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J. Eberhardsteiner

Application of Polyconvex Anisotropic Free Energies to Soft Tissues

J. Schröder*

Institut für Mechanik, Fachbereich 10
Universität Essen, 45117 Essen, Universitätsstr. 15, Germany
e-mail: j.schroeder@uni-essen.de

P. Neff

Fachbereich Mathematik
Technische Universität Darmstadt, 64289 Darmstadt, Schloßgartenstr. 7, Germany
e–mail: neff@mathematik.tu-darmstadt.de

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Abstract

In this talk we propose a framework for the three-dimensional modelling of biological soft tissues. For an overview of proposed models in the literature see e.g. HOLZAPFEL ET AL. [12] and the references therein. We discuss the construction of polyconvex, anisotropic free energy functions in an invariant setting. In order to guarantee the existence of solutions in large strain elasticity, the free energy function has to be quasiconvex. This condition is rather complicated to handle. Therefore, polyconvex functions which are always quasiconvex are usually considered, see BALL [1], DACOROGNA [5] and NEFF [10]. For isotropic materials, there exists a wide range of constitutive functions that satisfies the polyconvexity requirement, e.g. the Ogden type materials see CIARLET [4]. However, to the authors' knowledge, there does not exist a systematic treatment of anisotropic, polyconvex free energies in the literature. A variety of polyconvex transversely isotropic functions has been derived in SCHRÖDER & NEFF [14], [15]. The goal of the talk is the construction of constitutive functions for biological soft tissues in terms of the elements of a functional basis which automatically satisfy the polyconvexity condition. The functional basis consists of basic– and simultaneous invariants of the right Cauchy–Green tensor and a minimum set of structural tensors. For a general introduction to the invariant formulation of anisotropic constitutive equations with isotropic tensor functions see e.g. BOEHLER [3] and for specific model problems see e.g. SCHRÖDER [13]. After giving a general introduction we will focus on transverse isotropy, consider several model problems for biological soft tissues and present some numerical examples.

1 Introduction

In order to explain a variety of effects in physiology we require an accurate knowledge of the biological material behaviour on different scales: the nano-, ultra-, micro-, tissue-, and macro-scale, see e.g. MOW ET AL. [9]. The structural features on each level have an influence on the constitutive behaviour at the coarser scales. The body of interest consists of different phases like elastin, collagen, etc. In this context we can consider collagen as the basic structural element for soft tissues. The material behaviour of the collagen network in tension is characterized by a strongly nonlinear behaviour in fiber direction and by a much weaker stress-strain relation in the plane perpendicular to the fibers. Based on this observations soft tissues can be seen as transversely isotropic materials. The nonlinear tensile behaviour is often modelled by exponential type laws, see e.g. MOW ET AL. [9], FUNG [6], WEISS ET AL. [17], HOLZAPFEL & WEIZSÄCKER [11] and HOLZAPFEL ET AL. [12] and the references therein. For an overview in this field see also FUNG [6], and the references therein. In the following we concentrate on the nonlinear elasticity of soft tissues, thus we neglect any kind of history effects which is an intrinsic feature of biological materials. The main goal is the construction of a transversely isotropic, polyconvex free energy functions, see SCHRÖDER & NEFF [14], [15], which reflects the main characteristics of the soft tissues in tension.

2 Continuum Mechanics Preliminaries

The body of interest in the reference configuration is denoted with $\mathcal{B} \subset \mathbb{R}^3$, parametrized in $\mathbf{X}$ and the current configuration with $\mathcal{S} \subset \mathbb{R}^3$, parametrized in $\boldsymbol{x}$. The nonlinear deformation map $\boldsymbol{\varphi}_t : \mathcal{B} \to \mathcal{S}$ at time $t \in \mathbb{R}_+$ maps points $\boldsymbol{X} \in \mathcal{B}$ onto points $\boldsymbol{x} \in \mathcal{S}$. The deformation gradient $\boldsymbol{F}$ is defined by

$$\boldsymbol{F}(\boldsymbol{X}) := \nabla \boldsymbol{\varphi}_t(\boldsymbol{X}) \tag{1}$$

with the Jacobian $J(\boldsymbol{X}) := \det \boldsymbol{F}(\boldsymbol{X}) > 0$. The index notation of $\boldsymbol{F}$ is $F^a{}_A := \partial x^a / \partial X^A$. An important strain measure, the right Cauchy–Green tensor, is defined by

$$\boldsymbol{C} := \boldsymbol{F}^T \boldsymbol{F} \quad \text{with} \quad C_{AB} = F^a{}_A F^b{}_B g_{ab} \ , \tag{2}$$

where g_{ab} denotes the covariant metric tensor in the current configuration. The standard covariant metric tensor $\boldsymbol{G}$ within the Lagrange setting appears in the index representation G_{AB} and the contravariant metric tensor is denoted with $\boldsymbol{G}^{-1}$ with the index representation G^{AB}.
The principle of material frame indifference requires the invariance of the constitutive equation under superimposed rigid body motions onto the current configuration, Reduced constitutive equations which fulfill a priori this principle yield e.g. the functional dependence $\psi = \hat{\psi}(\boldsymbol{C}) = \hat{\psi}(\boldsymbol{C}(\boldsymbol{F}, \boldsymbol{g}))$. If we assume the free energy function to be a function of the right Cauchy–Green tensor $\hat{\psi}(\boldsymbol{C})$ we obtain the expression for the second Piola–Kirchhoff stresses

$$\boldsymbol{S} = 2\partial_C \hat{\psi}(\boldsymbol{C}) \ , \tag{3}$$

see e.g. MARSDEN & HUGHES [7]. Several restrictions on the form of the constitutive functions are required for anisotropic materials. Let $\mathcal{G}_{ti} \in \mathrm{SO}(3)$ be the material symmetry group for transversely isotropic material with respect to a local reference configuration. $\mathrm{SO}(3)$ denotes the special orthogonal group. The group $\mathcal{G}_{ti}$ is characterized by the unimodular tensors ${}^i\boldsymbol{Q} | i = 1, ...\infty$. The concept of material symmetry postulates the invariance condition

$$\hat{\psi}(\boldsymbol{F}\boldsymbol{Q}) = \hat{\psi}(\boldsymbol{F}) \quad \forall\, \boldsymbol{Q} \in \mathcal{G}_{ti}, \boldsymbol{F} \ . \tag{4}$$

In order to arrive at an isotropic tensor function representation for ψ we need an extension of the $\mathcal{G}_{ti}$-invariant function (4) to a function which is invariant under transformations of the special orthogonal group. This can be realized with the concept of structural tensors, in this context see e.g. the works of J.P. Boehler in 1978/1979. The material symmetry group $\mathcal{G}_{ti}$ can be represented by the structural tensor

$$\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a} \;, \tag{5}$$

where $\boldsymbol{a}$ is the preferred direction with $||\boldsymbol{a}|| = 1$. With (5) we arrive at the isotropic tensor function

$$\psi = \hat{\psi}(\boldsymbol{C}, \boldsymbol{M}) = \hat{\psi}(\boldsymbol{Q}^T \boldsymbol{C} \boldsymbol{Q}, \boldsymbol{Q}^T \boldsymbol{M} \boldsymbol{Q}) \;\; \forall \, \boldsymbol{Q} \;\in\; \mathrm{SO}(3) \;. \tag{6}$$

Thus we can express the functional dependence of ψ with respect to the argument tensors $(\boldsymbol{C}, \boldsymbol{M})$ in terms of the invariants

$$I_1 := \mathrm{tr}\,\boldsymbol{C}, \quad I_2 := \mathrm{tr}[\mathrm{Cof}\boldsymbol{C}], \quad I_3 := \mathrm{det}\boldsymbol{C}, \quad J_4 := \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}], \quad J_5 := \mathrm{tr}[\boldsymbol{C}^2 \boldsymbol{M}] \;, \tag{7}$$

i.e. $\psi = \hat{\psi}(I_1, I_2, I_3, J_4, J_5)$. The cofactor is defined for all invertible 3×3 tensors $\boldsymbol{C}$ as $\mathrm{Cof}(\boldsymbol{C}) = \det[\boldsymbol{C}]\boldsymbol{C}^{-T}$. In the following we focus on free energy functions which automatically satisfy the so-called polyconvexity condition.

3 Polyconvex Energies, Stresses and Moduli

We are interested in free energy functions ψ for transverse isotropy which a priori guarantee the existence of minimizers of some variational principles for finite deformations. In this framework the existence of minimizers is based on the concept of quasiconvexity, introduced by MORREY [8]. Quasiconvexity of a function ensures that the associated functional to be minimized is weakly lower semi-continuous and the rank one convexity of a function ensures that the Euler equations of the associated functional are elliptic, in this context see e.g. DACOROGNA [5] and SILHAVÝ [16]. The integral inequality condition of the quasiconvexity condition is rather complicated to handle. An important concept for pratical use is the so-called polyconvexity condition in the sense of BALL [2], [1], in this context see also CIARLET [4]. For isotropic material response functions there exist some models, e.g. the Ogden-type models, which satisfy this concept. For finite-valued, continuous functions we can recapitulate the important implications: i) a function ψ is convex if and only if ψ is polyconvex, ii) a function ψ is polyconvex if and only if ψ is quasiconvex, iii) a function ψ is quasiconvex if and only if ψ is rank one convex. Of course, the converse implications are not true.

Now we introduce $W \in C^2(\mathbb{M}^{3\times3}, \mathbb{R})$, a given scalar valued energy density. Here $\mathbb{M}^{3\times3}$ denotes the set of real 3×3 matrices and the adjugate of a matrix $\boldsymbol{F}$ is defined by $\mathrm{Adj}\boldsymbol{F} = \det[\boldsymbol{F}]\boldsymbol{F}^{-1} = \mathrm{Cof}(\boldsymbol{F})^T$.
Definition of Polyconvexity: $\boldsymbol{F} \mapsto W(\boldsymbol{F})$ is polyconvex if and only if there exists a function $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ (in general non-unique) such that

$$W(\boldsymbol{F}) = P(\boldsymbol{F}, \mathrm{Adj}\boldsymbol{F}, \det \boldsymbol{F})$$

and the function $\mathbb{R}^{19} \mapsto \mathbb{R},\; (\tilde{X}, \tilde{Y}, \tilde{Z}) \mapsto P(\tilde{X}, \tilde{Y}, \tilde{Z})$ is convex for all points $\boldsymbol{X} \in \mathbb{R}^3$.

In the above definition and in the following we drop the $\boldsymbol{X}$-dependence of the individual functions if there is no danger of confusion, i.e. we write $W \in C^2(\mathbb{M}^{3\times3}, \mathbb{R})$ instead of $W \in C^2(\mathbb{R}^3 \times \mathbb{M}^{3\times3}, \mathbb{R})$ and $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ instead of $P : \mathbb{R}^3 \times \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ in order to arrive at a more compact notation. In order to obtain various strain energy terms we assume an additively decoupled structure of ψ, i.e.

$$\psi = \sum_{j=1}^{n} \hat{\psi}_j(\boldsymbol{C}, \boldsymbol{M}) = \sum_{j=1}^{n} \hat{\psi}_j(I_1, I_2, I_3, J_4, J_5) \ , \tag{8}$$

where each term ψ_j for $j = 1, ..n$ has to fulfill the polyconvexity condition a priori. The stresses appear with applying the chain rule in the form

$$\boldsymbol{S} = 2 \sum_{j=1}^{n} \left\{ \frac{\partial \psi_j}{\partial I_1} \frac{\partial I_1}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial I_2} \frac{\partial I_2}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial I_3} \frac{\partial I_3}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial J_4} \frac{\partial J_4}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial J_5} \frac{\partial J_5}{\partial \boldsymbol{C}} \right\} . \tag{9}$$

With the derivatives of the invariants with respect to $\boldsymbol{C}$ and the identity

$$\text{tr}[\boldsymbol{C}^{-1}]\text{Cof}[\boldsymbol{C}] - \boldsymbol{C}^{-1}\text{Cof}[\boldsymbol{C}] = \text{tr}[\boldsymbol{C}]\boldsymbol{G}^{-1} - \boldsymbol{G}^{-1}\boldsymbol{C}\boldsymbol{G}^{-1} \ , \tag{10}$$

we arrive at the simplified expression

$$\boldsymbol{S} = 2 \textstyle\sum_{j=1}^{n} \left\{ \begin{array}{l} (\frac{\partial \psi_j}{\partial I_1} + \frac{\partial \psi_j}{\partial I_2} I_1)\boldsymbol{G}^{-1} - \frac{\partial \psi_j}{\partial I_2} \boldsymbol{G}^{-1}\boldsymbol{C}\boldsymbol{G}^{-1} + \frac{\partial \psi_j}{\partial I_3} \text{Cof}\boldsymbol{C} \\ \frac{\partial \psi_j}{\partial J_4} \boldsymbol{M} + \frac{\partial \psi_j}{\partial J_5} (\boldsymbol{C}\boldsymbol{M} + \boldsymbol{M}\boldsymbol{C}) \} \end{array} \right\} . \tag{11}$$

The tangent moduli are denoted in index-representation by $\mathbb{C}^{ABCD} := 2\partial_{C_{CD}} S^{AB}$, for details see SCHRÖDER & NEFF [14].

4 Transversely Isotropic Polyconvex Free Energy Functions

A three-dimensional constitutive model for transversely isotropic soft tissues for fully incompressible material behaviour has been proposed by WEISS ET AL. [17]. For their analysis they chose the function

$$\tilde{\psi}(I_1, I_2, I_3, J_4) = \beta_1(\frac{I_1}{I_3^{1/3}} - 3) + \beta_2(\frac{I_2}{I_3^{2/3}} - 3) + \beta_3(\exp[\frac{J_4}{I_3^{1/3}} - 1] - \frac{J_4}{I_3^{1/3}}) \ , \tag{12}$$

which is characterized by an exponential behaviour in fiber direction. In order to enforce fully incompressible behaviour they used the augmented Lagrangian method. The free energy (12) reflects the main characteristics of soft tissues in the physiological range very well. However, this function is not a priori polyconvex. For the following investigation we split the free energy ψ in an isotropic ψ^{iso} and an anisotropic part ψ^{ti}, i.e.

$$\hat{\psi}(I_1, I_2, I_3, J_4, J_5) = \hat{\psi}^{iso}(I_1, I_2, I_3) + \hat{\psi}^{ti}(I_1, I_2, I_3, J_4, J_5) \tag{13}$$

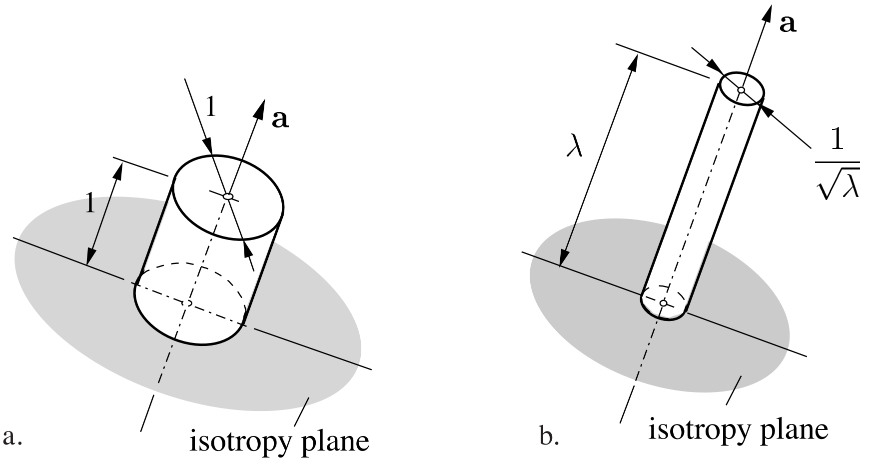
For the modelling of the isotropic part within a nearly incompressible formulation we choose the polyconvex function

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) + \alpha_4(I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2) \ . \tag{14}$$

The third and fouth term in (14) are introduced to penalize the volumetric deformation. For the transversely isotropic part we propose polynomial polyconcex invariants of the form

$$\alpha_6 ||\text{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2, \quad \alpha_7 \frac{||\boldsymbol{F}\boldsymbol{a}||^{2\alpha_8}}{(\det\boldsymbol{F})^{2/3}}, \quad \alpha_9 \{||\text{Cof}[\boldsymbol{F}]||^2 - ||\text{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2\}, \quad \alpha_{10} ||\boldsymbol{F}\boldsymbol{a}||^{2\alpha_{11}} \ . \tag{15}$$

Let us now consider the unimodular deformation of a cylinder with height and diameter equal one. The isochoric deformation is described by $\boldsymbol{F} = \mathrm{diag}[\lambda, 1/\sqrt{\lambda}, 1/\sqrt{\lambda}]$. A simple evaluation of the individual terms in (15) shows that $||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2$ is associated to the deformation of the cross section of the cylinder, $||\mathrm{Cof}[\boldsymbol{F}]||^2 - ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2$ is associated to the deformation of the generated surface and $||\boldsymbol{F}\boldsymbol{a}||^k$ to the stretch in $\boldsymbol{a}$-direction.



a. b.

Figure 1: Physical motivation of the polyconvex invariant functions (15) .

The individual functions (15) are now expressed in the elements of the functional basis, which leads to the explicit expression for the anisotropic part of the free energy

$$\psi^{ti} = \alpha_6(J_5 - I_1 J_4 + I_2) + \alpha_7 \frac{J_4^{\alpha_8}}{I_3^{1/3}} + \alpha_9(I_1 J_4 - J_5) + \alpha_{10} J_4^{\alpha_{11}} \; . \tag{16}$$

In contrast to the stresses appearing from (12) the stresses are generally not a priori zero if we use the proposed polyconvex functions. To enforce the condition of a stress free reference configuration, we have to evaluate (11) at the natural state. The natural state is characterized by $\boldsymbol{F} = \mathbf{1}$ and the invariants have the values

$$I_1 = 3, \quad I_2 = 3, \quad I_3 = 1, \quad J_4 = J_5 = \mathrm{tr}\boldsymbol{M} = 1 \; . \tag{17}$$

Consequently the stress condition for the natural state, i.e. $\boldsymbol{S}(\mathbf{1}) = \mathbf{0}$, leads to the equation

$$2 \sum_{j=1}^{n} \left\{ (\frac{\partial \psi_j}{\partial I_1} + 2\,\frac{\partial \psi_j}{\partial I_2} + \frac{\partial \psi_j}{\partial I_3})\mathbf{1} + (\frac{\partial \psi_j}{\partial J_4} + 2\frac{\partial \psi_j}{\partial J_5})\boldsymbol{M} \right\} = \mathbf{0} \; . \tag{18}$$

That states that two of the material parameters appering in (14) and (16) have to depend on the others, because the multipliers of the independent tensor generators $\mathbf{1}$ and $\boldsymbol{M}$ have to be zero. This leads to $\alpha_2 - \alpha_3 + \alpha_6 - \alpha_7/3 + \alpha_9 = 0$ and $-\alpha_6 + \alpha_7\alpha_8 + \alpha_9 + \alpha_{10}\alpha_{11} = 0$, respectively. These constrains are solved with respect to α_7 and α_6:

$$\left.\begin{array}{r} \alpha_7 = \dfrac{\alpha_3 - \alpha_2 - 2\alpha_9 - \alpha_{10}\alpha_{11}}{\alpha_8 - 1/3} \\ \alpha_6 = \dfrac{\alpha_3 - \alpha_2 - 2\alpha_9 - \alpha_{10}\alpha_{11}}{\alpha_8 - 1/3}\alpha_8 + \alpha_9 + \alpha_{10}\alpha_{11} \end{array}\right\} \; . \tag{19}$$

The dependent parameters α_7 and α_6 must be elements of $\mathbb{R}^+$, of course. The proof of the polyconvexity of the individual terms in (14) and (16) is given in SCHRÖDER & NEFF [14].

5 Numerical Examples

To verify that the proposed polyconvex free energy function is able to fit the characteristic behaviour of soft tissues we compare the stress response of our formulation with the one of WEISS ET AL. [17], based on (12), for two simple test problems.

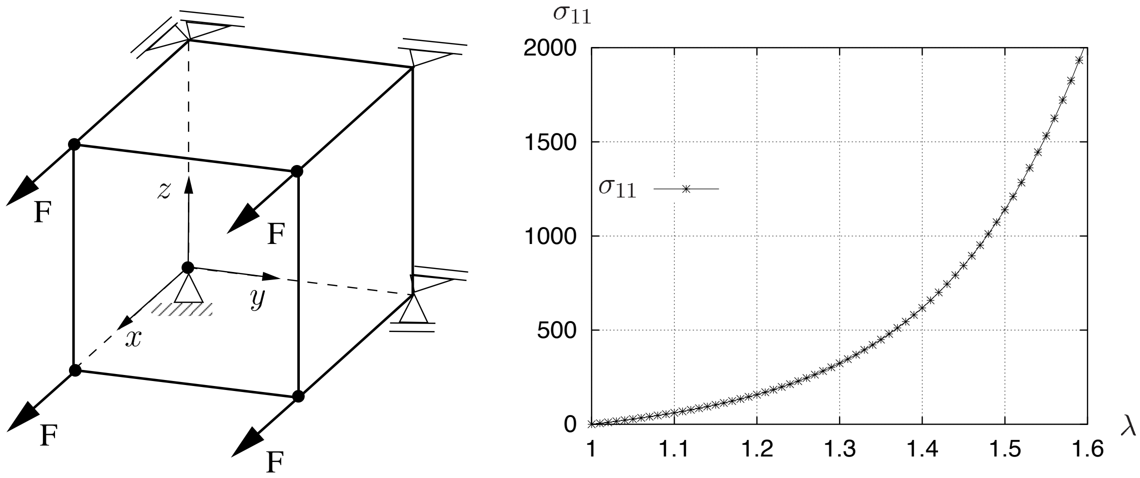


Figure 2: Unconstrained tension test: Cauchy stress σ_{11} versus stretch $\lambda := F_{11}$.

For the computations we set the prefered direction to $\boldsymbol{a} = (1,0,0)^T$. The material parameters for the isotropic part are set to

$$\alpha_1 = 10. \quad \alpha_2 = 1. \quad \alpha_3 = 30.5 \quad \alpha_4 = 10000. \,, \tag{20}$$

and for exponent of I_3 in the fourth term of (14) we choose the neutral element $\alpha_5 = 1$. The four independent parameters for the anisotropic part are

$$\alpha_8 = 5. \quad \alpha_9 = 1. \quad \alpha_{10} = 10. \quad \alpha_{11} = 2. \,. \tag{21}$$

Thus the dependent parameters are $\alpha_6 = 1.6071$ and $\alpha_7 = 29.0357$ and fulfill the condition $\alpha_6 > 0$ and $\alpha_7 > 0$.

As a first example we perform a simple tension test, where we stretch the element to 160% of its initial length, see Figure 2. It can be seen that the function models the nonlinear stress-strain behaviour in fiber direction, which is typical for a variety of soft tissues. The maximum variation from the incompressibility constraint $\det \boldsymbol{F} = 1$ is approximately 0.16%.

In the second example we consider a tension test, where the displacements in y-direction are hold fixed, see Figure 3. Here we have a similar characteristic for the stresses in fiber direction as in the previous example. The stress component σ_{22} is more or less linear and governed by a slight slope and the maximum variation from the incompressibility constraint is approximately 0.17%.

The above computation are compared with the formulation (12) with the parameters $\beta_1 = \beta_2 = 10.0$ and $\beta_3 = 100.0$, see WEISS ET AL. [17]. In contrast to their formulation we use a quasi-incompressible model by introducing a penalty term for the volumetric part similar to $(14)_{3,4}$ instead of an augmented Lagrangian formulation. The Cauchy-stress component σ_{11} for the simple tension test is plotted in Figure

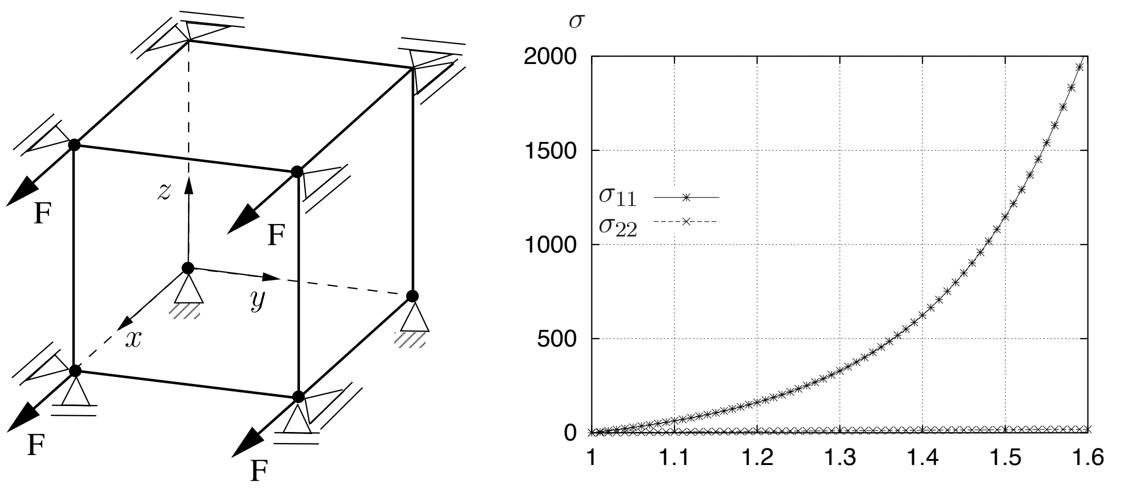


Figure 3: Constrained tension test: Cauchy stresses σ_{11} and σ_{22} versus stretch $\lambda := F_{11}$.

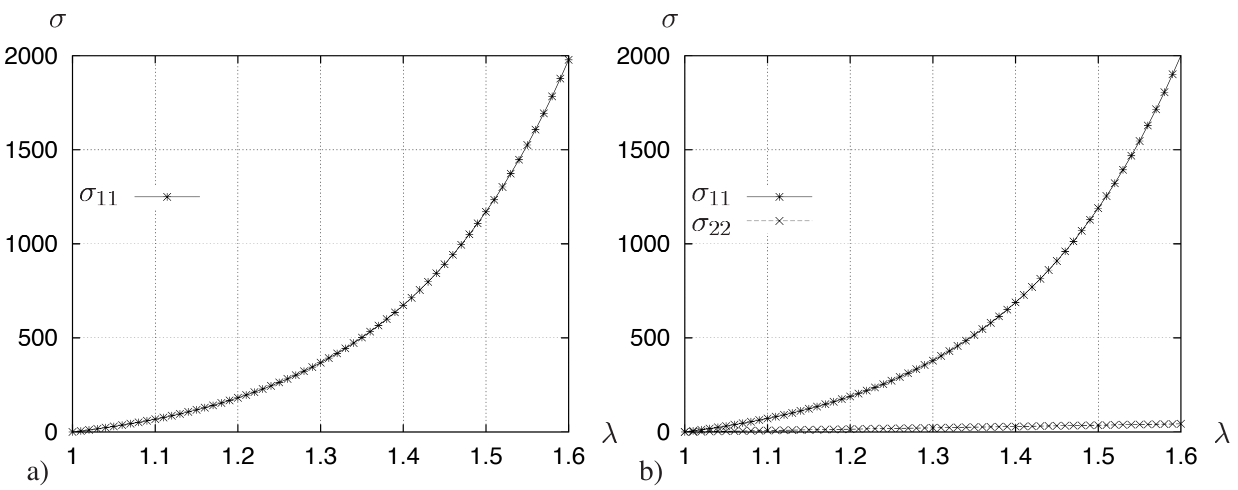


Figure 4: a) Unconstrained tension test: Cauchy stresses σ_{11} and b) constrained tension test: Cauchy stresses σ_{11} and σ_{22} versus stretch $\lambda := F_{11}$, respectively.

4a and the stress components σ_{11} and σ_{22} for the constrained tension test are depicted in Figure 4b. The variations from the incompressibility constraint are approximately 0.17% for both cases. A comparison of the results obtained with (13) and (12) shows that the characteristic behaviour of soft tissues in the physiological range can be modeled very well by polyconvex anisotropic free energy functions.

6 Conclusion

In this paper we have proposed a polyconvex transversely isotropic free energy for soft tissues based on [14], [15]. The obtained results have been compared with an exponential type transversely isotropic constitutive law given in [17]. For the considered examples we can conclude that the main characteristics of soft tissues in tension can be reproduced very well with the proposed model.

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