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Computational efficiency of numerical approximations of tangent moduli for finite element implementation of a fiber-reinforced hyperelastic material model

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Abstract

In this study, we evaluated computational efficiency of finite element (FE) simulations when a numerical approximation method was used to obtain the tangent moduli. A fiber-reinforced hyperelastic material model for nearly incompressible soft tissues was implemented for 3D solid elements using both the approximation method and the closed-form analytical method, and validated by comparing the components of the tangent modulus tensor (also referred to as the material Jacobian) between the two methods. The computational efficiency of the approximation method was evaluated with different perturbation parameters and approximation schemes, and quantified by the number of iteration steps and CPU time required to complete these simulations. From the simulation results, it can be seen that the overall accuracy of the approximation method is improved by adopting the central difference approximation scheme compared to the forward Euler approximation scheme. For small-scale simulations with about 10,000 DOFs, the approximation schemes could reduce the CPU time substantially compared to the closed-form solution, due to the fact that fewer calculation steps are needed at each integration point. However, for a large-scale simulation with about 300,000 DOFs, the advantages of the approximation schemes diminish because the factorization of the stiffness matrix will dominate the solution time. Overall, as it is material model independent, the approximation method simplifies the FE implementation of a complex constitutive model with comparable accuracy and computational efficiency to the closed-form solution, which makes it attractive in FE simulations with complex material models.

Keywords

Elasticity tensor; numerical approximation; biaxial testing; fiber-reinforced; hyperelastic material; finite element analysis

1. Introduction

Advances in noninvasive medical imaging techniques and computing power have substantially increased the capability of using computational tools to model and analyze

patient disease conditions, and develop treatment strategies (Xenos et al. 2010; Aguado-Sierra et al. 2011; Wang et al. 2014; Wang & Sun 2012; Liu et al. 2012; Sun et al. 2014). To construct a finite element (FE) model to model realistic patient conditions, patient-specific tissue geometries and experimentally derived, user-defined material models are necessary in order to obtain accurate simulation results. User-defined material models often involve complex functional forms, which can make implementation in commercial FE software packages such as ABAQUS challenging. Furthermore, patient-specific FE models usually employ a large number of elements to capture detailed anatomic features. Since a user-defined material model is evaluated at every integration point of the elements in a FE model, any improvement of numerical efficiency in the material model evaluation may lead to a substantial reduction of the simulation computational time.

Typically, to define material models in FE codes, the stress tensor and the tangent modulus tensor derived from the constitutive equation must be explicitly defined. While the stress evaluation is relatively straightforward, the specification of the tangent moduli is far more complicated, not only because it is a second-order derivation of the strain energy function with respect to the strain tensor, but also the coding of the resultant fourth-order tangent modulus tensor in a user-defined material subroutine is time-consuming and prone to coding errors. This is especially true for the material model implementations for the commercial FE codes: ABAQUS and ANSYS. For instance, in an ABAQUS user material subroutine UMAT, the tangent moduli associated with the Jaumann rate of Kirchhoff stress should be coded when used with continuum elements, while the tangent associated with the Green–Naghdi rate of Kirchhoff stress should be adopted for structural elements.

The tangent modulus tensor serves as an iterative operator for an implicit FE solver using the Newton-type method to solve the nonlinear initial-boundary value problems. An exact closed-form solution of the tangent moduli leads to a quadratic convergence (ABAQUS 2011); however, the exact tangent moduli are not mandatory to achieve accurate solutions due to the iterative nature of the Newton-type method. Therefore, approximation methods with various approximation schemes (Miehe 1996; Tanaka & Fujikawa 2011; Tanaka et al. 2014; Sun et al. 2008b) have been proposed as alternatives to analytical calculations of tangent moduli. Miehe (Miehe 1996) presented an approximation method to calculate the elasticity tensor associated with the convected rate of Kirchhoff stress. Sun et al. (2008b) presented a method to numerically approximate the material Jacobian for ABAQUS 3D solid elements and validated it using a simple isotropic Neo-Hookean material model. Tanaka and Fujikawa (Tanaka & Fujikawa 2011) proposed higher order approximation schemes, such as the second-order central difference (CD) and complex-step derivative approximation (CSDA). The approximation methods have been shown to be simple in coding and independent of material models. The open-source FE package, FEAP, calculates numerically approximated tangent for testing purposes. However, little is known about the computational efficiency of approximation methods compared to the closed-form solution.

In this paper, we adopted the approximation method (Sun et al. 2008b) and evaluated its computational efficiency using a fiber-reinforced hyperelastic material model implemented in the commercial FE code ABAQUS (Version 6.11, Pawtucket, RI). The constitutive model was coded for 3D solid elements using both the approximation method and the closed-form

analytical method, and validated by comparing the major components of the material Jacobian between the two methods. The computational efficiency of the approximation method was evaluated with different perturbation parameters and approximation schemes, i.e. the CD approximation scheme and the forward Euler approximation scheme. We quantified the computational efficiency by the number of iteration steps and CPU time required to complete the simulations.

2. Continuum mechanics framework

2.1. Description of the deformation

Deformation of a body is described by mapping χ from a material point $\mathbf{X}$ at its undeformed (referential) configuration Ω_0 to its position vector $\mathbf{x} = \chi(\mathbf{X}, t)$ at current deformed configuration Ω at time t . The deformation gradient $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ is used to describe the deformation. To account for the rate of deformation, the spatial velocity gradient is defined as: $\mathbf{L} = \text{grad}(\mathbf{v}) = \dot{\mathbf{F}}\mathbf{F}^{-1}$. Its symmetric and anti-symmetric parts are:

$$\mathbf{D} = \text{sym}(\mathbf{L}) = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T), \quad \mathbf{W} = \text{skew}(\mathbf{L}) = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T). \quad (1)$$

$\mathbf{D}$ and $\mathbf{W}$ are known as the rate of deformation tensor and the rate of rotation tensor, respectively.

Following Holzapfel (2000), we consider a multiplicative decomposition of the deformation gradient tensor $\mathbf{F} = (J^{1/3}\mathbf{I})\bar{\mathbf{F}}$, where $J = \det(\mathbf{F})$; $(J^{1/3}\mathbf{I})$ represents a dilational (volumetric) contribution, while $\bar{\mathbf{F}} = J^{-1/3}\mathbf{F}$ denotes a distortional (isochoric) contribution. The deviatoric part of right Cauchy–Green tensor and Green–Lagrange strain tensor is written as $\bar{\mathbf{C}} = \bar{\mathbf{F}}^T\bar{\mathbf{F}}$ and $\bar{\mathbf{E}} = \frac{1}{2}(\bar{\mathbf{C}} - \mathbf{I})$, respectively.

2.2. Hyperelastic stress response

Among various measures of stress, three of them are employed in this paper. They are: (1) second Piola–Kirchhoff stress, $\mathbf{S}$, defined in the referential configuration; (2) Kirchhoff stress, $\boldsymbol{\tau}$, which is a push-forward of second Piola–Kirchhoff stress; and (3) Cauchy stress $\boldsymbol{\sigma}$. These three measures of stress are expressed as:

$$\mathbf{S} = 2 \frac{\partial W(\mathbf{C})}{\partial \mathbf{C}}, \quad \boldsymbol{\tau} = \mathbf{F}\mathbf{S}\mathbf{F}^T, \quad \boldsymbol{\sigma} = J^{-1}\boldsymbol{\tau} \quad (2)$$

where W denotes a scalar valued strain-energy function postulated to exist for hyperelastic materials.

2.3. Tangent modulus tensor

Implementation of a user-defined material model in a FE code, such as ABAQUS, usually requires the user to explicitly specify: (1) Cauchy stress components calculated from a given

deformation and (2) the tangent modulus tensor derived from a constitutive equation of rate form. Various forms of objective rates were proposed to account for material rotation, such as Jaumann rate and Green–Naghdi rate. Note that even for the same material, different selections of stress and stress rate result in different tangent moduli. The constitutive equation with the Jaumann rate of Kirchhoff stress can be shown as below:

$$\tau^{\nabla \mathbf{J}} = \dot{\tau} - \mathbf{W}\tau - \tau\mathbf{W}^T = \mathbb{C}^{\tau \mathbf{J}} : \mathbf{D} \quad (3)$$

where the notation ∇ in the superscript denotes objective time derivative, while the notation ' $\dot{\cdot}$ ' stands for material time derivative; ∇ denotes the fourth-order tangent modulus tensor, with the superscripts represent the form of stress and stress rate utilized in the equation where $\mathbf{J}$ is for the Jaumann rate; the notation ' $:$ ' represents a double-dot product (also known as a scalar product) of tensors (Holzapfel 2000). To calculate the tangent moduli of a specific form, it starts with the evaluation of the elasticity tensor in the referential configuration:

$$\mathbb{C} = 2 \frac{\partial \mathbf{S}(\mathbf{C})}{\partial \mathbf{C}} = 4 \frac{\partial^2 W(\mathbf{C})}{\partial \mathbf{C} \partial \mathbf{C}} \quad (4)$$

The fourth-order referential tensor of elasticity possesses not only minor symmetry but also major symmetry, which implies $\mathbb{C}$ has 21 independent components (Sun et al. 2008b).

The corresponding elasticity tensor in the spatial description, $\mathbb{C}$, is then derived via the Piola transformation:

$$c_{abcd} = J^{-1} F_{aA} F_{bB} F_{cC} F_{dD} C_{ABCD} \quad (5)$$

$\mathbb{C}$ is associated with the objective Oldroyd (convective) rate (i.e. Lie time derivative) of Kirchhoff stress (Simo & Hughes 1998):

$$\mathcal{L}_v(\tau) = \mathbf{F} \dot{\mathbf{S}} \mathbf{F}^T = \dot{\tau} - \mathbf{L}\tau - \tau\mathbf{L}^T = J\mathbb{C} : \mathbf{D} \quad (6)$$

where $\mathcal{L}_v(\star)$ is the Lie time derivative of $\star$. $\mathcal{C}$ is then noted as $\mathbb{C}^{\tau c}$. Comparing Equation (3) with (6), a connection between $\mathbb{C}^{\tau \mathbf{J}}$ and $\mathbb{C}^{\tau c}$ can be established as:

$$c_{abcd}^{\tau \mathbf{J}} = c_{abcd}^{\tau c} + \frac{1}{2} (\delta_{ac} \tau_{bd} + \delta_{bd} \tau_{ac} + \delta_{ad} \tau_{bc} + \delta_{bc} \tau_{ad}) \quad (7)$$

The material Jacobian is then expressed as:

$$c_{abcd}^{MJ} = \frac{1}{J} c_{abcd}^{\tau J} \quad (8)$$

2.4. Approximation solution of tangent modulus tensor

The derivation and coding for the elasticity tensor of Equation (8) in a FE code are known to be time-consuming and prone to coding errors, which limits the widespread applications of complicated hyperelastic constitutive laws. Alternatively, an effective numerical approximation method can be employed to simplify the implementation process (Sun et al. 2008b).

To achieve the approximation, Equation (3) is linearized at first:

$$\Delta \tau - \Delta \mathbf{W} \tau - \tau \Delta \mathbf{W}^T = \Delta^{\tau J} : \Delta \mathbf{D} \quad (9)$$

where,

$$\begin{aligned} \Delta \mathbf{D} &= \frac{1}{2} \left(\Delta \mathbf{F} \mathbf{F}^{-1} + (\Delta \mathbf{F} \mathbf{F}^{-1})^T \right) \\ \Delta \mathbf{W} &= \frac{1}{2} \left(\Delta \mathbf{F} \mathbf{F}^{-1} - (\Delta \mathbf{F} \mathbf{F}^{-1})^T \right) \end{aligned}$$

with $\mathbf{F}$ the incremental form of deformation gradient tensor.

A perturbation to the $(\hat{i}, \hat{j})$ component of $\mathbf{D}$ is:

$$\Delta \mathbf{D}^{(\hat{i}\hat{j})} = \frac{1}{2} \left(\Delta \mathbf{F}^{(\hat{i}\hat{j})} \mathbf{F}^{-1} + (\Delta \mathbf{F}^{(\hat{i}\hat{j})} \mathbf{F}^{-1})^T \right) \quad (10)$$

(Note that $\hat{i}, \hat{j} = 1, 2, 3$ and no summation is assumed over $\hat{i}$ and $\hat{j}$ in this paper). With the perturbation to $\mathbf{F}$, $\mathbf{F}^{(\hat{i}\hat{j})}$ is expressed as:

$$\begin{aligned} \Delta \mathbf{F}^{(\hat{i}\hat{j})} &= \frac{\varepsilon}{2} \left(\mathbf{e}_{\hat{i}} \otimes \mathbf{e}_{\hat{j}} \cdot \mathbf{F} + \mathbf{e}_{\hat{j}} \otimes \mathbf{e}_{\hat{i}} \cdot \mathbf{F} \right) \\ \Delta F_{ab}^{(\hat{i}\hat{j})} &= \frac{\varepsilon}{2} \left(\delta_{a\hat{i}} F_{\hat{j}b} + \delta_{a\hat{j}} F_{\hat{i}b} \right) \end{aligned} \quad (11)$$

such that, perturbations to the rate of deformation and rotation is straightforward and can be updated as:

$$\Delta \mathbf{D}^{(\hat{i}\hat{j})} = \frac{\varepsilon}{2} \left(\mathbf{e}_{\hat{i}} \otimes \mathbf{e}_{\hat{j}} + \mathbf{e}_{\hat{j}} \otimes \mathbf{e}_{\hat{i}} \right), \quad \Delta \mathbf{W}^{(\hat{i}\hat{j})} = 0 \quad (12)$$

Perturbed deformation gradient $\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}})$ is defined as $\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}}) = \mathbf{F} + \hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}})$. Thus, the perturbation in Kirchhoff stress $\boldsymbol{\tau}$ can be approximated by the forward difference of the perturbed and unperturbed Kirchhoff stress:

$$\Delta\tau \cong \tau(\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}})) - \tau(\mathbf{F}) \quad (13)$$

Insert Equations (11) and (12) to (8):

$$\tau(\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}})) - \tau(\mathbf{F}) \cong \mathbb{C}^{\tau\mathbf{J}(\hat{\mathbf{I}}\hat{\mathbf{J}})} : \frac{\varepsilon}{2} (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i) \quad (14)$$

$\mathbb{C}^{\tau\mathbf{J}(\hat{\mathbf{I}}\hat{\mathbf{J}})}$ stands for the approximate tangent modulus tensor associated with the $\hat{\mathbf{I}}, \hat{\mathbf{J}}$ strain state. Due to its property of symmetry, $\mathbb{C}^{\tau\mathbf{J}(\hat{\mathbf{I}}\hat{\mathbf{J}})}$ can be shown in index form as:

$$c^{\tau\mathbf{J}(\hat{\mathbf{I}}\hat{\mathbf{J}})}_{ab} \hat{I} \hat{J} \cong \frac{1}{\varepsilon} [\tau(\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}}))_{ab} - \tau(\mathbf{F})_{ab}] \quad (15)$$

The material Jacobian defined in ABAQUS is now:

$$c^{MJ, \text{apm}}_{ab} \hat{I} \hat{J} = \frac{1}{J} c^{\tau\mathbf{J}(\hat{\mathbf{I}}\hat{\mathbf{J}})}_{ab} \hat{I} \hat{J} \cong \frac{1}{J\varepsilon} [\tau(\hat{\mathbf{F}}(\hat{\mathbf{I}}\hat{\mathbf{J}}))_{ab} - \tau(\mathbf{F})_{ab}] \quad (16)$$

2.5. Numerical approximation scheme

Recently, Tanaka and Fujikawa (2011) suggested to improve the approximation accuracy of the elasticity tensors by employing numerical approximation schemes of higher order. The approach was verified using an ABAQUS built-in model. Following Tanaka and Fujikawa (Tanaka & Fujikawa 2011), departing from Taylor's expansion,

$$f(x+\varepsilon) = f(x) + \frac{f'(x)\varepsilon}{1!} + \frac{f''(x)\varepsilon^2}{2!} + \frac{f'''(x)\varepsilon^3}{3!} + \dots \quad (17)$$

upon neglecting appropriate high-order small terms, the derivative of the function $f(x)$, $f'(x)$, can be expressed as:

$$f'(x) = \frac{f(x+\varepsilon) - f(x)}{\varepsilon} + O(\varepsilon) \quad (18)$$

Therefore, the approximation method of Equation (16) utilizes essentially a first-order forward Euler approximation scheme. To achieve higher order approximation, the CD scheme can be obtained by expanding:

$$f(x-\varepsilon) = f(x) - \frac{f'(x)\varepsilon}{1!} + \frac{f''(x)\varepsilon^2}{2!} - \frac{f'''(x)\varepsilon^3}{3!} + \dots \quad (19)$$

Minus Equation (19) with Equation (17), the derivative $f'(x)$ expressed in second-order CD method is:

$$f'(x) = \frac{f(x+\varepsilon) - f(x-\varepsilon)}{2\varepsilon} + O(\varepsilon^2) \quad (20)$$

The approximated tangent moduli are thus expressed as:

$$c^{MJ, \text{apm}}_{ab} \hat{I} \hat{J} = \frac{1}{J} c_{ab \hat{I} \hat{J}} \tau \mathbf{J}(\hat{I} \hat{J}) \cong \frac{1}{2J\varepsilon} \left[\tau \left(\hat{\mathbf{F}}^{(\hat{I} \hat{J})} \right)_{ab} - \tau \left(\hat{\mathbf{F}}^{(\hat{I} \hat{J})} \right)_{ab} \right] \quad (21)$$

where $\check{\mathbf{F}}^{(\hat{I} \hat{J})} = \mathbf{F} - \mathbf{F}^{(\hat{I} \hat{J})}$.

3. Examples – FE implementation of a fiber-reinforced hyperelastic material model

3.1. A fiber-reinforced hyperelastic material model

A fiber-reinforced invariant-based hyperelastic model (Gasser et al. 2006), which is widely used to model biological soft tissue, was adopted and modified in this study, and its strain energy function is expressed as:

$$W_0(\mathbf{C}, \mathbf{M}, \mathbf{N}, J) = c_{10} \left(\exp \left[c_{01} \left(\frac{\bar{I} - 3}{1} \right) \right] - 1 \right) + \frac{k_1}{2k_2} \left[\exp \left(k_2 \frac{\bar{\varepsilon}_1^2}{1} \right) - 1 \right] + \frac{k_1}{2k_2} \left[\exp \left(k_2 \frac{\bar{\varepsilon}_2^2}{2} \right) - 1 \right] + \frac{1}{D} (J - 1)^2 \quad (22)$$

where $\bar{\varepsilon}_1 := \kappa(\bar{I} - 3) + (1 - 3\kappa)(\bar{I}_4 - 1)$, $\bar{\varepsilon}_2 := \kappa(\bar{I} - 3) + (1 - 3\kappa)(\bar{I}_6 - 1)$, c_{01} , c_{10} , k_1 , k_2 , and D are the material parameters. κ ranging from 0 to 1/3 determines the dispersion of fibers; D is selected to enforce near incompressibility. The invariants of the distortional deformation are defined as $\bar{I}_1(\bar{\mathbf{C}}) := \text{tr}(\bar{\mathbf{C}})$, $\bar{I}_4(\bar{\mathbf{C}}, \mathbf{M}) := \mathbf{M} \cdot \bar{\mathbf{C}} \cdot \mathbf{M}$ and $\bar{I}_6(\bar{\mathbf{C}}, \mathbf{N}) := \mathbf{N} \cdot \bar{\mathbf{C}} \cdot \mathbf{N}$, where $\mathbf{M}$ and $\mathbf{N}$ denote the orientations of the two families of fibers in the material configuration, with the

$$\mathbf{M} = \begin{bmatrix} \cos \alpha \\ \sin \alpha \\ 0 \end{bmatrix}, \mathbf{N} = \begin{bmatrix} \cos \beta \\ \sin \beta \\ 0 \end{bmatrix};$$

α and β denote the angles between the orientation of the fibers in the undeformed state and the material axis. The derivation of stress components is given in Appendix 1 and the referential tensor of elasticity, $\mathbf{C}$, is presented in Appendix 2.

3.2. Utilization of planar biaxial testing data to obtain material model parameters

Planar biaxial testing, originally developed by Lanir and Fung (1974a, 1974b), is being increasingly utilized as a standard technique to characterize the mechanical properties of planar soft tissues (Sacks et al. 1997; Sacks 1999; Sun et al. 2003). In this study, we use the planar biaxial testing data of glutaraldehyde-treated bovine pericardium (GLBP) obtained previously to illustrate the modeling techniques and evaluate the approximation method. The testing protocol of a typical planar biaxial testing experiment has been reported previously (Sacks 1999; Sun et al. 2003). Briefly, the biaxial tests of GLBP tissues began with preconditioning of the 25 mm × 25 mm specimens with about 20 cycles of equibiaxial stress to the maximum first Piola–Kirchhoff stress level of about 1 MPa at a stress rate of 50 kPa/s. The subsequent stress-controlled testing protocols consisted of first Piola–Kirchhoff stress ratios $P_{11}:P_{22}$ held to constant values of 0.5:1, 0.75:1, 1:1, 1:0.75, and 1:0.5. The in-plane Green strain tensor $\mathbf{E}$ was calculated from the deformation gradient, $\mathbf{F}$. The first Piola–Kirchhoff stress tensor $\mathbf{P}$ was calculated as $P_i = f_i / (TL)$ where f_i are the current measured loads in each direction, T is the initial thickness of the specimen, and L are the unloaded reference specimen dimensions. The second Piola–Kirchhoff stress tensor $\mathbf{S}$ was obtained using $\mathbf{S} = \mathbf{F}^{-1} \cdot \mathbf{P}$.

Upon properly selecting parameter D (Doyle et al. 2010) as an infinitesimal value, the deformation Jacobian J approaches 1 so that the constitutive model of Equation (22) reaches its corresponding perfectly incompressible form:

$$W(\mathbf{C}, \mathbf{M}, \mathbf{N}, J) = c_{10} (\exp [c_{01} (\mathbf{I}_1 - 3)] - 1) + \frac{k_1}{2k_2} \left[\exp (k_2 \varepsilon_1^2) - 1 \right] + \frac{k_1}{2k_2} \left[\exp (k_2 \varepsilon_2^2) - 1 \right] - p(J - 1) \quad (23)$$

where $J = 1$ and p is a Lagrangian multiplier which can be determined from the boundary condition of planar biaxial tests.

The detailed derivation of stress using Equation (23) is shown in Appendix 3. In this study, the material parameters of Equation (23) were obtained by the means of the nonlinear least-square fitting method in MATLAB (The MathWorks, Inc., Natick, MA). The fitted material constants are summarized in the Table 1. The material parameters were tested for convexity using the method presented in Sun and Sacks (Sun & Sacks 2005). The fitted Cauchy stress–Green strain curves are shown in Figure 1. From Table 1 and Figure 1, it is noted that the fitted curve (denoted as analytical) obtained from incompressible hyperelastic theory is in excellent agreement with that from the experiment.

3.3. FE model setup and simulation results

A FE model was established to simulate the biaxial experiments: the specimen had the dimensions of 25 mm × 25 mm × 0.4 mm. Four evenly spaced nodal forces, 5 mm apart from each other and 2.5 mm inside the specimen edge, were imposed on each side. Each nodal force was 2.5 N, to induce a 1 MPa Lagrangian stress on each edge. The global

coordinate axes were chosen to align with the loading directions. The geometry domain was discretized with 40×40 eight-node brick elements (C3D8) in ABAQUS. The material constants were taken as inputs to the FE model. In the simulations, the ABAQUS/ UMAT was employed to incorporate the approximation method. The simulations were performed on a Windows 64-bit desktop computer equipped with an Intel Core i7-2600 processor (3.40 GHz) and 8 GB memory.

The average FE-predicted stress–strain response was extracted from the simulation results for the 8×8 element ($5 \text{ mm} \times 5 \text{ mm}$) region in the center of the model for comparison with the experimental data. This region was specifically selected to represent the square region enclosed by the four optical markers in the biaxial test for strain measurement. As shown in Figure 1, the numerical predictions match well with both the experimental and analytical results. The contour of the Mises stress made from the numerical simulation is shown in Figure 2. It can be seen that despite symmetric loading, the sample in the simulated biaxial test deformed asymmetrically due to material anisotropy, which was also observed in the experiment (Sun & Sacks 2005).

3.4. Validation of approximation method

The good match achieved between the numerical solution and the analytical/experimental results presented in Figure 1 demonstrates the effectiveness of the approximation method. However, it does not guarantee that the approximation of the material Jacobian is correct, since inaccurate definition of the tangent moduli leads to slower (if not no) convergence in the Newton scheme without changing the converged results. Therefore, it is necessary to compare the approximate tangent moduli with the closed-form solutions to validate the approximation. Accordingly, the same simulation was repeated using a different UMAT subroutine coded with the closed form, analytical evaluation of the tangent moduli. The relative error ϵ of the approximation was defined following Tanaka et al. (2014) to facilitate the comparison:

$$\epsilon = \left(\sum_{a,b,c,d} \left(c_{abcd}^{MJ} - c_{abcd}^{MJ,apm} \right)^2 \right)^{1/2} / \left(\sum_{a,b,c,d} \left(c_{abcd}^{MJ} \right)^2 \right)^{1/2} \quad (24)$$

The relative error obtained using the approximation scheme was plotted against variable perturbation parameters ϵ in Figure 3. The first-order approximation errors are of the same order as ϵ based on Equation (18), which suggests a preference for a small value of ϵ . However, when ϵ becomes too small, the evaluation is prone to numerical truncation errors. There exists an optimal value for ϵ . It is shown in Figure 3 that the first-order approximation achieved its optimal accuracy when ϵ was selected to be 1×10^{-8} , which was also observed by Tanaka and Fujikawa (2011).

3.5. Computational efficiency

The approximated tangent moduli tended to result in slower convergence than the analytical values that provide overall second-order convergence. However, it is shown in Figure 4 that

although the first-order approximation method required more iterations (Figure 4(a)), it reduced the CPU time by about 80% ($\varepsilon = 1 \times 10^{-8}$, Figure 4(b)) due to the fact that fewer calculations were made at each integration point for each iteration. The approximation method evaluates the stress tensor twice (Equation 16), i.e. the first derivative of the scalar valued strain energy function with respect to the second-order strain tensor is calculated two times. However, for the analytical method, in addition to estimating the stress tensor, the fourth-order tangent modulus tensor, i.e. the second derivative of the strain function (Hessian) with respect to the strain tensor, must be calculated. This is not only much more complicated but also considerably more costly. Therefore, the more complicated the constitutive equation is, the more computational efficiency the approximation method possesses over the analytical evaluation.

3.6. Higher order approximation

In order to improve the accuracy of approximation to the tangent, the second-order CD scheme of Equation (21) was coded in UMAT. The numerical simulation of the biaxial test was repeated and the tangent moduli were again evaluated at the same integration point of the same element. It is noticed from Figure 3 that the overall accuracy of approximation was improved by adopting the CD method compared to the first-order forward Euler method. The simulation results were most accurate when $\varepsilon = 1 \times 10^{-6}$, which was in good agreement with that found in Tanaka and Fujikawa (2011). Using this perturbation parameter value, the simulation also took less iterations to converge, compared to not only the forward Euler approximated method, but also the analytical method. Despite the rapid convergence, the simulation using the CD method with $\varepsilon = 1 \times 10^{-6}$ took about 13% more CPU time than that with the forward Euler method with $\varepsilon = 1 \times 10^{-8}$. This is because the CD method involves additional calculations of the perturbed deformation gradient and Kirchhoff stress compared with the forward Euler method. Despite this, the CD method was considerably more time efficient than the direct analytical evaluation (74% less in CPU time). Recently, Tanaka et al. (2014) presented a comparison of approximation methods using the first-order forward Euler method and the second-order CSDA method. Tanaka et al. demonstrated the superiority of the second-order CSDA method over the forward Euler method in terms of accuracy and robustness. However, it was shown that the CSDA method took about 100% longer CPU time than the forward Euler method when it was run on a mesh size of 2000 elements that is similar to that adopted in our simulations.

3.7. Approximation method in larger scale computation

The approximation method has been shown to be more computationally efficient than the analytical method in previous sections using a mesh size of around 2000 C3D8 elements with around 10,000 DOFs. However, in large-scale simulations, factorization time of the stiffness matrix may dominate the FEA solution time. In this case, the advantage of the approximation method over the analytical method could be diminished. To demonstrate this, we constructed an FE model (C3D8 elements) of a cylindrical tube based on the geometry of a rat carotid artery segment (Sun et al. 2008a). The vessel was fixed at both ends in the axial direction and was inflated up to 25 KPa with pressure acting on the inner surface. Using the same material model of Equation (22) and material parameters as previous, the simulation

was carried out on two different meshes: Mesh 1 with 99,330 DOFs and Mesh 2 with 319,950 DOFs.

When the computational scale was increased, the overall CPU time saved using the approximation methods was reduced (Table 2). The CPU time saved per iteration using the first- and second-order approximations were reduced from 12.1 to 6.8% in Mesh 1–8.3% and 3.9% in Mesh 2, respectively. Table 2 shows that the closed-form solution required the least amount of iterations before achieving convergence for both meshes. It follows that as the computational scale continues to increase, the difference in CPU time between the approximate and analytical calculation methods would eventually become negligibly small, provided that the approximation methods did not delay the convergence further.

It is worth noting that the beauty of the approximation method is its feature of material independence. Although the form of the constitutive model is problem dependent, its implementation using the approximation method could be achieved by updating the stress evaluation only without changing any other part of the UMAT code. Whereas, implementing a user-defined material model analytically requires the renewal of not only the stress, but also the tangent moduli, which essentially demands a UMAT recoding all together.

4. Conclusion

In this study, we evaluated the computational efficiency and accuracy of numerical approximation methods to obtain the consistent tangent moduli. The first-order forward Euler method was shown to give acceptable accuracy for the numerical examples. Adopting the second-order CD method could increase accuracy at the cost of more CPU time. The value of the perturbation parameter ϵ is important in controlling the approximation accuracy as well as the numerical efficiency of the simulations. Because fewer calculations are involved in the approximation method at every integration point, the approximation method was found to reduce the CPU time considerably compared to the analytical approach for small-scale FE meshes. However, for large-scale meshes, the solution time is dominated by the factorization of the stiffness matrix, so the CPU time saved by using the approximation method was less significant. Overall, the approximation schemes for the tangent moduli can result in acceptable accuracy and comparable computational efficiency compared to analytical methods. Owing to its added feature of material model independence and ease in coding, the approximation method could facilitate the FE implementation of complex constitutive relations in biomechanical applications.

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Appendix 1. Stress calculation using the fiber-reinforced material model

The strain energy function is composed of three parts: an isotropic term contributed from the matrix W_m , an anisotropic term from the collagen fiber contribution W_f and a penalty term U :

$$W_0(\mathbf{C}, \mathbf{M}, \mathbf{N}, J) = W_m(\bar{I}_1) + W_f(\bar{I}_1, \bar{I}_4, \bar{I}_6) + U(J) \quad (\text{A1})$$

It can be further grouped as an isochoric part and a volumetric part as:

$$W_0 = W_{\text{iso}} + W_{\text{vol}} \quad (\text{A2})$$

where, $W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6) = W_m(\bar{I}_1) + W_f(\bar{I}_1, \bar{I}_4, \bar{I}_6)$, $W_{\text{vol}}(J) = U(J)$. Fictitious second Piola–Krichhoff stress is presented as:

$$\bar{\mathbf{S}} = 2 \frac{\partial W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{\mathbf{C}}} = 2 \left(\bar{W}_1 \frac{\partial \bar{I}_1}{\partial \bar{\mathbf{C}}} + \bar{W}_4 \frac{\partial \bar{I}_4}{\partial \bar{\mathbf{C}}} + \bar{W}_6 \frac{\partial \bar{I}_6}{\partial \bar{\mathbf{C}}} \right) \quad (\text{A3})$$

where,

$$\begin{aligned} \bar{W}_1 &= \frac{\partial W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_1} = c_{10} c_{01} \left(\exp \left[c_{01} (\bar{I}_1 - 3) \right] - 1 \right) + k_1 \kappa \left[\bar{\varepsilon}_1 \exp(k_2 \bar{\varepsilon}_1^2) + \bar{\varepsilon}_2 \exp(k_2 \bar{\varepsilon}_2^2) \right], \\ \bar{W}_4 &= \frac{\partial W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_4} = k_1 (1 - 3\kappa) \bar{\varepsilon}_1 \exp(k_2 \bar{\varepsilon}_1^2), \\ \bar{W}_6 &= \frac{\partial W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_6} = k_1 (1 - 3\kappa) \bar{\varepsilon}_2 \exp(k_2 \bar{\varepsilon}_2^2) \end{aligned} \quad (\text{A4})$$

Utilizing the expressions:

$$\frac{\partial \bar{I}_1(\bar{\mathbf{C}})}{\partial \bar{\mathbf{C}}} = \mathbf{I}, \quad \frac{\partial \bar{I}_4(\bar{\mathbf{C}}, \mathbf{M})}{\partial \bar{\mathbf{C}}} = \mathbf{M} \otimes \mathbf{M}, \quad \frac{\partial \bar{I}_6(\bar{\mathbf{C}}, \mathbf{N})}{\partial \bar{\mathbf{C}}} = \mathbf{N} \otimes \mathbf{N}, \quad \frac{\partial J(\mathbf{F})}{\partial \mathbf{C}} = \frac{1}{2} J \mathbf{C}^{-1} \quad (\text{A5})$$

it follows

$$\bar{\mathbf{S}} = 2 \left(\bar{W}_1 \mathbf{I} + \bar{W}_4 \mathbf{M} \otimes \mathbf{M} + \bar{W}_6 \mathbf{N} \otimes \mathbf{N} \right) \quad (\text{A6})$$

Therefore, we obtain the deviatoric part and volumetric part of the second P–K stress:

$$\mathbf{S}_{\text{iso}} = 2 \frac{\partial W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \mathbf{C}} = J^{-2/3} \text{Dev} \bar{\mathbf{S}} \quad (\text{A7})$$

$$\mathbf{S}_{\text{vol}} = 2 \frac{\partial W_{\text{vol}}(J)}{\partial \mathbf{C}} = 2 \frac{\partial W_{\text{vol}}}{\partial J} \frac{\partial J}{\partial \mathbf{C}} = \frac{2}{D} J(J-1) \mathbf{C}^{-1} \quad (\text{A8})$$

with $\text{Dev}[\ast] = [\ast] - \frac{1}{3}([\ast]:\mathbf{C})\mathbf{C}^{-1}$.

The Second Piola–Kirchhoff stress along with Cauchy stress and Kirchhoff stress are calculated from:

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{vol}} \quad (\text{A9})$$

$$\boldsymbol{\sigma} = J^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T \quad (\text{A10})$$

$$\boldsymbol{\tau} = J \boldsymbol{\sigma} \quad (\text{A11})$$

Appendix 2. Calculation of referential tensor of elasticity for the model

Following the isochoric-volumetric split from Equation (A2),

$$\mathbb{C} = \mathbb{C}_{\text{iso}} + \mathbb{C}_{\text{vol}} \quad (\text{A12})$$

and

$$\begin{aligned} \mathbb{C}_{\text{iso}} &= \mathbb{P} : \bar{\mathbb{C}} : \mathbb{P}^T + \frac{2}{3} J^{-\frac{2}{3}} (\bar{\mathbf{S}} : \bar{\mathbf{C}}) \tilde{\mathbb{P}} - \frac{2}{3} (\mathbf{C}^{-1} \otimes \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{iso}} \otimes \mathbf{C}^{-1}) \\ \mathbb{C}_{\text{vol}} &= J \left(\frac{\partial W_{\text{vol}}}{\partial J} + J \frac{\partial^2 W_{\text{vol}}}{\partial J^2} \right) \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} + 2J \frac{\partial W_{\text{vol}}}{\partial J} \frac{\partial \mathbf{C}^{-1}}{\partial \mathbf{C}} \end{aligned} \quad (\text{A13})$$

where

$$\begin{aligned}
(\mathbb{P})_{abcd} &= \frac{1}{2} (\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}) - \frac{1}{3} C_{ab}^{-1} C_{cd} \\
(\tilde{\mathbb{P}})_{abcd} &= \frac{1}{2} (C_{ac}^{-1} C_{bd}^{-1} + C_{ad}^{-1} C_{bc}^{-1}) - \frac{1}{3} C_{ab}^{-1} C_{cd}^{-1} \\
(\bar{\mathbb{C}})_{abcd} &= 4J^{-4/3} \frac{\partial^2 W_{\text{iso}}}{\partial C_{ab} \partial C_{cd}} \\
\left(\frac{\partial \mathbf{C}^{-1}}{\partial \mathbf{C}}\right)_{abcd} &= -\frac{1}{2} (C_{ac}^{-1} C_{bd}^{-1} + C_{ad}^{-1} C_{bc}^{-1}) \quad (\text{A14})
\end{aligned}$$

To obtain $\frac{\partial^2 W_{\text{iso}}}{\partial \mathbf{C} \partial \mathbf{C}}$, the following second derivatives of W_{iso} with respect to the invariants I_1, I_4 and I_6 can be expressed as:

$$\begin{aligned}
\bar{W}_{11} &= \frac{\partial^2 W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_1^2} = c_{10} c_{01}^2 \exp \left[c_{01} (\bar{I}_1 - 3) \right] + k_1 \kappa^2 \left[(1 + 2k_2 \bar{\varepsilon}_1^2) \exp(k_2 \bar{\varepsilon}_1^2) + (1 + 2k_2 \bar{\varepsilon}_2^2) \exp(k_2 \bar{\varepsilon}_2^2) \right] \\
\bar{W}_{44} &= \frac{\partial^2 W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_4^2} = k_1 (1 - 3\kappa)^2 (1 + 2k_2 \bar{\varepsilon}_1^2) \exp(k_2 \bar{\varepsilon}_1^2) \\
\bar{W}_{66} &= \frac{\partial^2 W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_6^2} = k_1 (1 - 3\kappa)^2 (1 + 2k_2 \bar{\varepsilon}_2^2) \exp(k_2 \bar{\varepsilon}_2^2) \\
\bar{W}_{14} &= \frac{\partial^2 W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_1 \partial \bar{I}_4} = k_1 \kappa (1 - 3\kappa) (1 + 2k_2 \bar{\varepsilon}_1^2) \exp(k_2 \bar{\varepsilon}_1^2) \\
\bar{W}_{16} &= \frac{\partial^2 W_{\text{iso}}(\bar{I}_1, \bar{I}_4, \bar{I}_6)}{\partial \bar{I}_1 \partial \bar{I}_6} = k_1 \kappa (1 - 3\kappa) (1 + 2k_2 \bar{\varepsilon}_2^2) \exp(k_2 \bar{\varepsilon}_2^2) \\
\bar{W}_{41} &= \bar{W}_{14} \\
\bar{W}_{61} &= \bar{W}_{16}
\end{aligned} \quad (\text{A15})$$

Appendix 3. Analytical evaluation of stress using the model in the scenario of a planar biaxial test

Departing from Equation (23), the second Piola–Kirchhoff stress under experimentally measured deformation in the biaxial test can be calculated as:

$$\mathbf{S} = 2 \frac{\partial W(\mathbf{C}, \mathbf{M}, \mathbf{N}, J)}{\partial \mathbf{C}} = 2 \left(W_1 \frac{\partial I_1}{\partial \mathbf{C}} + W_4 \frac{\partial I_4}{\partial \mathbf{C}} + W_6 \frac{\partial I_6}{\partial \mathbf{C}} + W_J \frac{\partial J}{\partial \mathbf{C}} \right), \quad (\text{A16})$$

where

$$W_J = \frac{\partial W(\mathbf{C}, \mathbf{M}, \mathbf{N}, J)}{\partial J} = -p \quad (\text{A17})$$

We then can obtain

$$\mathbf{S} = 2 (W_1 \mathbf{I} + W_4 \mathbf{M} \otimes \mathbf{M} + W_6 \mathbf{N} \otimes \mathbf{N}) + W_J J \mathbf{C}^{-1} \quad (\text{A18})$$

Therefore,

$$\begin{aligned}\boldsymbol{\sigma} &= 2(W_1 \mathbf{b} + W_4 \mathbf{m} \otimes \mathbf{m} + W_6 \mathbf{n} \otimes \mathbf{n}) + W_J \mathbf{I}, \\ \text{or, } \sigma_{ij} &= 2(W_1 b_{ij} + W_4 m_i m_j + W_6 n_i n_j) + W_J \delta_{ij} \quad (\text{A19})\end{aligned}$$

Note that $\mathbf{m} = \mathbf{F}\mathbf{M}$ and $\mathbf{n} = \mathbf{F}\mathbf{N}$ are the images of $\mathbf{M}$ and $\mathbf{N}$ in the deformed configuration.

For planar biaxial tests, it resembles a plane stress problem for which it is stress-free in the direction normal to the 1–2 plane, thus,

$$\sigma_{33} = 2(W_1 b_{33} + W_4 m_3 m_3 + W_6 n_3 n_3) - p = 0 \quad (\text{A20})$$

Due to the fact that the deformation takes place in the 1–2 plane, m_3 and n_3 are zero. p , therefore, can be expressed as:

$$p = 2W_1 b_{33} \quad (\text{A21})$$

Therefore, the Cauchy stress components in the plane stress problem are:

$$\sigma_{ij} = 2(W_1 b_{ij} + W_4 m_i m_j + W_6 n_i n_j) - 2\delta_{ij} W_1 b_{33} \quad (\text{A22})$$

Figure 1. Curves of Cauchy stress vs. Green strain resulted from experiment (black dashed), analytical fitting (red dashed) and numerical simulation (blue solid).

Figure 2.

FE meshes used in the biaxial test simulation: red arrows denote the loading directions with their round roots showing the sites of loading, yellow box enclosed region represents the area delineated by the four markers in the biaxial test (a); Von Mises stress contour in the deformed configuration (b).

Figure 3. Relative error of the Jacobian approximation vs. logarithmic perturbation using different approximation scheme.

Figure 4. Iteration number (a) and CPU time (b) vs. logarithmic perturbation using different approximation scheme. Note: Dash lines represent the levels reached by analytical method.

Table 1
Fitted material parameters for the modified HGO model using equi-biaxial testing data.

c_{01}	c_{10} (KPa)	k_1 (KPa)	k_2	κ	α (degree)	β (degree)	r^2
14.87	1.16	4.48	62.20	0	23.38	88.66	0.994

Table 2

CPU time and iteration numbers taken by the two meshes using varying methods to calculate the tangent moduli—highlighted and underlined values are the percentage ratio of saved CPU time by approximation method compared with analytical method.

Mesh #	1 (with 99,330 DOFs)					2 (with 319,950 DOFs)				
	Iteration number	CPU time (s)	Total saved CPU time	CPU time per iteration (s)	Saved CPU time per iteration	Iteration number	CPU time (s)	Total saved CPU time	CPU time per iteration (s)	Saved CPU time per iteration
Forward Euler	90	1504.0	11%	16.7	12.1%	91	7485.7	7.3%	82.3	8.2%
Central difference	90	1596.9	5.5%	17.7	6.8%	91	7847.6	2.8%	86.2	3.9%
Analytical	89	1690.5	—	19.0	—	90	8074.1	—	89.7	—