume may evolve with time as interstitial fluid flows into or out of the tissue (Mow, Kuei, Lai and Armstrong 1980). When modeling nearly incompressible tissues, an uncoupled form of the strain energy density is often employed in finite element implementations to avoid the phenomenon of mesh locking (Bonet and Wood 1997),

$$W(\mathbf{E}) = U(J) + \int_0^{2\pi} \int_0^\pi R(\mathbf{n}^0) \Psi(\tilde{E}_n) H(\tilde{E}_n) \sin\phi d\phi d\theta, \quad (2)$$

where $J = \det \mathbf{F}$, $\mathbf{F}$ is the deformation gradient, and $\tilde{E}_n$ is the normal component of $\tilde{\mathbf{E}}$ along the fiber direction $\mathbf{n}^0$. Here, $\tilde{\mathbf{E}} = (\tilde{\mathbf{F}}^T \cdot \tilde{\mathbf{F}} - \mathbf{I})/2$ where $\tilde{\mathbf{F}} = J^{-1/3} \mathbf{F}$, such that $\det \tilde{\mathbf{F}} = 1$. For these uncoupled formulations, a typical form adopted for $U(J)$ is

$$U(J) = \frac{\kappa}{2} (\ln J)^2 \quad (3)$$

where κ is the bulk modulus. When the value of κ is selected to be much larger than other elastic moduli appearing in $\Psi(\tilde{E}_n)$, the response of these materials is nearly isochoric, $J \approx 1$, so that $\tilde{E}_n \approx E_n$. The integration schemes presented below are equally applicable to the formulations of Eq.(1) and Eq.(2).

In order to numerically approximate the spherical integration described above, Lanir (1983) discretized the spherical angles over the rectangular domain of the (θ, ϕ) -plane, and performed a summation of the integrand at each integration point,

$$I(f) = \int_0^{2\pi} \int_0^\pi f(\theta, \phi) \sin\phi d\phi d\theta \approx \sum_{\theta} \sum_{\phi} f(\theta, \phi) \sin\phi \Delta\theta \Delta\phi. \quad (4)$$

Bazant and Oh (1986) showed that numerical formulas with uniformly distributed integration points on the sphere are superior to this approach, since the uniform discretization over the rectangular (θ, ϕ) -plane produces a distribution wastefully crowded near the poles of the sphere. Formulas with uniformly distributed integration points over a unit sphere may be described as the finite element integration (FEI) scheme (Atkinson 1982),

$$I(f) = \sum_{i=1}^N f(Q_i) \cdot \Delta A_i, \quad (5)$$

where A_i is the element area, Q_i is the centroid for each element, and N is the number of elements.

Methods for generating the integration points or elements on a unit sphere have been discussed in a series of articles. Bazant and Oh (1986) considered integration points on the edges and faces of polyhedra with uniform distribution and high degrees of symmetry. Fliege and Maier (1999) considered points as electrical charges and numerically calculated the point distribution by minimizing the potential energy of the charge distribution. Hannay and Nye (2004) derived these points by considering the Fibonacci sampling lattice with non-uniform scaling. Ehret, Itskov and Schmid (2010) investigated and compared a series of formulas for the FEI scheme, with applications to a full network model of rubber elasticity and to an exponential model for soft tissues. They demonstrated that asymmetric point

distributions are most detrimental for inducing anisotropic responses in isotropic material laws. They also showed that symmetric distributions using a small number of integration points may also break the expected symmetry of the response.

Although these FEI schemes have been proven more accurate and efficient than uniform discretization over the rectangular (θ, φ) -plane, we find three major drawbacks to the FEI scheme. First, they usually require a large number of elements N to achieve sufficient accuracy ($N > 1200$), resulting in a large computational cost in a finite element (FE) analysis. Second, fibers may not be in tension in some regions on the unit sphere, where the integration becomes wasteful, thus diminishing computational efficiency. Third, a significant discretization error may arise when the tensed fiber bundles span a small region compared to the area of the elements on the sphere.

In our prior study (Ateshian 2007), we analyzed the material symmetry of fibrous tissues undergoing tension and compression, showing that the region where fibers are in tension can be expressed as a function of the eigenvalues of the strain tensor in a basis aligned with the eigenvectors of the strain. Based on this finding, our aim in this study was to develop an integration scheme exclusively for the CFD framework, that can significantly mitigate the first drawback of the FEI scheme, while eliminating the second and third completely.

In this presentation, we include one particular FEI scheme for comparison, where we evaluated the distribution of integration points on the sphere using an icosahedron to produce 20 and 60 uniformly distributed points, and a publicly-shared program (Semechko 2013) (function ‘Particle-SampleSphere’ within ‘Uniform Sampling of a Sphere’) to produce 196 to 1796 nearly uniformly distributed points by increments of 200. Semechko’s method generates approximately uniformly distributed points on a unit sphere by minimizing the potential energy of a system of charged particles. Though this algorithm does not produce fully symmetric point distributions, it can generate a broader range of integration points than fully symmetric formulations (Heo and Xu 2001).

2. Formulation

As shown previously (Ateshian 2007), there are four ranges of integration based on the Lagrangian strain eigenvalues E_i ($i = 1, 2, 3$), in the basis $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3\}$ of eigenvectors of $\mathbf{E}$:

1. T case: all eigenvalues are positive, $E_i > 0$. Fibers are in tension along all spatial directions, and the region of integration is the whole sphere, $\theta \in [0, 2\pi]$, $\varphi \in [0, \pi]$.
2. TC case: two eigenvalues are negative and one is positive, $E_1, E_2 < 0 < E_3$. Fibers are in tension inside an elliptical double cone whose apexes meet at the origin, and whose axis is along $\mathbf{m}_3$, Figure 1(a). The region of integration is inside the double cone, $\theta \in [0, 2\pi]$, $\varphi \in [0, \varphi_0] \cup [\pi - \varphi_0, \pi]$, where

$$\phi_0(\theta) = \tan^{-1} \sqrt{-E_3 / (E_1 \cos^2 \theta + E_2 \sin^2 \theta)}. \quad (6)$$

3. CT case: two eigenvalues are positive and one is negative, $E_3 = 0 < E_1, E_2$. Fibers are in tension outside the double cone, which is the complementary region of the TC case, Figure 1(b). The region of integration becomes $\theta \in [0, 2\pi]$, $\varphi \in [\varphi_0, \pi - \varphi_0]$.
4. C case: all eigenvalues are negative, $E_i < 0$. In this case, fibers are in compression along all directions, and none contribute to the integration.

Since the two directions $\pm \mathbf{n}^0$ represent the same fiber bundle, the integral over $\varphi \in [0, \pi]$ in Eq.(1) may be evaluated from twice the integral over $\varphi \in [0, \pi/2]$. To numerically approximate the integration within these regions, we effected a change of variable from φ to $\zeta \in [-1, 1]$,

$$\zeta = 2 \frac{\cos \phi - \cos \phi_a}{\cos \phi_b - \cos \phi_a} - 1, \quad (7)$$

where $\varphi \in [\varphi_a, \varphi_b]$ and φ_a and φ_b depend on the cases described above: $\varphi_a = 0$ in the T and TC cases and $\varphi_a = \varphi_0$ in the CT case; $\varphi_b = \pi/2$ in the T and CT cases, and $\varphi_b = \varphi_0$ in the TC case. In all cases, $\zeta \in [-1, 1]$, such that

$$I(f) = \int_0^{2\pi} \int_{-1}^1 (\cos \phi_a - \cos \phi_b) f(\theta, \phi) d\zeta d\theta. \quad (8)$$

The integration scheme we adopted here for the evaluation of $I(f)$ uses Gauss-Kronrod quadrature along ζ and the trapezoidal rule along θ (Dahlquist and Björck 2008); we refer to it as the GKT scheme,

$$I(f) \approx \frac{\pi}{m_T} \sum_{j=1}^{m_T} \sum_{i=1}^{n_{GK}} w_i (\cos \phi_a - \cos \phi_b) f(\theta_j, \phi_i), \quad (9)$$

$$\phi_i = \cos^{-1} \left(\frac{\cos \phi_b - \cos \phi_a}{2} \zeta_i + \frac{\cos \phi_a + \cos \phi_b}{2} \right), \quad (10)$$

where φ_a and φ_b may depend on θ_j . Here, m_T is the number of uniformly distributed integration points along θ , with $\theta_j = 2\pi j/m_T$, and n_{GK} is the number of integration points along ζ , with ζ_i representing the Gauss-Kronrod quadrature points and w_i representing the corresponding weights. We only chose odd values for m_T , starting from 3, as they produced more accurate results than even values for integration along θ . The Gauss-Kronrod rule extends the n points of a Gauss rule by adding $n + 1$ integration points, $n_{GK} = 2n + 1$, producing exact results for polynomials of degree $3n + 1$ if n is even and $3n + 2$ if n is odd. In this study, we only used odd values of n ($n = 3, 5, \dots, 13$), such that $n_{GK} = 7, 11, \dots, 27$. For the GKT scheme, the number of integration points is thus $N = m_T \cdot n_{GK}$. In the analyses presented below, we first chose $n_{GK} = 7$, and increased it only when increasing m_T produced no further reduction in error.

3. Single element analysis

The accuracy and computational efficiency of the GKT versus FEI schemes may be influenced by the choice of constitutive relation for the fiber stress-strain response, since a highly nonlinear response with strain can produce highly nonlinear spatial distributions of stress over the unit sphere. Accuracy and computational efficiency may also be influenced by the anisotropy of the fiber density distribution, especially when preferred fiber directions are not aligned with eigenvectors of the strain. First, we investigated the influence of the fiber stress-strain response, assuming an isotropic fiber distribution, $R(\mathbf{n}^0) = \frac{1}{4\pi}$. Then, for a given stress-strain response, we investigated the influence of $R(\mathbf{n}^0)$ for initially transversely isotropic fiber distributions, while we rotated the eigenvectors of the strain relative to the preferred fiber distribution directions.

We analyzed a single finite element in the shape of a unit cube, under prescribed displacements. The face normals of the cube were aligned with the eigenvectors of $\mathbf{E}$, and the eigenvalues E_i were evaluated from prescribed stretches λ_i along those directions, $E_i = (\lambda_i^2 - 1)/2$. The normal strain along each fiber direction E_n was evaluated from

$$E_n = E_1 \cos^2 \theta \sin^2 \phi + E_2 \sin^2 \theta \sin^2 \phi + E_3 \cos^2 \phi, \quad (11)$$

where (θ, ϕ) are the spherical angles along the direction $\mathbf{n}^0$ of the fiber (Ateshian 2007).

We adopted three representative strain conditions to evaluate the T case, with $\lambda_1 = \lambda_2 = \lambda_3 = 1.1$, TC case with $\lambda_1 = 0.5$, $\lambda_2 = 0.9$, $\lambda_3 = 1.1$, and CT case with $\lambda_1 = 1.1$, $\lambda_2 = 1.3$, $\lambda_3 = 0.5$. We illustrate the cube deformation, the range of integration over ϕ as a function of θ (Eq. (6)), and the region of integration in Table 1. We used MATLAB to perform the above GKT and FEI integrations for the unit cube analysis, and we compared principal normal stresses to the numerical value obtained with the MATLAB numerical double integration function 'integral2', evaluated with relative error of 10^{-5} , henceforth described as exact values.

3.1 Strain energy density

We chose a fiber strain energy density $\Psi(E_n)$ that includes the exponential (Sacks and Sun 2003; Holzapfel, Gasser and Ogden 2000; Stylianopoulos and Barocas 2007) and power-law (Ateshian, Rajan, et al. 2009) relations commonly used in soft tissue mechanics,

$$\Psi(E_n) = \frac{\xi}{\alpha\beta} \left[\exp(\alpha(2E_n)^\beta) - 1 \right], \quad \beta \geq 2, \xi, \alpha \geq 0, \quad (12)$$

where α, β, ξ are the material parameters.

When $\alpha = k_2$, $\beta = 2$, and $\xi = k_1$, Eq.(12) reduces to the exponential function described by Holzapfel, Gasser and Ogden (2000). When $\alpha = 1$, $\beta = 2$, and $\xi = c$, it also reduces to the Fung-type strain energy density described in (Holzapfel, Gasser and Ogden 2004; Sacks and Sun 2003), in which the exponential term is a combination of quadratic forms of all strain components. Letting $\alpha = 0$, $\beta = \bar{\alpha}$, and $\xi = \bar{\alpha}\bar{\xi}$ recovers the formulation of Ateshian, Rajan, et

al. (2009) (where $\bar{\alpha}, \bar{\xi}$ are the α, ξ defined in that study). From all these articles, the range of α falls within $[0, 17]$ and that of β is within $[2, 3.5]$. In this analysis, we set these ranges to $\alpha = [0, 20]$ and $\beta = [2, 4]$, to capture the values used in practice; specific combinations of α and β used in the simulations appear in Table 2. Since ξ is a constant factor that does not affect the accuracy, it was set to 1.

We evaluated the largest relative error (RE) in the principal normal stresses against the corresponding exact values. We determined the number of integration points NI required to produce RE = 1% for a range of material properties and all three strain conditions (Figure 2). NI_{GKT} was smaller than or equal to NI_{FEI} in all cases, with the largest difference most apparent in the TC and CT cases. There was no variation with fiber properties in the T and TC cases, though in the CT case NI exhibited a higher value for $\alpha = 20$, which represents a highly nonlinear stress-strain response. The number of Gauss-Kronrod points was $n_{GK} = 7$ for all cases, and the number of trapezoidal points m_T ranged from 3 to 11.

3.2 Fiber density distribution

Two commonly used 3D continuous fiber distributions $R(\mathbf{n}^0)$ in soft tissue mechanics include the transversely isotropic *von Mises* (Gasser, Ogden and Holzapfel 2006) and the orthotropic ellipsoidal (Ateshian, Rajan, et al. 2009) distributions. Let $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ represent the orthonormal basis defining the preferred fiber directions (e.g., the normals to the planes of orthotropic symmetry) in the reference configuration. In this section, we analyzed the influence of the functional form of $R(\mathbf{n}^0)$, as well as the relative orientation of the bases $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ and $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3\}$, for GKT and FEI integration schemes. We used the fiber strain energy density corresponding to $\alpha = 0, \beta = 2, \xi = 1$ in these cases. The relative orientation of the two bases was defined using spherical angles (θ_f, φ_f) as illustrated in Figure 3, where $\mathbf{f}_1$ lies in the $(\mathbf{m}_1, \mathbf{m}_2)$ -plane; the combinations of θ_f and φ_f we used in the simulations appear in Table 3, where we set the ranges to $\theta_f \in [0, \pi]$ and $\varphi_f \in [0, \pi/2]$. For fiber distributions that are transversely isotropic about $\mathbf{f}_3$, and given the orthogonality of the principal planes of normal strain, constraining $\mathbf{f}_1$ and (θ_f, φ_f) in this manner did not reduce the generality of this analysis.

3.2.1 von Mises distribution—The transversely isotropic π -periodic *von Mises* fiber distribution is given by

$$R(\mathbf{n}^0) = \frac{1}{\pi} \sqrt{\frac{b}{2\pi}} \frac{\exp \left[\frac{2b (\mathbf{n}^0 \cdot \mathbf{f}_3)^2}{\text{erfi}(\sqrt{2b})} \right]}{\text{erfi}(\sqrt{2b})}, \quad (13)$$

where $\text{erfi}(x)$ is the imaginary error function and $b > 0$ is the concentration parameter (Gasser, Ogden and Holzapfel 2006). When $b \rightarrow 0$, the fiber distribution becomes isotropic, with $R(\mathbf{n}^0) \rightarrow \frac{1}{4\pi}$ (Gasser, Ogden and Holzapfel 2006). With increasing values of b , the fibers become more aligned with $\mathbf{f}_3$, and the integrand in Eq.(1) exhibits increasing nonlinearity. In this analysis, we selected a most critical condition with $b = 5$ (Federico and Gasser 2010), to test the robustness of the integration schemes.

We calculated the total stress numerically with the GKT and FEI schemes for T, TC, and CT cases. We evaluated the measures RE and NI, defined above, for both integration schemes, with NI reported in Figure 4. NI_{GKT} was smaller than NI_{FEI} in all cases, with the largest difference most apparent in the TC and CT cases. The pattern for NI_{GKT} also showed less variation with fiber orientation relative to the principal planes of normal strain than that for NI_{FEI} . In these analyses, $n_{GK} = 7$ was sufficient for all cases, and m_T ranged from 3 to 15.

3.2.2 Ellipsoidal distribution—The orthotropic ellipsoidal fiber density distribution (Ateshian, Rajan, et al. 2009) is given by

$$R(\mathbf{n}^0) = C^{-1} \left[\left(\frac{n_1^0}{a} \right)^2 + \left(\frac{n_2^0}{b} \right)^2 + \left(\frac{n_3^0}{c} \right)^2 \right]^{-1/2}, \quad (14)$$

where (n_1^0, n_2^0, n_3^0) are the components of $\mathbf{n}^0$ in the fiber axes basis $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$, a , b and c are the semi-principal axes of the ellipsoid, and C is obtained by satisfying $\int_A R(\mathbf{n}^0) dA = 1$ over the unit sphere. When $a = b = 1$, the distribution is transversely isotropic about $\mathbf{f}_3$; increasing values of c produce increasingly aligned fiber distributions. In this analysis, we selected a most critical condition with $c = 10$.

The resulting values of NI are presented in Figure 5. Similarly to the *von Mises* distribution, NI_{GKT} was smaller than NI_{FEI} in all cases, with the largest difference most apparent in the TC and CT cases. In these analyses, $n_{GK} = 7$ was sufficient in most cases, except that $n_{GK} = 11$ was required when $\varphi_f = 0, \pi/4$ in the T case; m_T ranged from 3 to 15.

4. Multi-elements analysis

To examine the performance of the GKT and FEI schemes in a multiple elements analysis, we implemented these integration schemes in the open source finite element software FEBio (<http://www.febio.org>). We used a cube meshed with a large number of elements to examine the performance and computational efficiency of these integration schemes. Furthermore, we modeled an annular disk subjected to a prescribed axial compression to examine the axisymmetry of the principal components of stress for both integration schemes.

4.1 Compressible Unit cube

We subjected a unit cube, meshed with $20 \times 20 \times 20$ 8-node hexahedral elements, to the same strain conditions described above, using the fiber strain energy density function in Eq.(12), superposed on a compressible neo-Hookean ground matrix as described by Bonet and Wood (1997) with Lamé-like coefficients $\lambda = 0$ and $\mu = 0.5 \times 10^{-3}$ (Young's modulus $E_Y = 10^{-3}$ and Poisson's ratio $\nu = 0$); we investigated isotropic (spherical), *von Mises* ($b = 5$) and ellipsoidal ($a = b = 1, c = 10$) fiber density distributions, with fiber axes orientation similarly varied. Specific values of fiber properties α and β (with $\xi = 1$) and fiber axes orientations used in each of the simulations are presented in Table 4. The units of length and stress are arbitrary in this analysis; for example, the unit cube may be $1 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm}$ and the units of E_Y and ξ may be kPa or MPa.

Principal normal stresses were evaluated numerically using the GKT and FEI schemes, for T, TC, and CT strain cases. We performed a convergence analysis on the number of integration points required to produce a relative change $RC < 1\%$ in the principal stresses. We increased the number of integration points N between consecutive iterations i in the convergence analysis based on the GKT scheme: $N_{i-1} = m_T \cdot n_{GK}$ and $N_i = (m_T + 2) \cdot n_{GK}$ (since only odd values of m_T were employed); the same increment $N = N_i - N_{i-1}$ was applied to the FEI scheme. The largest value of RC among all three principal stresses was derived by subtracting the stress at the current N_i relative to that at the previous N_{i-1} , and normalizing the absolute value of that difference by the stress at the current N_i . The value of N_i when convergence was achieved ($RC = 1\%$) was denoted by NI, and the running (clock) time required to evaluate the converged case was denoted by RT. We purposefully selected Young's modulus E_Y of the ground matrix to be much smaller than the fiber modulus ξ , to minimize the influence of E_Y on the value of RC, since the GKT and FEI integration schemes only affected the calculation of stress in the fibers.

In most cases, NI_{GKT} was smaller than NI_{FEI} , often by one order of magnitude (Figure 6) and with the largest difference found in the TC and CT cases; the only exception occurred in the T case with isotropic fiber density, where NI had similar small values for both schemes. In the T case, both schemes had higher values of NI with transversely isotropic fiber density distributions. In the TC and CT cases, NI_{FEI} showed larger variation with fiber properties and basis orientations. RT had the same pattern as NI for both schemes, therefore RT_{GKT} was smaller than RT_{FEI} in most cases, with the largest differences observed in the TC and CT cases.

The relative change RC is also reported in Figure 7 when the number of integration points N_i was prescribed to be nearly the same for both schemes, with $(n_{GK}, m_T) = (11, 35)$ for GKT and 396 for FEI. We found that $RC_{GKT} \approx 0$ for most cases, except with the ellipsoidal fiber distribution density. RC_{FEI} was consistently larger than RC_{GKT} in all cases.

4.2 Nearly Incompressible Unit Cube

A unit cube meshed with $20 \times 20 \times 20$ 8-node hexahedral elements was subjected either to a tensile stretch ($\lambda_3 = 1.3$) or a compressive stretch ($\lambda_3 = 0.7$) along the z -axis, while faces initially normal to the x - and y -axes were traction-free. The cube was modeled with the uncoupled strain energy density formulation of Eq.(2), superposed on a nearly incompressible neo-Hookean ground matrix ($\Psi(\tilde{\mathbf{C}}) = c(\tilde{I}_1 - 3)/2$, where $\tilde{I}_1 = \text{tr}\tilde{\mathbf{C}}$ and $\tilde{\mathbf{C}} = \tilde{\mathbf{F}}^T \cdot \tilde{\mathbf{F}}$) with $c = 1$. The bulk modulus in $U(J)$ was set to $\kappa = 3000$. Isotropic (spherical), *von Mises* ($b = 5$) and ellipsoidal ($a = b = 1$, $c = 10$) fiber density distributions were also investigated, and the fiber axes orientation was similarly varied. Specific values of fiber properties α and β (with $\xi = 10$) and fiber axes orientations used in each of the simulations are presented in Table 4. As in the previous section, units are arbitrary for the cube size (e.g., mm), and the properties c , κ , and ξ (e.g., kPa or MPa).

Principal normal components of the Cauchy stress were evaluated numerically using the GKT and FEI schemes, for the stretch and compression cases. A convergence analysis was performed similar to that described in the previous section. In all cases, NI_{GKT} was smaller than NI_{FEI} , often by more than one order of magnitude (Figure 6). In both loading

configurations, the FEI scheme had much higher values of NI with isotropic fiber density when $\alpha = 20$ and $\beta = 2$, and also with transversely isotropic fiber density when $\varphi_f = 0$ and $\pi/4$. RT followed a similar pattern as NI for both schemes, therefore RT_{GKT} was smaller than RT_{FEI} in all cases, with the largest differences observed in conditions B, D and H. In all these analyses, the volume ratio J ranged from 0.99925 to 1.02947; the latter value, achieved in case B where the fiber response was most nonlinear, could be brought closer to unity by increasing κ , however the same value of κ was adopted across all cases in this evaluation, for consistent comparison.

4.3 Nearly Incompressible Annular disk

An annular disk with a thickness of 0.5 mm, and inner and outer diameters of 4 and 10 mm, was meshed with 336 hexahedral elements. The material model employed the same solid uncoupled solid mixture described in the previous section, with the neo-Hookean parameter set to $c = 1$ kPa and bulk modulus $\kappa = 10^4$ kPa; fiber material parameters were set to $\alpha = 4$, $\beta = 4$, $\xi = 10$ kPa, with an isotropic fiber density distribution. The bottom of the disk was fixed in the axial direction and the inner rim was constrained in the radial and tangential directions, while the top face had a prescribed displacement of -0.15 mm (compression). This problem is similar, but not identical, to the finite element model analyzed by Ehret, Itskov and Schmid (2010). We used the GKT scheme with $(n_{GK}, m_T) = (7, 9)$ and the FEI scheme with $N_{FEI} = 60$. The maximum principal normal Cauchy stress is reported in Figure 9. The FEI scheme exhibited a fluctuating distribution circumferentially, whereas the GKT scheme produced the expected axisymmetric distribution. The value of J ranged from 0.9982 at the inner rim, to 0.9999 at the outer rim, for both integration schemes.

5. Discussion

In this study, we introduced an integration scheme specialized to continuous fiber distributions where fibers may only sustain tension. We restricted the integration to the subdomain of the unit sphere where the normal strain is tensile (Figure 1); we used Gauss-Kronrod quadrature across latitudes and the trapezoidal rule across longitudes. We compared this GKT scheme to the most commonly used integration method, the finite element integration scheme, which employs uniformly (or nearly-uniformly) distributed integration points on the unit sphere. Despite its advantages relative to integration over the rectangular domain of spherical angles, there are three major drawbacks to the FEI scheme: a high computational cost due to the usually large number of integration points needed to achieve sufficient accuracy, a waste of integration over the domain of the unit sphere where fibers are not in tension, and a discretization error when tensed fiber bundles span a small region compared to the discretized surface of the unit sphere.

As shown from the results of this study, the GKT scheme significantly mitigated the first drawback, by demonstrating that fewer integration points were needed to achieve the same accuracy as the FEI scheme ($NI_{GKT} - NI_{FEI}$) in all cases (Figure 2, 4, 5, 6). By design (Figure 1 and Table 1), the GKT scheme also eliminated the second and third drawbacks completely. The smaller value of NI achieved in the GKT scheme translated into reduced computational time ($RT_{GKT} < RT_{FEI}$, Figure 6), despite the fact that the GKT scheme required the additional evaluation of eigenvalues and eigenvectors of the strain.

We performed analyses on a single cubic element to evaluate the accuracies of both schemes under various choices of nonlinear fiber responses (Figure 2) and fiber distribution densities (Figure 4 and 5). Evaluations of these integration schemes were performed using fully coupled as well as uncoupled strain energy density formulations, commonly used for modeling compressible and nearly incompressible solids in finite element analyses, respectively. To achieve the same accuracy, the FEI scheme generally required more integration points than the GKT scheme, especially in the TC and CT cases. More generally, the accuracy of the stress calculation may not be determinable, in which case a convergence analysis may be performed by varying the number of integration points. As illustrated in Figure 6 and Figure 8, the GKT scheme required fewer integration points to achieve a desired convergence threshold than the FEI scheme in all cases except for the T case with isotropic fiber density distribution and a compressible material model, where the performances of the two schemes were comparable. Alternatively, when the number of integration points was fixed in advance, the GKT scheme always achieved better results than the FEI scheme, often by orders of magnitude as illustrated in Figure 7.

The GKT scheme was less sensitive to the nonlinearity of the fiber stress response than the FEI scheme when the strains switched between T, TC and CT cases and the fiber distribution was isotropic (Figure 2). We may attribute this differential sensitivity to the fact that the nonlinear variation of the fiber stress along the different fiber directions was captured more accurately by the higher-order Gauss-Kronrod integration scheme than the midpoint-rule FEI scheme.

Both schemes were found to be variably sensitive to the orientation of the principal direction of transversely isotropic fiber distributions relative to the principal directions of normal strain (Figure 4 and 5), though the GKT scheme consistently performed better in all cases. As addressed in the study of Ehret, Itskov and Schmid (2010), FEI schemes are not all equal, as some of them may break the expected symmetry of the stress distribution. As shown here, the GKT scheme maintained symmetry when expected (Figure 9).

In practice, a user may not know in advance how many integration points N are needed to achieve a desired accuracy for a particular problem. Based on this study, we recommend that a convergence analysis be performed, as illustrated in the case of the finite element analysis of a cube. When convergence analyses are not convenient or practical, the value of N may be selected from the most conservative case of this study. For the GKT scheme, these values were $n_{GK} = 11$ and $m_T = 31$, thus corresponding to $N = 341$.

The Gauss-Kronrod rule used in the GKT scheme is known to be one of the easiest and most effective methods of numerical integration (Dahlquist and Björck 2008). For example, it is used in the double integration function ‘integral2’ in MATLAB (www.mathworks.com), which applies this rule across both directions of integration (Shampine 2008), called the GKKG scheme. In this study, we adopted the Gauss-Kronrod rule only across latitudes, while we used the trapezoidal rule across longitudes, because the integrand of the CFD framework is 2π -periodic, and the trapezoidal rule has super convergence property for integrating periodic trigonometric polynomials (Dahlquist and Björck 2008). Though not

shown here, the GKT scheme was found to converge with fewer integration points than the GKGK scheme in most cases of this study.

In summary, in this study we introduced a GKT integration scheme specialized to the analysis of stresses in continuous fiber distributions, where fibers can only sustain tension. We showed that this scheme performed consistently more efficiently than the conventional FEI scheme in a range of analyses that examined nonlinear and anisotropic fiber responses, for compressible and nearly incompressible material models.

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Figure 1. Domain of integration of total strain energy function in (a) TC case and (b) CT case, corresponding to directions along which the fiber normal strain E_n is positive.

Figure 2.

Number of integration points (NI) required to produce a relative error (RE) 1% in the principal normal stresses, when comparing GKT and FEI schemes to the MATLAB function 'integral2'. The fiber density distribution is isotropic. Cases A–F correspond to the combinations of material coefficients appearing in Table 2. T, TC and CT cases represent three conditions that produce tensile normal strains in fibers, as described in Table 1.

Figure 3.

Orientation of fiber axes $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ relative to the basis $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3\}$ of eigenvector of $\mathbf{E}$.

Figure 4.

Number of integration points (NI) required to produce a relative error (RE) 1% in the principal normal stresses, when comparing GKT and FEI schemes to the MATLAB function 'integral2'. Fibers follow a transversely isotropic *von Mises* density distribution. Cases A–I correspond to dominant fiber axes orientations given in Table 3. T, TC and CT cases represent three conditions that produce tensile normal strains in fibers, as described in Table 1.

Figure 5.

Number of integration points (NI) required to produce a relative error (RE) 1% in the principal normal stresses, when comparing GKT and FEI schemes to the MATLAB function 'integral2'. Fibers follow a transversely isotropic ellipsoidal density distribution. Cases A–I correspond to dominant fiber axes orientations given in Table 3. T, TC and CT cases represent three conditions that produce tensile normal strains in fibers, as described in Table 1.

Figure 6.

Number of integration points NI (bars) required to achieve a relative change (RC) 1% in the calculation of the principal normal stresses, in the multi-element convergence analysis of a compressible unit cube. The clock time CT (curves, black for FEI, gray for GKT) required to complete the analysis of the corresponding converged case is also reported. Cases A–I correspond to the various combinations of fiber properties, fiber density distributions and fiber basis orientations given in Table 4. Results are reported for both GKT and FEI schemes, for three representative conditions that produce tensile normal strains in fibers (Table 1).

Figure 7.

Relative change RC in principal normal stresses between consecutive iterations N_{i-1} and N_i , when N_i was prescribed close to 390 for GKT and FEI schemes. Cases A–I correspond to the various combinations of fiber properties, fiber density distributions and fiber basis orientations given in Table 4. For analyses A through F, the value of RC_{GKT} was nearly zero. Results are reported for both GKT and FEI schemes, for three representative conditions that produce tensile normal strains in fibers (Table 1).

Figure 8.

Number of integration points NI (bars) required to achieve a relative change (RC) $\leq 1\%$ in the calculation of the principal normal stresses, in the multi-element convergence analysis of a nearly incompressible cube. The clock time CT (curves, black for FEI, gray for GKT) required to complete the analysis of the corresponding converged case is also reported. Cases A-I correspond to the various combinations of fiber properties, fiber density distributions and fiber basis orientations given in Table 4. Results are reported for both GKT and FEI schemes, for two representative loading conditions that produce tensile normal strains in fibers (Table 1).

Figure 9. Maximum principal normal Cauchy stress evaluated using (a) the FEI scheme ($N_{\text{FEI}} = 60$), and (b) the GKT scheme, $(n_{\text{GK}}, m_{\text{T}}) = (7, 9)$.

Three strain conditions may produce tensile strains in fibers passing through a given point, as determined from the values of the principal normal strains: In the T case, all fibers passing through that point are in tension; in the TC case, fibers oriented within an elliptical double cone are in tension; and in the CT case, fibers oriented outside the elliptical double cone are in tension.

Table 1

	reference configuration	current configuration	range of φ	region of integration
T case
TC case
CT case

Table 2

Six different combinations (A–F) of material coefficients α and β are employed with the strain energy density of Eq.(12), to assess the numerical performance of the Gauss-Kronrod-Trapezoidal (GKT) and Finite Element Integration (FEI) schemes.

	Material coefficients
A	$\alpha = 0, \beta = 2$
B	$\alpha = 1, \beta = 2$
C	$\alpha = 20, \beta = 2$
D	$\alpha = 0, \beta = 4$
E	$\alpha = 1, \beta = 4$
F	$\alpha = 20, \beta = 4$

Table 3

Fiber axes orientations (θ_f , ϕ_f) relative to eigenvectors of the strain, used in the comparison of GKT and FEI schemes for *von Mises* and ellipsoidal fiber distribution densities.

	Fiber axes orientations
A	$\phi_f = 0, \theta_f = 0$
B	$\phi_f = \pi/4, \theta_f = 0$
C	$\phi_f = \pi/4, \theta_f = \pi/4$
D	$\phi_f = \pi/4, \theta_f = \pi/2$
E	$\phi_f = \pi/4, \theta_f = 3\pi/4$
F	$\phi_f = \pi/2, \theta_f = 0$
G	$\phi_f = \pi/2, \theta_f = \pi/4$
H	$\phi_f = \pi/2, \theta_f = \pi/2$
I	$\phi_f = \pi/2, \theta_f = 3\pi/4$

Table 4

Material coefficients, fiber density distributions and fiber material axes directions used in the multi-element analysis.

	Material coefficients	Fiber distribution	Fiber axes orientation
A	$\alpha = 0, \beta = 2$	spherical	NA
B	$\alpha = 20, \beta = 2$	spherical	NA
C	$\alpha = 20, \beta = 4$	spherical	NA
D	$\alpha = 0, \beta = 2$	<i>von Mises</i>	$\varphi_f = 0, \theta_f = 0$
E		<i>von Mises</i>	$\varphi_f = \pi/4, \theta_f = 0$
F		<i>von Mises</i>	$\varphi_f = \pi/2, \theta_f = 0$
G		ellipsoidal	$\varphi_f = 0, \theta_f = 0$
H		ellipsoidal	$\varphi_f = \pi/4, \theta_f = 0$
I		ellipsoidal	$\varphi_f = \pi/2, \theta_f = 0$