Efficient integration of evolution equations for a fiber-like Maxwell body

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Abstract. Fiber-like Maxwell body is frequently used to model the mechanical behaviour of advanced composite materials, which appear in engineering and bio-mechanical applications. Here we consider a material model of the fiber-like Maxwell body based on the Sidoroff decomposition of the deformation gradient. In our case this decomposition yields a multiplicative split of the fiber stretch into inelastic and elastic parts. One of the advantages of the model is that various hyperelastic potentials can be employed for a greater accuracy. Three different potentials are analyzed in this paper: the classical Holzapfel potential and its modifications. The first modification accounts for a fiber slackness and the second one is intended for applications with a local fiber buckling. In terms of these three potentials, we analyze the performance of a universal iteration-free time-stepping scheme. Robustness and accuracy of this algorithm are tested. The iteration-free method is shown to compare favourably to the classical Euler-backward which includes the Newton iteration process.

1. Introduction

Fiber-based composites may exhibit a number of properties which are not available for classical monolithic materials. An accurate modelling of mechanical response of such materials subjected to large inelastic strains is a topic of ongoing research. The so-called iso-strain approach is frequently used in material modelling [1]. According to that approach, the overall stress response is a combination of individual responses of the matrix and fiber subjected to the same strain. Within a large-scale FEM analysis of applied problems a computational efficiency is a substantial issue. Large computational costs appear due to a big amount of calls of material subroutine on the Gauss-point level. Especially large number of calls appear when working with a dispersed arrangement of fibers (cf. [10]). In case of the globally explicit FEM, the Gauss-point integration may even take over most of the CPU-time. A substantial progress has been achieved dealing with the isotropic Maxwell models used to describe the matrix material. In particular highly efficient and robust algorithms are available for multiplicative inelasticity [5,6]. At the same time, Newton-like iterations are used for the numerical analysis of behaviour of fibers, which are time consuming [4]. Therefore, the current paper is focused on the efficient numerics for anisotropic models of fibers. We implement the material model of a fiber-like Maxwell body advocated in [7]. The hyperelastic properties of a single fiber are captured using three different potentials. The first potential was proposed by Holzapfel and co-workers in [3] and it is popular in engineering and bio-mechanics. Its modification was considered in [8,9] to account for fiber-slackness by assuming zero stresses for stretches below a certain threshold. Later another modification
was introduced by Tagiltsev et al. in [7] to account for fiber-matrix interaction under local compression involving fiber buckling. All three potentials are highly nonlinear and exhibit an exponential growth of stresses under tension. In order to simulate the evolution of the inelastic strain, a stiff ordinary differential equation needs to be integrated. Whereas the classical Euler-backward method requires a computationally expensive iterative process of Newton type, the newly proposed method is iteration free.

2. Fiber-like Maxwell body
In this section we consider a material model which was already advocated in [7]. Let $\hat{a}$ be a unit vector directed along the fiber in the reference configuration. Using it we introduce the structure tensor $M := \hat{a} \otimes \hat{a}$. The fiber stretch $\lambda$ can be computed as $\lambda = \sqrt{C : M}$, where $C$ is the right Cauchy-Green tensor. The model is based on the multiplicative decomposition of the deformation gradient tensor.\(^1\) This decomposition implies the following multiplicative split for the fiber stretch $\lambda$ into the inelastic stretch $\lambda_i$ and the elastic stretch $\lambda_e$:

$$\lambda = \lambda_i \lambda_e. \quad (1)$$

We assume that the Helmholtz free energy per unit mass is a function of $\lambda_e$:

$$\Psi_{fiber} = \Psi_{fiber}(\lambda_e^2). \quad (2)$$

It is convenient to introduce the following derivative

$$f := \frac{d \Psi_{fiber}(\lambda_e^2)}{d(\lambda_e^2)}. \quad (3)$$

Using the Coleman-Noll procedure the second Piola-Kirchhoff stress tensor $\tilde{T}$ can be evaluated as

$$\tilde{T} = \frac{2\rho_R f}{\lambda^2} P_C : M, \quad P_C : M = M - \frac{1}{3} \text{tr}(CM)C^{-1}, \quad (4)$$

where $\rho_R$ is the mass density in the reference configuration. As shown in [7], the evolution equation for the inelastic stretch takes the form

$$\frac{\dot{\lambda}_i}{\lambda_i} = \frac{1}{\eta} f \left( \frac{\lambda}{\lambda_i} \right)^2 \cdot \frac{\lambda^2}{\lambda_i^2} \rho_R, \quad (5)$$

where $\eta$ is the Newtonian viscosity. Here, for simplicity, we assume that $\eta$ is constant. In case of constant stretch $\lambda$ we can re-write this equation in the equivalent form:

$$\frac{\dot{\lambda}_e}{\lambda_e} = -\frac{\rho_R}{\eta} f(\lambda_e^2) \lambda_e^2. \quad (6)$$

This material model is thermodynamically consistent and objective. Note that a similar mathematical framework was recently considered for the fiber-like Maxwell material in [4]. Three different potentials are considered in this paper:

- Holzapfel potential (cf. [3]) is characterized by the following relations:

$$\Psi_{Holzapfel}(\lambda_e^2) = \frac{k_1}{2k_2} (e^{k_2(\lambda_e^2-1)^2} - 1), \quad f = 2k_1(\lambda_e^2 - 1)e^{k_2(\lambda_e^2-1)^2}, \quad (7)$$

where $k_1 \geq 0$ is the stiffness parameter; $k_2 > 0$ is a non-dimensional parameter attributed to the nonlinearity of the stress response under uniaxial tension.

\(^1\) An alternative approach to viscosity of fibers is based on convolution integrals [2].
• potential with fiber slackness (cf. [8,9]) is given by
\[ \Psi_{Holzapfel}^{\text{Holzapfel}}(\lambda_e^2) = \frac{t_3}{t_1^2} (e^{k_2(\lambda_e^2-k_3)^2} - 1), \]
\[ f_{Holzapfel}^{\text{Holzapfel}}(\lambda_e^2) = 2k_1(\lambda_e^2 - k_3 - 1)e^{k_2(\lambda_e^2-k_3)^2}, \] (8)
where \( \langle a \rangle := \max\{a, 0\} \); \( k_1 \) and \( k_2 \) are similar to the parameters of the Holzapfel potential; \( k_3 \geq 0 \) is the so-called slackness parameter. The stress vanishes for stretches below \( \sqrt{1+k_3}. \)

• potential with arctangent (cf. [7]) is defined by
\[ f_{arctan}(\lambda_e^2) = 2k_1(\lambda_e^2 - 1)e^{k_2(\lambda_e^2-1)^2} \frac{arctan(k(\lambda_e^2-1)+\pi/2)}{\pi}, \]
\[ \Psi_{arctan}(\lambda_e^2) = \int_0^{\lambda_e^2} f_{arctan}(\xi)d\xi. \] (9)
In this potential, \( k_3 \geq 0 \) is a fitting parameter used to adjust the critical compressive stress corresponding to the fiber buckling; \( k_1 \) and \( k_2 \) possess the same meaning as above. The potential \( \Psi_{arctan} \) converges to \( \Psi_{Holzapfel}^{\text{Holzapfel}} \) (with \( k_3 = 0 \) in (8)) shown above as \( k_3 \to \infty \) in (9).

3. Numerical integration of evolution equations
Evolution equations (5) and (6) are stiff. Therefore explicit time-stepping would yield poor results. In this section we discuss their implicit integration. Consider a typical time step
\[ t_n \to t_{n+1}, \Delta t = t_{n+1} - t_n > 0. \] Assume that \( n+1 \lambda \) and \( n \lambda_i \) are known. We need to update the inelastic stretch \( \lambda_i \) and to compute the current stress \( n+1 \mathbf{T}. \)

3.1. Euler-backward method for equation (5) combined with Newton iteration
The classical Euler-backward yields the following discretized version of the evolution equation (5):
\[ n+1 \lambda_i = n \lambda_i + \frac{\Delta t \rho R}{\eta} f^{n+1} \lambda^2 \bigg/ \bigg( \frac{n+1 \lambda^2}{n+1 \lambda_i^2} \bigg). \] (10)
This non-linear algebraic equation is solved using the Newton method with \( n \lambda_i \) as initial approximation for the unknown \( n+1 \lambda_i \). Numerical tests show that the Newton iteration process usually converges in approximately 6 iterations.

3.2. Iteration-free method for equation (6)
The integration within the time step is subdivided into two substeps: elastic predictor and inelastic corrector. Within the elastic predictor, we assume that \( \lambda \) changes instantly from \( n \lambda \) to \( n+1 \lambda \). This yields the following trial elastic stretch \( \lambda_e^{\text{trial}} = n+1 \lambda / n \lambda_i \). Next, within the inelastic corrector, the stretch is hold constant with \( \lambda = n+1 \lambda \) and the correct value of \( n+1 \lambda_e \) is computed using evolution equation (6) and the initial condition \( \lambda_e |t=t_n = \lambda_e^{\text{trial}} \). The discretized version of (6) takes the form
\[ n+1 \lambda_e = \lambda_e^{\text{trial}} - \frac{\Delta t \rho R}{\eta} f^{n+1} \lambda_e^2, \] (11)

The classical Newton method provides a computational procedure to evaluate the function \( n+1 \lambda_e = n+1 \lambda_e^{\text{trial}} \). The idea of the iteration-free method is to pre-compute the values of this function at a limited number of points and to use these results in subsequent computations.
Toward that end we assume that \( \lambda_e^{\text{trial}} \) remains in the interval \([0.1, 3]\). Following [7] we subdivide the interval into five subintervals: \([0.1, 0.5], [0.5, 1], [1, 1.5], [1.5, 2], [2, 3]\) and employ cubic spline to interpolate the \( n+1 \lambda_e (\lambda_e^{\text{trial}}) \) function between the mentioned key points. An example of such an interpolation is shown in Figure 1.
Implementing the pre-computed spline we obtain an approximate solution of (11): \( n^{+1}\lambda^e_{est} = \text{Spline(}\lambda^{trial}_e) \). Next, in order to reduce the error, we carry out a single Newton iteration which provides \( n^{+1}\lambda_e \). Note that this method requires only one Newton iteration and it can be used for any regular function \( f \).

4. Testing the algorithm for viscoelastic fiber models

Now let us demonstrate the applicability and efficiency of described method. The work started in [7] is being extended here and numerical simulations are carried out for three types of fiber potentials mentioned above: (7), (8), and (9). In numerical experiments a single fiber is subjected to a uniaxial isochoric strain-controlled non-monotonic loading. The deformation gradient tensor \( \mathbf{F} \) is set here by a prescribed stretch \( \lambda = l/l_0 \) as \( \mathbf{F} = \lambda \hat{\mathbf{a}} \otimes \hat{\mathbf{a}} + \lambda^{-1/2}(1 - \hat{\mathbf{a}} \otimes \hat{\mathbf{a}}) \), where \( \hat{\mathbf{a}} \) is the unit vector defining the fiber orientation in the reference configuration. Figure 2 shows the loading program for the logarithmic strain \( \varepsilon = \ln \lambda \). The employed material parameters for the
analyzed fiber potentials are given in Table 1.

Table 1. Set of material parameters of a single fiber used for accuracy testing

| Potential                                | $k_1$    | $k_2$    | $\eta$    | $k_3$    |
|------------------------------------------|----------|----------|------------|----------|
| Holzapfel potential (7)                  | 130.0 KPa| 0.5      | 5.0 KPa -s | -        |
| potential with fiber slackness (8)       | 130.0 KPa| 0.5      | 5.0 KPa -s | 0.21     |
| potential with arctangent (9)            | 130.0 KPa| 0.5      | 5.0 KPa -s | 50.0     |

The numerical solution obtained by the classical Euler backward method combined with the Newton iteration and extremely small time step size $\Delta t = 10^{-6}$ s is considered to be exact and denoted by $\sigma^{exact}$. The primary interest here is the axial stress $\sigma = T : (\bar{a} \otimes \bar{a})$, where $T$ stands for the true stress (here we benefit from $\bar{a}$ being an eigenvector of $F$). Stress histories obtained using the classical EBM and the iteration-free method with step size $\Delta t = 2^{-7}$ s for fiber potentials (7), (8), (9) are presented on the left-hand sides of Figures 3, 4, 5. Denoting numerical error as $\Delta \sigma := |\sigma^{exact} - \sigma^{numerical}|$ we can also present the deviation of the numerical solution from the exact solution. The deviation is shown for every simulation on the right-hand side of Figures 3, 4, 5.

As is seen from the figures, the errors for both methods are of the same order of magnitude. Although the potential with fiber slackness (8) exhibits a singularity at the threshold stretch, sufficiently accurate results still can be obtained. Figure 5 (right) indicates that for the potential with arctangent the numerical error of the new method can be slightly larger than the error of the classical method. This happens for states with $\lambda_e$ close to 1. The error can be explained by insufficient accuracy of the spline approximation used for the transition curve near $\lambda_e = 1$, see.
Figure 4. Simulation results for energy potential with fiber slackness (8). Left: computed stress history. Right: numerical error of two methods.

Figure 5. Simulation results for energy potential with arctangent (9). Left: computed stress history. Right: numerical error of two methods.
Figure 1. Obviously, the error can be reduced by taking a more accurate spline approximation.

5. Conclusion
New testing results for a series of hyperelastic potentials are presented. It is shown that for potentials with exponential growth stable and accurate numerical simulations are possible. Even for large time steps no convergence problems were detected when solving the non-linear equation using the standard Newton iteration. As expected, the Euler backward is unconditionally stable and first-order accurate. The recently proposed iteration-free algorithm inherits these advantages. At the same time the new method is more efficient due to its iteration-free nature. For simplicity, a Newtonian viscosity is considered here. As a generalisation one may introduce a stress-dependent viscosity: \( \eta = \eta(\sigma) \). This generalisation involving the non-Newtonian viscosity would allow us to capture a more broad class of phenomena like elasto-visco-plasticity. This will be brought forward in the follow-up publications. In conclusion, the iteration-free method is promising for modelling of a large-strain viscoelastic behaviour of fiber-reinforced composites, especially within a full-scale FEM.

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