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Matrix decompositions in constitutive relations for continuous medium

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Title: Matrix decompositions in constitutive relations for continuous medium

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Abstract: We study the application of the QR decomposition in the theory of Green elastic solids with emphasis on transversely isotropic materials such as fiber-reinforced materials. We provide a methodology, how to use the QR decomposition to describe materials with general fiber orientation including curved fibers. We then focus on the so-called conjugate stress / strain basis model, and we show that for isotropic materials the model is equivalent to the standard model of Green elastic solid. We also provide a methodology, how to describe transversely isotropic materials using the QR decomposition. Next, we consider the popular standard reinforcing material model with spatially-varying fiber directions and fiber stiffnesses, and we perform numerical experiments in various geometries. To our best knowledge, our implementation is the first implementation of numerical solvers for QR based models with spatially-varying fiber directions. Finally, we compare the results for the conjugate stress / strain model with the results for the standard model of Green elasticity and linear elasticity.

Keywords: continuum mechanics, matrix decomposition, constitutive relations

Contents

Introduction

Elasticity and matrix decompositions

The most frequently studied response of continuous solid bodies is arguably the elastic response. The elastic response can be vaguely characterized as the ”ability of a deformed material body to return to its original shape and size when the forces causing the deformation are removed” (Bri [2022]).

The mathematical study of elastic response starts in 1660 by English polymath Robert Hooke (1635–1703) who formulated Hooke law for the one dimensional response of elastic solids. An important landmark in the research of the elastic solids is the discovery of Doyle-Ericksen formula, which effectively describes the fully three-dimensional response of elastic solids to finite deformations. The Doyle-Ericksen formula gives a relation between a thermodynamic potential (Helmholtz free energy), the deformation and the Cauchy stress tensor. The elastic solid materials wherein the stress is given as a derivative of a potential with respect to a deformation measure are referred to as the Green elastic solids or hyperelastic solids.

The description of material response is then fully encoded in the chosen formula for the potential. Traditionally, the potential is written as a function of the standard invariants of the left Cauchy–Green tensor, and the deformation gradient is traditionally decomposed using the polar decomposition. The polar decomposition splits the deformation gradient into an orthogonal matrix (rotation) and a symmetric positive definite matrix (stretch), hence it allows one to make the material response independent of rigid body rotations.

Some aspects of the traditional approach are however not convenient in practice. In particular, Criscione [2004] has shown that the use of principal matrix invariants is not optimal from the perspective of experimental analysis as it may lead to an experimental error propagation. Furthermore, the description of anisotropic materials with standard pseudo-invariants might be clumsy and inconvenient.

As an alternative to the standard polar decomposition of deformation gradient, one might also use other matrix decompositions such as the QR decomposition. The QR decomposition splits the deformation gradient into a product of an orthogonal matrix (rotation) and an upper-triangular matrix (stretch), and in continuum mechanics context it has been first investigated by McLellan [1976]. Recently the use of QR decomposition has been revisited by Srinivasa [2012], who has argued that the QR decomposition indeed addresses the aforementioned issues related to the use of standard polar decomposition.

In this thesis we study the applications of the QR decomposition in the elasticity and compare it with the standard theory of Green elastic solids and the linear elasticity. We focus on the model presented in Erel and Freed [2017], which uses the QR decomposition of the deformation gradient to model anisotropic planar materials (such as biological membranes). We study the equivalence of both approaches to Green elasticity and, in particular, we investigate the possibility of numerical solution of governing equations arising in material models based on the QR decomposition.

Thesis outline

The thesis is divided into four chapters. The first chapter provides an overview of both matrix decompositions as well as theirs physical interpretation.

The second chapter is devoted to the standard theory of Green elastic solids and linear elasticity. We introduce both theories and specify, how they describe transversely isotropic materials (e.g. fiber-reinforced materials). We also briefly discuss both problems mentioned above, i.e. the propagation of measurement errors and the description of anisotropic materials.

In the third chapter we finally focus on the QR decomposition. We provide a way how we can handle transversely isotropic materials with axis of symmetry, which is not straight. Then we study the conjugate stress / strain basis model presented in Erel and Freed [2017]. We show, that for isotropic materials, the model is equivalent to the standard model of Green elastic solid. Furthermore we show, how we can describe transversely isotropic materials in this framework.

The last chapter contains numerical experiments. We perform numerical computations with all three mentioned models (standard Green elasticity, linear elasticity and conjugate stress / strain basis model) and compare the results. All computations are performed with the so-called standard reinforcing material, which is a popular example of transversely isotropic material.

1. Matrix decompositions

QR decomposition can be used to solve systems of linear equations and it is a basis for QR algorithm, which is used to compute eigenvectors and eigenvalues of matrices. It is direct and important consequence of Gram-Schmidt process.

History of Gram-Schmidt process dates back to the 18th century to the French polymath Pierre-Simon Laplace (1749 - 1827) who used it on a least square problem. It was however the article *Zur Theorie der linearen und nichtlinearen Integralgleichungen* published in 1907 by German mathematician Erhard Schmidt (1876 - 1959) which popularized this orthonormalization technique. In the article, focused on study of integral equations, the author mentions that the technique was already used in paper *Über die entwickelung reeler funktionen in reihen mittelstder methode der kleinsten quadrate* published in 1883 by Danish actuary and mathematician Jørgen Pedersen Gram (1850 - 1916).[1] Nowadays Gram-Schmidt process is a part of standard curriculum of linear algebra courses.

This chapter introduces both polar and QR decompositions. We compare them and present a way, how we can interpret both decompositions.

1.1 Notation

In this section we define basic concepts and notation that we use (unless mentioned otherwise).

Real numbers are denoted as $\mathbb{R}$ and $\mathbb{R}^{m\times n}$ denotes a matrix with m rows and n columns. Scalars are marked with italic letters, vector with bold letters and tensors with double struck letters.

Transposition of a matrix $\mathbb{A}$ is denoted as $\mathbb{A}^\top$ and $\mathbb{A}^{-1}$ means an inverse matrix of $\mathbb{A}$ (assuming it exists). A transposed inverse matrix is marked as $\mathbb{A}^{-\top}$. Determinant of a square matrix $\mathbb{A}$ is denoted as $\det \mathbb{A}$, $\operatorname{Tr} \mathbb{A}$ denotes a trace of $\mathbb{A}$ and its cofactor is marked as $\operatorname{cof} \mathbb{A}$, which is defined as $\operatorname{cof} \mathbb{A} = (\det \mathbb{A})\mathbb{A}^{-\top}$. An identity matrix is denoted as $\mathbb{I}$ and zero matrix as $\mathbb{O}$.

An inner product of vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted as $\mathbf{a}\cdot\mathbf{b}$. Standard Euclidean norm of a vector is marked as $\|\mathbf{a}\|$. By tensor product of two vectors we mean $\mathbf{a}\otimes\mathbf{b} := \mathbf{a}\mathbf{b}^\top$. We use the following inner product on a space of matrices: $\mathbb{A} : \mathbb{B} = \operatorname{Tr}\left(\mathbb{A}^\top\mathbb{B}\right)$. This inner product leads directly to the Frobenius norm $\|\mathbb{A}\| := \sqrt{\operatorname{Tr}\,(\mathbb{A}^\top\mathbb{A})}$.

The symbol $\mathbf{u}$ means displacement, deformation gradient is denoted as $\mathbb{F}$, spatial velocity gradient as $\mathbb{L}$, left and right Cauchy-Green strain tensors as $\mathbb{B}$ and $\mathbb{C}$. Cauchy stress tensor is marked as $\mathbb{T}$, Kirchhoff stress tensor as $\mathbb{S}$ and first Piola-Kirchhoff stress tensor as $\mathbb{T}_R$.

Helmholtz free energy is marked as ψ, entropy as S, internal energy as U and work as W.

Density is denoted as ρ. Bulk modulus is denoted as K, P-wave modulus as M, Young modulus as E, Poisson ratio as ν, shear modulus as G and Lamé's parameter as λ.

[1]Informations taken from Leon et al. [2013].

The subscript R is used to denote quantities in the reference configuration, i.e. ρ_R means the density in the reference configuration.

We use the Einstein summation convention. That it, the repeated index in a single expression (that is not used elsewhere) implies summation over that index. We do not distinguish between the lower and upper indices of vectors and tensors.

Remark. In matrix analysis, orthogonal matrices are usually denoted by Q and upper triangular matrices by R. However in continuum mechanics R typically means a rotation, which is an orthogonal matrix, which causes a conflict in notation.

There are two ways how to solve this problem. One possibility is to denote the QR decomposition of the deformation gradient as $\mathbb{F} = \mathbb{Q}\widetilde{\mathbb{F}}$. This is used for example in Srinivasa [2012] or Erel and Freed [2017].

Another possibility is to denote the QR decomposition as $\mathbb{F} = \mathcal{RU}$. This is used for example in Freed et al. [2019], where the term "Laplace stretch" for the $\mathcal{U}$ was coined. In this work we use the this variant.

1.2 Polar decomposition

The polar decomposition is a useful tool in the continuum mechanics. It allows us to decompose the deformation gradient $\mathbb{F}$ to a rotation $\mathbb{R}$ and stretch $\mathbb{U}$. The matrix $\mathbb{R}$ is a unitary matrix with determinant equal to 1. This means that the matrix preserves volume and thus can be interpreted as a rotation. The matrix $\mathbb{U}$ is a symmetric positive definite matrix. Since $\mathbb{R}$ preserves a volume, any changes in the shape must be induced by the matrix $\mathbb{U}$. The polar decomposition thus allows us to "filter out" the rotation to get the stretch, which is most of the time of our interest.

Theorem 1 (Polar decomposition)**.** *Let* $\mathbb{A} \in \mathbb{R}^{n\times n}$ *be such that* $\det \mathbb{A} > 0$*. Then there exist unique symmetric positive definite matrices* $\mathbb{U}$ *and* $\mathbb{V}$ *and an orthogonal matrix* $\mathbb{R}$*,* $\det \mathbb{R} = 1$ *such that*

$$\mathbb{A} = \mathbb{R}\mathbb{U},$$
$$\mathbb{A} = \mathbb{V}\mathbb{R}.$$

Proof. Let $\widetilde{\mathbb{V}}\widetilde{\mathbb{D}}\widetilde{\mathbb{U}}$ be the singular value decomposition of $\mathbb{A}$. Then $\widetilde{\mathbb{V}}$ and $\widetilde{\mathbb{U}}$ are orthogonal matrices and $\widetilde{\mathbb{D}}$ is a diagonal matrix with positive elements on the main diagonal. We can then define $\mathbb{U}, \mathbb{V}$ and $\mathbb{R}$ in the following way:

$$\mathbb{U} = \widetilde{\mathbb{U}}^\top \widetilde{\mathbb{D}}\widetilde{\mathbb{U}},$$
$$\mathbb{V} = \widetilde{\mathbb{V}}\widetilde{\mathbb{D}}\widetilde{\mathbb{V}}^\top,$$
$$\mathbb{R} = \widetilde{\mathbb{V}}\widetilde{\mathbb{U}}.$$

Then $\mathbb{A} = \mathbb{R}\mathbb{U} = \mathbb{V}\mathbb{R}$, $\mathbb{U}$ and $\mathbb{V}$ are symmetric and positive definite (because $\widetilde{\mathbb{D}}$ has positive elements on its diagonal) and $\mathbb{R}$ is a proper orthogonal matrix, because $\det \mathbb{A} = \det \mathbb{R} \det \mathbb{U}$ and $\det \mathbb{A}, \det \mathbb{U} > 0$, which implies that $\det \mathbb{R} = 1$.

The only thing that remains to show is the uniqueness. It is sufficient to prove the uniqueness of $\mathbb{U}$ and $\mathbb{V}$, because we then can set $\mathbb{R}$ to be equal to $\mathbb{A}\mathbb{U}^{-1}$. Let $\mathbb{R}\mathbb{U}$ and $\mathbb{R}'\mathbb{U}'$ be two distinct polar decompositions of $\mathbb{A}$. Then $\mathbb{A}^\top\mathbb{A} = \mathbb{U}^\top\mathbb{U} = \mathbb{U}^2 = \mathbb{U}'^\top\mathbb{U}' = \mathbb{U}'^2$. Since $\mathbb{U}$ and $\mathbb{U}'$ are positive definite, we can write $\mathbb{U} = \sqrt{\mathbb{A}^\top\mathbb{A}}$

and $\mathbb{U}' = \sqrt{\mathbb{A}^\top \mathbb{A}}$. However the square root of a positive definite matrix is unique, which implies $\mathbb{U} = \mathbb{U}'$. The uniqueness of $\mathbb{V}$ can be shown in a similar way. $\square$

In the continuum mechanics setting, the polar decomposition is closely related to the left and right Cauchy strain tensors $\mathbb{B}$ and $\mathbb{C}$:

$$\mathbb{B} = \mathbb{F}\mathbb{F}^\top = \mathbb{V}\mathbb{R}\left(\mathbb{V}\mathbb{R}\right)^\top = \mathbb{V}\mathbb{V}^\top = \mathbb{V}^2,$$
$$\mathbb{C} = \mathbb{F}^\top\mathbb{F} = \left(\mathbb{R}\mathbb{U}\right)^\top \mathbb{R}\mathbb{U} = \mathbb{U}^\top\mathbb{U} = \mathbb{U}^2.$$

An advantage of the polar decomposition is that once we know it in one basis, it is easy to compute in another basis. Let $\mathbb{Q}$ be an orthogonal matrix. Then the polar decomposition of a matrix $\mathbb{F}' = \mathbb{Q}\mathbb{F}\mathbb{Q}^\top$ has the following form:

$$\mathbb{F}' = \mathbb{Q}\mathbb{R}\mathbb{U}\mathbb{Q}^\top = \mathbb{Q}\mathbb{R}\mathbb{Q}^\top\mathbb{Q}\mathbb{U}\mathbb{Q}^\top = \mathbb{R}'\mathbb{U}'.$$

1.3 QR decomposition

The polar decomposition is not the only way how we can decompose the deformation gradient into a rotation and a strain, as we can use the QR decomposition. The QR decomposition factors a matrix to a product of an orthogonal matrix and an upper triangular matrix. Thus using the QR decomposition we can decompose the deformation gradient $\mathbb{F}$ to the rotation $\mathcal{R}$ and the stretch $\mathcal{U}$, which is sometimes called the Laplace stretch.

One advantage of using the QR decomposition instead of the polar decomposition, is that the Laplace stretch $\mathcal{U}$ is nothing else than Cholesky factorization of a right Cauchy-Green strain tensor $\mathbb{C}$:

$$\mathbb{C} = \mathbb{F}^\top\mathbb{F} = (\mathcal{R}\mathcal{U})^\top\mathcal{R}\mathcal{U} = \mathcal{U}^\top\mathcal{U}. \tag{1.1}$$

Contrary to the polar decomposition, it is not easy to transform the QR decomposition into another basis.

1.3.1 Gram-Schmidt process

The QR decomposition is nothing else than an application of the Gram-Schmidt process on a matrix. The process is a method, how to orthonormalize a set of vectors. It takes a finite and linearly independent set of vectors and returns a set of vectors, that are mutually orthonormal and span the same space as the vectors before the orthonormalization.

If $\mathbf{u}_1, \ldots, \mathbf{u}_n$ are linearly independent vectors, then the Gram-Schmidt process can be written in the following way:

1. $\mathbf{v}_1 = \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|}$,
2. $\mathbf{w}_k = \mathbf{u}_k - \sum_{i=1}^{k-1} \left(\mathbf{u}_k \cdot \mathbf{v}_i\right) \mathbf{v}_i \qquad k = 1, \ldots, n$,
3. $\mathbf{v}_k = \frac{\mathbf{w}_k}{\|\mathbf{w}_k\|}$.

The vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ are the resulting orthonormal vectors.

Theorem 2 (QR decomposition)**.** *Let $\mathbb{A} \in \mathbb{R}^{n\times n}$ be an invertible matrix. Then there exist an orthogonal matrix $\mathbb{Q}$ and an upper triangular matrix $\mathbb{R}$ with positive elements on its diagonal, such that $\mathbb{A} = \mathbb{Q}\mathbb{R}$. These matrices are unique.*

Proof. Let us denote column vectors of the matrix $\mathbb{A}$ by $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Now we can use the Gram-Schmidt process to get the orthonormal vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ and unnormalized orthogonal vectors $\mathbf{w}_1, \ldots, \mathbf{w}_n$. Then we can write

$$\mathbf{u}_k = \mathbf{v}_1 \cdot \mathbf{u}_k \mathbf{v}_1 + \ldots + \mathbf{v}_{k-1} \cdot \mathbf{u}_k \mathbf{v}_{k-1} + \|\mathbf{w}_k\| \mathbf{v}_k.$$

This can be written in a matrix in the following way:

$$(\mathbf{u}_1|\ldots|\mathbf{u}_n) = (\mathbf{v}_1|\ldots|\mathbf{v}_n)\begin{pmatrix} \|\mathbf{w}_1\| & \mathbf{v}_1\cdot\mathbf{u}_2 & \ldots & \mathbf{v}_1\cdot\mathbf{u}_n \\ 0 & \|\mathbf{w}_2\| & \ldots & \mathbf{v}_2\cdot\mathbf{u}_n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \|\mathbf{w}_n\| \end{pmatrix}.$$

It remains to prove the uniqueness. Let $\mathbb{A} = \mathbb{Q}\mathbb{R} = \mathbb{Q}'\mathbb{R}'$ be two distinct QR decompositions of the matrix $\mathbb{A}$. Then $\mathbb{Q}^\top\mathbb{Q}' = \mathbb{R}\mathbb{R}'^{-1} =: \mathbb{B}$. This matrix is orthogonal and upper triangular. This implies that $B_{11} = 1$ and $B_{k1} = 0, k = 2, \ldots, n$. Due to the orthonormality of the column vectors, we see that $B_{21} = 0$. But also $B_{k2} = 0, k = 3, \ldots, n$. This means that $B_{22} = 1$, because the upper triangular matrices $\mathbb{R}$ and $\mathbb{R}'$ (and therefore also $\mathbb{B}$) have positive elements on the diagonal (this can be seen from the construction). Using an induction and the same reasoning, we conclude that $\mathbb{B} = \mathbb{I}$. ☐

1.3.2 QR decomposition in two dimensions

The case of two dimensions is trivial enough that the analytic formulas for the QR decomposition of the deformation gradient have a very simple form:

$$\mathbb{F} = \mathcal{R}\mathcal{U}, \tag{1.2a}$$

$$\mathcal{R} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{1.2b}$$

$$\mathcal{U} = \begin{pmatrix} a & a\gamma \\ 0 & b \end{pmatrix}, \tag{1.2c}$$

where

$$\sin\theta = \frac{-F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}}, \tag{1.3a}$$

$$\cos\theta = \frac{F_{11}}{\sqrt{F_{11}^2 + F_{21}^2}}, \tag{1.3b}$$

$$a = \sqrt{F_{11}^2 + F_{21}^2}, \tag{1.3c}$$

$$b = \frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}}, \tag{1.3d}$$

$$\gamma = \frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2}. \tag{1.3e}$$

Since $\mathcal{U}$ is by (1.1) also Cholesky factorization of $\mathbb{C}$, we can also write its elements in terms of elements of $\mathbb{C}$:

$$\begin{aligned} a &= \sqrt{C_{11}}, \\ \gamma &= \frac{C_{12}}{C_{11}}, \\ b &= \sqrt{C_{22} - \frac{C_{12}^2}{C_{11}}}. \end{aligned}$$

Because $\mathcal{U}$ is upper triangular matrix, it is easy to compute its inverse (which is also upper triangular) and the right Cauchy-Green strain tensor $\mathbb{C}$:

$$\mathcal{U}^{-1} = \begin{pmatrix} \frac{1}{a} & -\frac{\gamma}{b} \\ 0 & \frac{1}{b} \end{pmatrix}, \tag{1.4}$$

$$\mathbb{C} = \mathcal{U}^\top \mathcal{U} = \begin{pmatrix} a^2 & a^2\gamma \\ a^2\gamma & a^2\gamma^2 + b^2 \end{pmatrix}. \tag{1.5}$$

Principal invariants[2] of $\mathbb{C}$ can be expressed in terms of elements of Laplace stretch $\mathcal{U}$:

$$I_1(\mathbb{C}) = \operatorname{Tr}\mathbb{C} = \operatorname{Tr}\left(\mathcal{U}^\top\mathcal{U}\right) = a^2\left(1+\gamma^2\right) + b^2, \tag{1.6a}$$

$$I_3(\mathbb{C}) = \det\mathbb{C} = \det\left(\mathcal{U}^\top\mathcal{U}\right) = a^2b^2. \tag{1.6b}$$

1.4 Geometrical interpretation of polar and QR decompositions

Both matrix decompositions serve the similar manner. That is, to decompose the deformation gradient into the rotation and the strain, as both decompositions results in product of the orthogonal matrix and either symmetric positive definite or upper triangular matrix. Thus we would expect that we can physically interpret them in a similar way. The orthogonal matrices $\mathbb{R}$ and $\mathcal{R}$ can of course be interpreted as rotations, as they both preserve volume.

The interpretation of $\mathbb{U}$ (or $\mathbb{V}$) and $\mathcal{U}$ is a little bit more complicated. We provide the interpretation only in three dimensions, as the case of two dimensions is analogous.

1.4.1 Polar decomposition

To interpret the polar decomposition of the deformation gradient, we have to perform the diagonalization of $\mathbb{U}$ (or $\mathbb{V}$). Let $\mathbb{Q}^\top\mathbb{D}\mathbb{Q}$ be the diagonalization of $\mathbb{U}$. Since $\mathbb{U}$ is symmetric positive definite, the matrix $\mathbb{Q}$ is orthogonal and all eigenvalues of $\mathbb{U}$ (elements on the diagonal of $\mathbb{D}$) are positive. Thus we can interpret $\mathbb{U}$ as performing a rotation $\mathbb{Q}$, then performing a stretch $\mathbb{D}$ and then finally performing a rotation $\mathbb{Q}^\top$. The matrix $\mathbb{V}$ can be interpreted in the similar way.

[2] for precise definition of principal invariants see Definition 1

1.4.2 QR decomposition

To interpret the Laplace stretch $\mathcal{U}$, we have to decompose it into a product of the following three matrices:

$$\mathcal{U} = \begin{pmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 1 & 0 & \beta \\ 0 & 1 & \alpha \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} =: \Lambda \mathcal{U}^{\alpha\beta} \mathcal{U}^{\gamma}.$$

Denoting the standard Cartesian basis as $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$, we can see, that the Laplace stretch $\mathcal{U}$ first performs a simple shear in the $\mathbf{e}_1 - \mathbf{e}_3$ plane by $\gamma\mathbf{e}_1$, then a shear in the $\mathbf{e}_1 - \mathbf{e}_2$ plane by $\beta\mathbf{e}_1 + \alpha\mathbf{e}_2$ and finally a stretch in all three directions. This is shown in the Figure 1.1.

Remark. Sometimes a convention $\mathcal{U} = \begin{pmatrix} a & \gamma & \beta \\ 0 & b & \alpha \\ 0 & 0 & c \end{pmatrix}$ is used. This can be seen for example in Paul and Freed [2020].

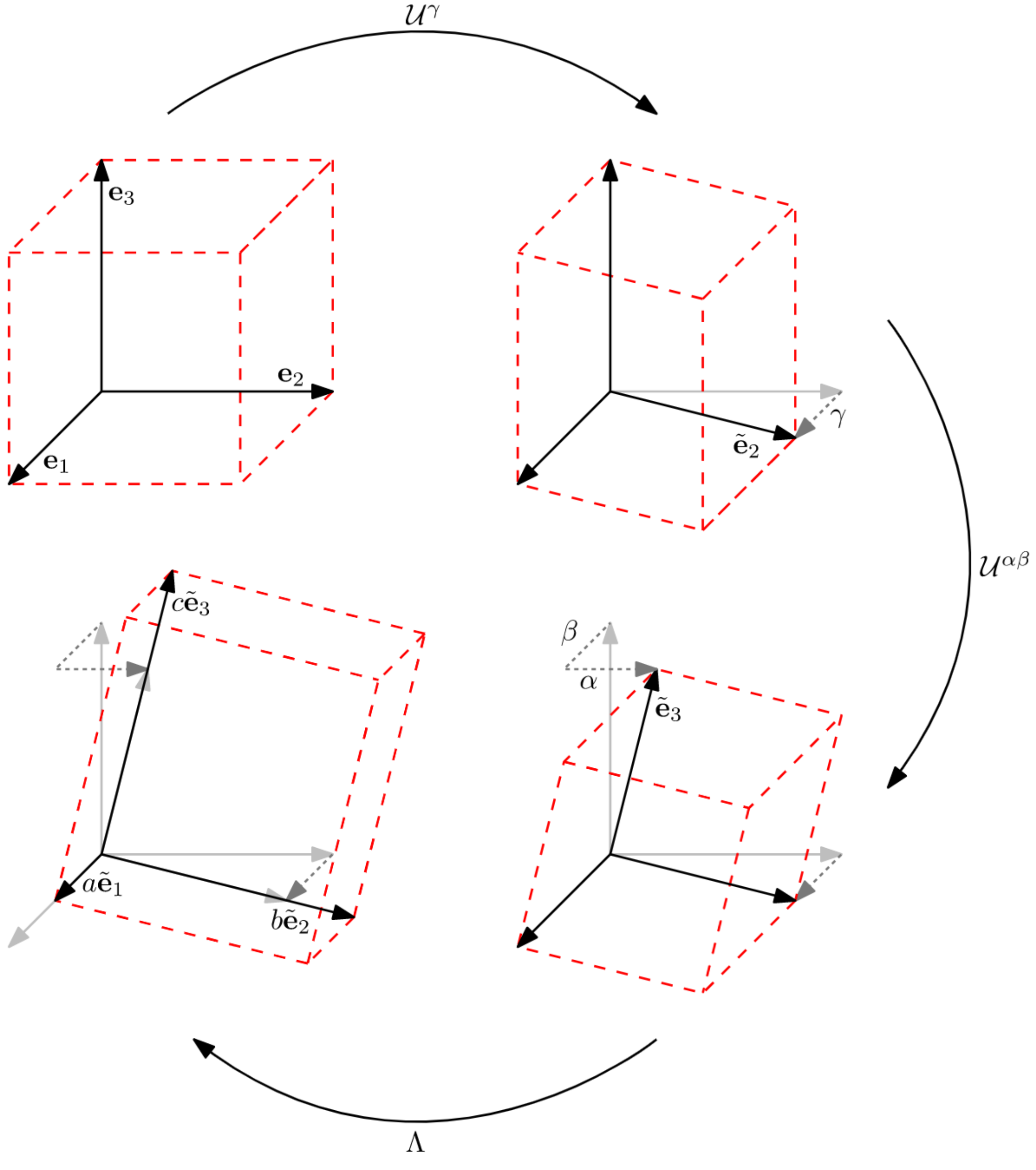


Figure 1.1: Interpretation of the Laplace stretch $\mathcal{U}$. First, two shears are applied and then a stretch in all three directions.

2. Standard theory of elasticity

In what follows we mostly focus on transversely isotropic materials, which are symmetric about an axis that is normal to the plane of isotropy. A typical example of such material is a material that is reinforced by fibers. These materials are composed of fibers and matrix material, in which the fibers are present. We assume that at each point there is a matrix material and a fiber (which is infinitely thin) at the same time. The fibers are assumed to be aligned in along a family of curves, which may not consist of straight lines.

We start by describing the theory of principal matrix invariants including the representation theorems. Some basic technical results, such as formulae for the derivatives of invariants with respect to the matrix, can be found in Appendix A.

Then we proceed with the theory of Green elastic solids. We summarize the theory for isotropic materials and we also introduce the model of fiber-reinforced materials presented in Spencer [1972]. Then we proceed with the theory of linear elasticity. We derive formulas for general anisotropic, transversely isotropic and fully isotropic material in two dimensions.

The end of this chapter is devoted to analysis of problems of the standard theory. Namely the propagation of measurement errors and the description of anisotropic materials. We discuss these problems and mention, how the QR decomposition can solve then.

2.1 Principal matrix invariants

Some quantities (for example energy) should not depend on observer. In other words, if two different people look at the same object at the same time, they should observe the same thing. Therefore we look for some quantity that is preserved even when we change the basis. We cannot simply take elements of a matrix, because they depend on a choice of basis. There are many of these quantities that satisfy out requirements, but the most important are the so-called principal invariants.

Definition 1 (Principal invariants)**.** *Let $\mathbb{A} \in \mathbb{R}^{3\times 3}$ be a matrix. We define the principal invariants I_1, I_2 and I_3 of $\mathbb{A}$ in the following way:*

$$\begin{aligned} I_1(\mathbb{A}) &= \operatorname{Tr} \mathbb{A}, \\ I_2(\mathbb{A}) &= \frac{1}{2}\left[(\operatorname{Tr} \mathbb{A})^2 - \operatorname{Tr}\left(\mathbb{A}^2\right)\right] = \operatorname{Tr}\left(\operatorname{cof} \mathbb{A}\right), \\ I_3(\mathbb{A}) &= \det \mathbb{A}. \end{aligned}$$

These invariants satisfy our requirements, because $I_i\left(\mathbb{Q}\mathbb{A}\mathbb{Q}^\top\right) = I_i(\mathbb{A})$ for any orthogonal matrix $\mathbb{Q}$, thanks to the cyclic property of trace and the fact, that $\det(\mathbb{A}\mathbb{B}) = \det \mathbb{A} \det \mathbb{B}$.

The notion of matrix invariants directly leads to a definition of an isotropic function, which formalizes the reasoning done at the beginning of this section.

Definition 2 (Isotropic function)**.** *Let $\varphi\colon \mathbb{R}^{3\times 3} \to \mathbb{R}$ be a scalar function of a tensor variable. The function φ is called isotropic, if and only if $\varphi(\mathbb{Q}\mathbb{A}\mathbb{Q}^\top) = \varphi(\mathbb{A})$ holds for every matrix $\mathbb{A} \in \mathbb{R}^{3\times 3}$ and every proper orthogonal matrix $\mathbb{Q} \in \mathbb{R}^{3\times 3}$.*

A tensor function of a tensor variable $f\colon \mathbb{R}^{3\times3} \to \mathbb{R}^{3\times3}$ is called isotropic, if and only if $f(\mathbb{Q}\mathbb{A}\mathbb{Q}^\top) = \mathbb{Q}f(\mathbb{A})\mathbb{Q}^\top$ holds for every matrix $\mathbb{A} \in \mathbb{R}^{3\times3}$ and every proper orthogonal matrix $\mathbb{Q} \in \mathbb{R}^{3\times3}$.

It is important to know, how we can represent isotropic function. The following theorem answers this question.

Theorem 3 (Representation of isotropic functions)**.** *A scalar function of a tensor variable $\varphi\colon \mathbb{A} \in \mathbb{R}^{3\times3}_{sym} \to \mathbb{R}$, where $\mathbb{A}$ is a symmetric matrix, is isotropic if and only if it can be expressed as a function of the principal invariants of $\mathbb{A}$.*

A tensor function of a tensor variable $f\colon \mathbb{A} \in \mathbb{R}^{3\times3}_{sym} \mapsto \mathbb{B} \in \mathbb{R}^{3\times3}_{sym}$, where $\mathbb{A}$ and $\mathbb{B}$ are symmetric matrices, is isotropic if and only if it has a representation of the following form:

$$f(\mathbb{A}) = \varphi_0\mathbb{I} + \varphi_1\mathbb{A} + \varphi_2\mathbb{A}^2,$$

where $\{\varphi_i\}_{i=0}^3$ are scalar functions of the principal invariants of $\mathbb{A}$.

Proof. The proof for the first part can be found for example in Truesdell and Noll [2004]. The proof for the second part can be found in Rivlin and Ericksen [1997] and Spencer [1971]. □

Remark. In case of two dimensions, only two invariants are sufficient, as the third invariant can be expressed as a function of the other invariants. Furthermore if f is an isotropic tensor function, then it has a form $f = \varphi_0\mathbb{I} + \varphi_1\mathbb{A}$, as the term with $\mathbb{A}^2$ can be expressed using Caley-Hamilton theorem in terms of $\mathbb{I}$ and $\mathbb{A}$.

There is a nontrivial relation between the principal invariants of a diagonalizable matrix and its eigenvalues. Let $\mathbb{A}$ be a 3 by 3 diagonalizable matrix and denote by λ_1, λ_2 and λ_3 its eigenvalues. If we denote $\mathbb{U}^{-1}\mathbb{D}\mathbb{U}$ the diagonalization of $\mathbb{A}$ and use the cyclic property of a trace and the fact, that $\det(\mathbb{A}\mathbb{B}) = \det\mathbb{A}\det\mathbb{B}$, then we get

$$\begin{aligned}
I_1(\mathbb{A}) &= \mathrm{Tr}\,(\mathbb{U}^{-1}\mathbb{D}\mathbb{U}) = \mathrm{Tr}\,(\mathbb{D}) = \lambda_1 + \lambda_2 + \lambda_3,\\
I_3(\mathbb{A}) &= \det\left(\mathbb{U}^{-1}\mathbb{D}\mathbb{U}\right) = \det\mathbb{D} = \lambda_1\lambda_2\lambda_3,\\
I_2(\mathbb{A}) &= \mathrm{Tr}\,\mathrm{cof}\,\left(\mathbb{U}^{-1}\mathbb{D}\mathbb{U}\right) = \mathrm{Tr}\,\left[\det\mathbb{D}\left(\mathbb{U}^{-1}\mathbb{D}\mathbb{U}\right)^{-\top}\right] = \mathrm{Tr}\,\left[\mathbb{U}^\top\left(\det\mathbb{D}\mathbb{D}^{-1}\right)\mathbb{U}^{-\top}\right]\\
&= \mathrm{Tr}\,\left(\det\mathbb{D}\mathbb{D}^{-1}\right) = \lambda_2\lambda_3 + \lambda_1\lambda_3 + \lambda_1\lambda_2.
\end{aligned}$$

Unsurprisingly, there is a connection to a characteristic polynomial of a matrix.

$$\begin{aligned}
\det(\mathbb{A} - \mu\mathbb{I}) &= \det\left(\mathbb{U}^{-1}\mathbb{D}\mathbb{U} - \mu\mathbb{U}^{-1}\mathbb{U}\right) = \det\mathbb{U}^{-1}\det\left(\mathbb{D} - \mu\mathbb{I}\right)\det\mathbb{U}\\
&= -\sum_{i=1}^{3}(\mu - \lambda_i) = -\mu^3 + (\lambda_1 + \lambda_2 + \lambda_3)\,\mu^2\\
&\quad - (\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1)\,\mu + \lambda_1\lambda_2\lambda_3\\
&= -\,\mu^3 + (\mathrm{Tr}\,\mathbb{A})\mu^2 - (\mathrm{Tr}\,\mathrm{cof}\,\mathbb{A})\mu + \det\mathbb{A}
\end{aligned}$$

We see, that we can easily switch from the description in terms of invariants to the description in terms of eigenvalues. This however does not mean that both descriptions are equally suitable, because one form can be much simpler than the another.

2.2 Green elastic solid

Green elastic material is a material that does not produce entropy in mechanical processes. Therefore it is a model of ideal elastic behavior. Common examples include rubber or biological tissues. It is well known, that the formula for Cauchy stress tensor of the Green elastic solid, known as Doyle-Ericksen formula, can be written in the following way:[1]

$$\mathbb{T} = \frac{2\rho_R}{\sqrt{\det \mathbb{B}}} \frac{\partial \psi(\mathbb{B})}{\partial \mathbb{B}} \mathbb{B}, \tag{2.1}$$

where ρ_R is density in the reference configuration, $\mathbb{B} = \mathbb{F}\mathbb{F}^\top$ is left Cauchy-Green tensor and ψ is Helmholtz free energy depending on $\mathbb{B}$.

The free energy describes how the material stores energy. Therefore if the solid is isotropic, then the free energy also should be isotropic. Thus ψ is an isotropic function and, using Representation Theorem 3, it can be written as a function of invariants: $\psi(\mathbb{B}) = \psi\left(I_1(\mathbb{B}), I_2(\mathbb{B}), I_3(\mathbb{B})\right)$. Using the chain rule we get

$$\mathbb{T} = \frac{2\rho_R}{\sqrt{\det \mathbb{B}}} \left(\frac{\partial \psi}{\partial I_1} \frac{\partial I_1}{\partial \mathbb{B}} + \frac{\partial \psi}{\partial I_2} \frac{\partial I_2}{\partial \mathbb{B}} + \frac{\partial \psi}{\partial I_3} \frac{\partial I_3}{\partial \mathbb{B}} \right) \mathbb{B}$$

Now we can use Theorem A.1 to obtain

$$\begin{aligned}
\mathbb{T} &= \frac{2\rho_R}{\sqrt{\det \mathbb{B}}} \left(\frac{\partial \psi}{\partial I_1} \mathbb{I} + \frac{\partial \psi}{\partial I_2} ((\operatorname{Tr} \mathbb{B})\mathbb{I} - \mathbb{B}) + \frac{\partial \psi}{\partial I_3} (\det \mathbb{B}) \mathbb{B}^{-1} \right) \mathbb{B} \\
&= \frac{2\rho_R}{\sqrt{\det \mathbb{B}}} \left(\frac{\partial \psi}{\partial I_1} \mathbb{B} + \frac{\partial \psi}{\partial I_2} ((\operatorname{Tr} \mathbb{B})\mathbb{B} - \mathbb{B}^2) + \frac{\partial \psi}{\partial I_3} (\det \mathbb{B}) \mathbb{I} \right) \\
&= \frac{2\rho_R}{\sqrt{\det \mathbb{B}}} \left[\frac{\partial \psi}{\partial I_3} \det(\mathbb{B}) \mathbb{I} + \left(\frac{\partial \psi}{\partial I_1} + \frac{\partial \psi}{\partial I_2} \operatorname{Tr} \mathbb{B} \right) \mathbb{B} - \frac{\partial \psi}{\partial I_2} \mathbb{B}^2 \right].
\end{aligned}$$

Thus we see, that the Cauchy stress tensor is also an isotropic function. An alternative variant, where $\mathbb{B}^2$ is, using the Cayley-Hamilton theorem, expressed in terms of $\mathbb{I}, \mathbb{B}, \mathbb{B}^{-1}$, can also be used.

Sometimes it is useful to assume, that ψ depends on the right Cauchy-Green strain tensor $\mathbb{C} = \mathbb{F}^\top \mathbb{F}$ instead of $\mathbb{B}$. This assumption leads to the following form:

$$\mathbb{T} = \frac{2\rho_R}{\sqrt{\det \mathbb{C}}} \mathbb{F} \frac{\partial \psi(\mathbb{C})}{\partial \mathbb{C}} \mathbb{F}^\top.$$

This is equivalent to the previous formula (2.1), because $I_i(\mathbb{C}) = I_i(\mathbb{B}), i = 1, 2, 3$ and

$$\begin{aligned}
\mathbb{F}\mathbb{I}\mathbb{F}^\top &= \mathbb{B}, \\
\mathbb{F}\mathbb{C}\mathbb{F}^\top &= \mathbb{F}\mathbb{F}^\top\mathbb{F}\mathbb{F}^\top = \mathbb{B}^2, \\
\mathbb{F}\mathbb{C}^{-1}\mathbb{F}^\top &= \mathbb{F}\mathbb{F}^{-1}\mathbb{F}^{\top}\mathbb{F}^{-\top} = \mathbb{I}.
\end{aligned}$$

[1]For derivation see e.g. Gurtin et al. [2010].

2.2.1 Requirements on free energy

There are several requirements on the free energy. First, imagine that we stretch out material to infinity. Then the energy stored in the material should also be infinite. Thus we require $\psi \to \infty$ as $\det \mathbb{F} \to \infty$.

Now consider a situation, in which we compress the material into a single point. Then the stored energy also should be infinite. Therefore we require that $\psi \to \infty$ as $\det \mathbb{F} \to 0^+$.

2.3 Spencer's model of fiber-reinforced material

In the previous section, we have discussed a theory of isotropic Green elastic solid. In this section we expand this theory to allow fiber-reinforced materials. An extensive theory of fiber-reinforced materials can be found in Spencer [1972]. Basic overview can also be found in Holzapfel [2000].

To introduce fibers into our material, we have to know their direction. This fiber direction is defined by a unit vector $\mathbf{A}$ in reference configuration, which is at each point tangent to the direction of fibers.

Helmholtz free energy ψ of isotropic material depends only on invariants I_1, I_2 and I_3. In case of fiber-reinforced materials, the free energy must depend also on some other expressions, which depends on the fiber direction. Spencer [1972] introduced the so-called pseudo-invariants I_4 and I_5 on which ψ also depends:

$$I_4(\mathbb{C}, \mathbf{A}) = \mathbf{A} \cdot \mathbb{C}\mathbf{A}, \tag{2.2a}$$

$$I_5(\mathbb{C}, \mathbf{A}) = \mathbf{A} \cdot \mathbb{C}^2\mathbf{A}. \tag{2.2b}$$

The pseudo-invariant I_4 is equal to the square of stretch $\lambda = \|\mathbb{F}\mathbf{A}\|$ in the fiber direction $\mathbf{A}$.

$$\mathbf{A} \cdot \mathbb{C}\mathbf{A} = \mathbb{F}\mathbf{A} \cdot \mathbb{F}\mathbf{A} = \lambda^2.$$

Now, with the help of Theorem A.2, we can write the formula for the Cauchy stress tensor:

$$\begin{aligned}
\mathbb{T} &= \frac{2\rho_R}{\sqrt{\det \mathbb{C}}} \mathbb{F} \frac{\partial \psi(\mathbb{C})}{\partial \mathbb{C}} \mathbb{F}^\top \\
&= \frac{2\rho_R}{\sqrt{\det \mathbb{C}}} \mathbb{F} \left(\frac{\partial \psi}{\partial I_1}\frac{\partial I_1}{\partial \mathbb{C}} + \frac{\partial \psi}{\partial I_2}\frac{\partial I_2}{\partial \mathbb{C}} + \frac{\partial \psi}{\partial I_3}\frac{\partial I_3}{\partial \mathbb{C}} + \frac{\partial \psi}{\partial I_4}\frac{\partial I_4}{\partial \mathbb{C}} + \frac{\partial \psi}{\partial I_5}\frac{\partial I_5}{\partial \mathbb{C}} \right) \mathbb{F}^\top \\
&= \frac{2\rho_R}{\sqrt{\det \mathbb{C}}} \left[\frac{\partial \psi}{\partial I_3} \det(\mathbb{C})\mathbb{I} + \left(\frac{\partial \psi}{\partial I_1} + \frac{\partial \psi}{\partial I_2} \operatorname{Tr} \mathbb{C} \right) \mathbb{B} - \frac{\partial \psi}{\partial I_2} \mathbb{B}^2 \right. \\
&\quad \left. + \frac{\partial \psi}{\partial I_4} \mathbf{A} \otimes \mathbf{A} + \frac{\partial \psi}{\partial I_5} \left(\mathbf{A} \otimes \mathbb{C}\mathbf{A} + \mathbb{C}\mathbf{A} \otimes \mathbf{A} \right) \right].
\end{aligned} \tag{2.3}$$

2.4 Linear elasticity

Equations, that are used mechanics of solids, are highly nonlinear, which means, that they are difficult to solve. However if the strain is small, we can use simplified theory called linear elasticity. The idea is to linearise the equations with respect to some small quantity. For small strains an appropriate choice is displacement, thus we assume, that the norm of displacement $\mathbf{u}$ is small:

$$\|\nabla \mathbf{u}\| \ll 1.$$

Since the deformation gradient $\mathbb{F}$ can also be computed as

$$\mathbb{F} = \mathbb{I} + \nabla \mathbf{u},$$

we see, that $\mathbb{F}$ is close to identity.

Using the gradient of displacement, we can define the linearized strain tensor (also called infinitesimal strain tensor or small strain tensor) as

$$\mathbb{e} = \frac{1}{2}\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top\right).$$

From the definition we see, that $\mathbb{e}$ is symmetric.

For the rest of the thesis, we focus for simplicity only on two dimensional problems. Therefore we only provide the description of the linear elasticity only in two dimensions. The case of three dimensions is however analogous.

2.4.1 Elasticity tensor

We are looking for a linear constitutive equation, that would allow us to compute stress from strain and vice versa. In linear elasticity we do not distinguish between Cauchy, Kirchhoff or first Piola-Kirchhoff stress tensors, since the reference and current configurations are almost the same. There is just one stress tensor, which we will denote by $\mathbb{T}$, that is symmetric.

When it comes to the stress-strain relation, a great place to start is Hooke's law. It can be generalized to

$$\tau_{ij} = C_{ijkl}\epsilon_{kl} \qquad i, j = 1, 2, \tag{2.4}$$

where C_{ijkl} are elements of a fourth-order tensor with 16 independent elements called elasticity tensor.

From (2.4) we see, that the elasticity tensor C_{ijkl} must be symmetric in indices i and j and also in indices k and l, because both $\mathbb{T}$ and $\mathbb{e}$ are symmetric. This reduces the number of independent elements to 9. Furthermore the elasticity tensor must be symmetric with respect to index pairs ij and kl, since the $\mathbb{T}$ is the derivative of the free energy: $\tau_{ij} = \frac{\partial \rho\psi}{\partial \epsilon_{ij}}$. This further reduces the number of independent elements to 6.

To represent the tensor, we can use Voigt notation, which is used to represent a symmetric tensor by reducing its order. In our case we can write the elasticity tensor as a 3×3 matrix $c_{\alpha\beta}$, where $\alpha = i$, if $i = j$ and $\alpha = 3$, if $i \neq j$. The same way for β. (We use Greek letters and small letter c to distinguish between indices of the elasticity matrix from indices of the fourth-order elasticity tensor.) We obtain

$$\begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{12} & c_{22} & c_{23} \\ c_{13} & c_{23} & c_{33} \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{pmatrix}.$$

This is the most general form with no symmetry. If the material possesses some symmetries, then there other restriction on the elasticity matrix $c_{\alpha\beta}$.

Remark. Sometimes an inverted relation with the compliance matrix $d_{\alpha\beta}$ is used.

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & d_{13} \\ d_{12} & d_{22} & d_{23} \\ d_{13} & d_{23} & d_{33} \end{pmatrix} \begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix}.$$

2.4.2 Transversely isotropic material

The elasticity tensor C_{ijkl} transforms by the rule

$$C'_{ijkl} = a_{im}a_{jn}a_{kr}a_{ls}C_{mnrs} \qquad i,j,k,l = 1,2, \tag{2.5}$$

where a_{ij} are elements of an orthogonal transformation. If the material possesses some kind of symmetry, then $C'_{ijkl} = C_{ijkl}$ for this symmetry. This puts additional constrains on the elasticity matrix $c_{\alpha\beta}$.

Now suppose that the material si transversely isotropic and assume, that the axis of symmetry in the $(1,0)^\top$ direction. In our case we expect, that if we reflect the stress and strain tensors along the axis of symmetry, we obtain the same tensors. Thus they should be invariant with respect to the reflection $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Using (2.5) we see, that we only have to consider elements of C_{ijkl} with odd number of ones. Therefore

$$\begin{aligned} C'_{1112} &= -C_{1112} &&\Longrightarrow C_{1112} = c_{13} = 0, \\ C'_{2221} &= -C_{2221} &&\Longrightarrow C_{2221} = c_{23} = 0, \end{aligned}$$

We see, that the stress - strain relation has the following form:

$$\begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & 0 \\ c_{12} & c_{22} & 0 \\ 0 & 0 & c_{33} \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{pmatrix}. \tag{2.6}$$

Remark. We would obtain the same result, if we used $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ as the transformation matrix.

2.4.3 Isotropic materials

In the case of fully isotropic material, it has to hold $C'_{ijkl} = C_{ijkl}$ not only for reflection, but also for arbitrary rotation $\begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}$.

We start from the equation (2.6), since it already has some restrictions. Using the transformation rule (2.5) yields

$$\begin{aligned} C'_{1111} = c'_{11} = c_{11} =& c_{11}\cos^4\varphi + c_{22}\sin^4\varphi + c_{12}\sin^2\varphi\cos^2\varphi \\ &+ c_{21}\sin^2\varphi\cos^2\varphi + 4c_{33}\sin^2\varphi\cos^2\varphi, \\ C'_{2222} = c'_{22} = c_{22} =& c_{11}\sin^4\varphi + c_{22}\cos^4\varphi + c_{12}\sin^2\varphi\cos^2\varphi \\ &+ c_{21}\sin^2\varphi\cos^2\varphi + 4c_{33}\sin^2\varphi\cos^2\varphi, \\ C'_{1122} = c'_{12} = c_{12} =& c_{11}\sin^2\varphi\cos^2\varphi + c_{22}\sin^2\varphi\cos^2\varphi + c_{12}\cos^4\varphi \\ &+ c_{21}\sin^4\varphi - 4c_{33}\sin^2\varphi\cos^2\varphi, \\ C'_{1212} = c'_{33} = c_{33} =& c_{11}\sin^2\varphi\cos^2\varphi + c_{22}\sin^2\varphi\cos^2\varphi \\ &- c_{12}\sin^2\varphi\cos^2\varphi - c_{21}\sin^2\varphi\cos^2\varphi + 4c_{33}\cos^4\varphi. \end{aligned}$$

Adding equations for c_{12} and c_{11} gives

$$\begin{aligned} c_{11}+c_{12} &= c_{11}\cos^4\varphi + c_{22}\sin^4\varphi + c_{12}\sin^2\varphi\cos^2\varphi + c_{12}\sin^2\varphi\cos^2\varphi \\ &\quad + 4c_{33}\sin^2\cos^2\varphi + c_{11}\sin^2\varphi\cos^2\varphi + c_{22}\sin^2\varphi\cos^2\varphi + c_{12}\cos^4\varphi \\ &\quad + c_{12}\sin^4\varphi - 4c_{33}\sin^2\cos^2\varphi \\ &= c_{11}\cos^2\varphi + c_{22}\sin^2\varphi + c_{12} \\ c_{11} &= c_{11}\cos^2\varphi + c_{22}\sin^2\varphi = c_{11}(1-\sin^2\varphi) + c_{22}\sin^2\varphi. \end{aligned}$$

This implies that $c_{11} = c_{22}$.

Finally, subtracting the equation for c_{12} from the equation for c_{11} yields

$$\begin{aligned} c_{11}-c_{12} &= c_{11}\cos^4\varphi + c_{11}\sin^4\varphi + c_{12}\sin^2\varphi\cos^2\varphi + c_{12}\sin^2\varphi\cos^2\varphi \\ &\quad + 4c_{33}\sin^2\cos^2\varphi - c_{11}\sin^2\varphi\cos^2\varphi - c_{11}\sin^2\varphi\cos^2\varphi - c_{12}\cos^4\varphi \\ &\quad - c_{12}\sin^4\varphi + 4c_{33}\sin^2\cos^2\varphi \\ &= c_{11}(\sin^2\varphi - \cos^2\varphi)^2 - c_{12}(\sin^2\varphi-\cos^2\varphi)^2 + 8c_{33}\sin^2\varphi\cos^2\varphi \\ &= c_{11}\cos^2(2\varphi) - c_{12}\cos^2(2\varphi) + 2c_{33}\sin^2(2\varphi) \\ &= (c_{11}-c_{12})(1-\sin^2(2\varphi)) + 2c_{33}\sin^2(2\varphi). \end{aligned}$$

Thus $c_{11} - c_{12} = 2c_{33}$.

Setting $c_{33} = G$ and $c_{12} = \lambda$ gives the following relation:

$$\begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} = \begin{pmatrix} \lambda+2G & \lambda & 0 \\ \lambda & \lambda+2G & 0 \\ 0 & 0 & G \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{pmatrix},$$

which can also be written as

$$\mathbb{T} = \lambda\,(\operatorname{Tr}\mathbb{E})\,\mathbb{I} + 2G\mathbb{E}.$$

This well-known formula can be found for example in Gurtin et al. [2010].

2.5 Potential problems of the standard theory of Green elastic solids

The final section of this chapter is devoted to the discussion of potential problems of the standard theory of Green elastic solids.

2.5.1 Propagation of measurement errors

The first problem, that may occur it the propagation of measurement errors. We can define the covariance of two tensors by

$$R_C(\mathbb{A},\mathbb{B}) = \frac{\|\mathbb{A}:\mathbb{B}\|}{\|\mathbb{A}\|\|\mathbb{B}\|}.$$

Using the Cauchy-Schwartz inequality we see, that

$$\begin{aligned} &R_C(\mathbb{A},\mathbb{B}) \in [0,1], \\ &R_C(\mathbb{A},\mathbb{B}) = 0 \iff \|\mathbb{A}:\mathbb{B}\| = 0 \iff \text{the tensors are mutually orthogonal}, \\ &R_C(\mathbb{A},\mathbb{B}) = 1 \iff \exists c\colon \mathbb{A} = c\mathbb{B} \iff \text{the tensors are linearly dependent}. \end{aligned}$$

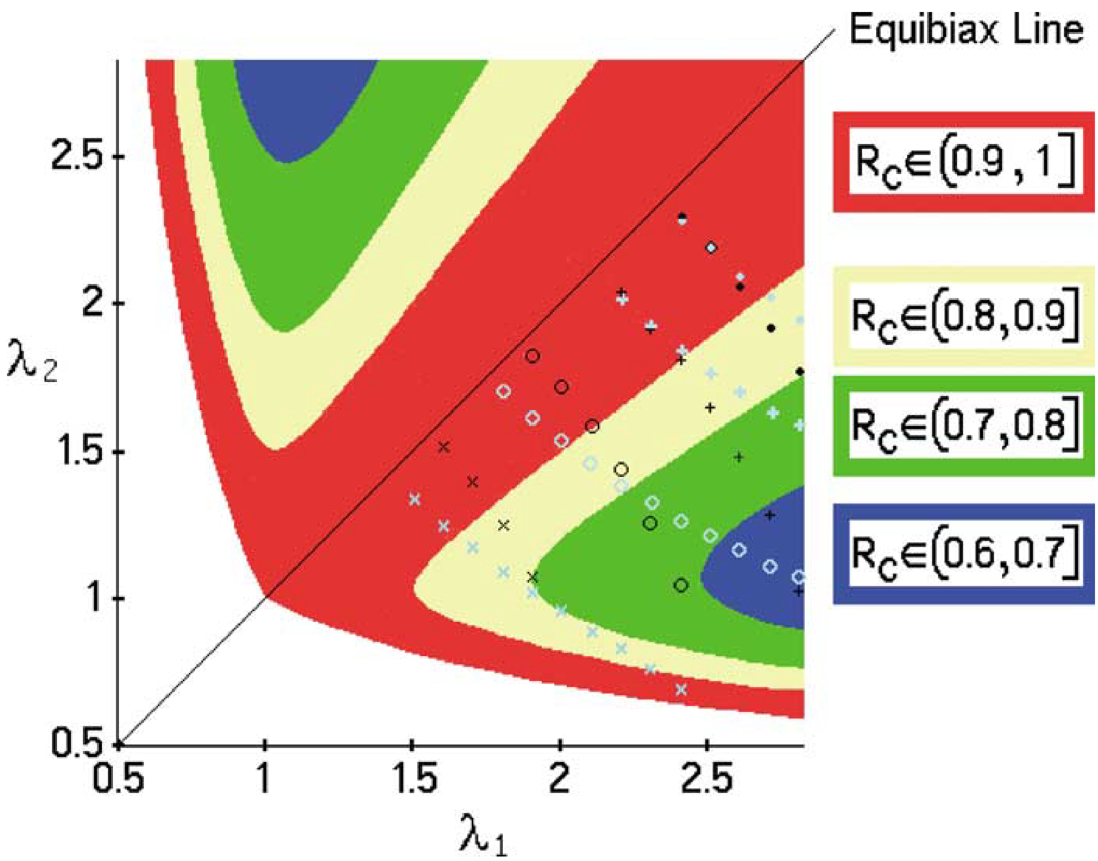


Figure 2.1: A covariance of response terms I_1 and I_2 for a biaxial stretch. λ_1 and λ_2 are stretch ratios. Figure taken from Criscione [2004].

The covariance thus measures, how much mutually orthogonal the tensors $\mathbb{A}$ and $\mathbb{B}$ are.

Now we can consider a general constitutive law of the form

$$\mathbb{T} = -q\mathbb{I} + \alpha_1\mathbb{A}_1 + \alpha_2\mathbb{A}_2,$$

where $\mathbb{T}$ is a Cauchy stress tensor, $\mathbb{A}_1$ and $\mathbb{A}_2$ are symmetric and deviatoric tensors. Criscione [2004] has shown, that the error in stress measurements is magnified by a factor

$$\left[1 - R_C\left(\mathbb{A}_1, \mathbb{A}_2\right)^2\right]^{-1/2}.$$

Thus if the tensors $\mathbb{A}_1$ and $\mathbb{A}_2$ are close to being linearly dependent, then the measurement error will be greatly magnified.

In Figure 2.1 we can see a covariance of the I_1 and I_2 response terms for a biaxial stretch of an incompressible sheet with a constitutive material law of the following form:

$$\mathbb{T} = -p\mathbb{I} + 2\frac{\partial \rho\psi}{\partial I_1}\mathbb{B} - 2\frac{\partial \rho\psi}{\partial I_2}\mathbb{B}^{-1},$$

where $\psi = \psi(I_1, I_2)$. As we can see, the magnification of measurement errors is significant.

Srinivasa [2012] has shown, that the use of the QR decomposition does not suffer from this problem and thus may be better from the experimental point of view.

2.5.2 Description of anisotropic materials

The second potential problem is the description of the anisotropic materials. The Spencer's model of transversely isotropic material described in Section 2.3 might feel clumsy, as it requires to define the fiber direction vector $\mathbf{A}$, which is rather artificial.

This is however not the case of the QR decomposition based approach, because, as Srinivasa [2012] has shown, the material anisotropy reduces to the parity of the Helmholtz free energy ψ. The introduction of the vector $\mathbf{A}$ is not necessary.

Orthotropy

Let us consider orthotropic material. Orthotropic materials are materials with three planes of symmetry wich are mutually orthogonal. If we assume a coordinate system such that its basis vectors are orthogonal to the planes of symmetry, then the free energy has the following form:

$$\psi = \psi_o \left(a, b, c, \alpha^2, \beta^2, \gamma^2, \alpha\beta\gamma\right),$$

or, if ψ is analytic in the last invariant,

$$\psi = \psi_{o1} \left(a, b, c, \alpha^2, \beta^2, \gamma^2\right) + \psi_{o2} \left(a, b, c, \alpha^2, \beta^2, \gamma^2\right) \alpha\beta\gamma.$$

Transverse isotropy

In the case of the transversely isotropic material symmetric about an x_3 axis, the free energy can be written as

$$\psi = \psi_T \left(\frac{\log a + \log b}{2}, \frac{\log a - \log b}{2}, \log c, \beta^2 + \gamma^2, \beta^2 - \gamma^2\right).$$

For more details see Srinivasa [2012].

3. Green elasticity based on the QR decomposition

This chapter is devoted to the application of the QR decomposition in the theory of Green elastic solids. Like in the previous chapter we focus on the transversely isotropic materials with the typical example being fiber-reinforced material.

We begin with the problem of the privileged basis and provide a solution. Then we proceed with the study of the model developed by Erel and Freed [2017]. We describe the model and show that for isotropic materials it is equivalent to the standard model of Green elasticity. We also present a way how to describe transversely isotropic materials.

3.1 Privileged basis

An occurring theme in the articles regarding the QR decomposition[1] is the necessity to choose the basis in such a way that one of the basis vector is in the direction of fibers. This basis is usually called the privileged or laboratory basis. This choice of basis however might not be always convenient. Consider a square piece of material reinforced by fibers at an angle of $\pi/4$ with the sides of the square. It is much more convenient to choose and use a basis such that basis vectors are parallel to the sides of the square than the privileged basis.

To overcome this problem we first have to choose two bases, one in the reference configuration and once in the current configuration. We denote the basis in the reference configuration as $\left\{\mathbf{E}_i^C\right\}_{i=1}^2$ and the basis in the current configuration as $\left\{\mathbf{e}_i^C\right\}_{i=1}^2$. These are the bases, in wich we want to perform computations, thus we call the computational bases. We assume that these bases are identical:

$$\mathbf{E}_i^C = \mathbf{e}_i^C \qquad i = 1, 2.$$

The deformation gradient has the following form in these bases:

$$\mathbb{F}^C = F_{ij}^C \mathbf{e}_i^C \otimes \mathbf{E}_j^C.$$

We use the superscript C to stress the fact, that the deformation gradient is expressed in terms of computational bases. But since this is the standard deformation gradient, we usually suppress the superscript and denote it as $\mathbb{F}$. We use this convention also for other tensors, e.g. stress tensors.

Now it is time to incorporate fibers and their directions. Let $\mathbb{Q}^{A\top}$ be an orthogonal matrix, which defines the direction of the fibers. That is, let $\mathbb{Q}^{A\top}$ be an orthogonal matrix, such that $\mathbb{Q}^{A\top}\mathbf{E}_1^C$ is a tangent vector to fibers. We do not require the matrix $\mathbb{Q}^{A\top}$ to be constant. We can then define two new bases:

$$\mathbf{E}_i^A = \mathbb{Q}^{A\top}\mathbf{E}_i^C \qquad i = 1, 2,$$
$$\mathbf{e}_i^A = \mathbb{Q}^{A\top}\mathbf{e}_i^C \qquad i = 1, 2.$$

[1]see for example Erel and Freed [2017] or Srinivasa [2012]

These are the privileged bases, that were mentioned at the beginning of the section. We also call them the anisotropy bases, as they are given by the anisotropy of the material. It is easy to see, that these bases can also be identified with each other.

Now we can define the anisotropic deformation gradient $\mathbb{F}^A$. The basis vectors transform using the matrix ${\mathbb{Q}^A}^\top$. The entries of the deformation gradient, in order to be invariant under the choice of basis, thus must transform using the matrix $\mathbb{Q}^A$, which gives the following transformation rule:

$$
\begin{aligned}
\mathbb{F}^A &= \mathbb{Q}^A \mathbb{F} {\mathbb{Q}^A}^\top, \\
\mathbb{F}^A &= F^A_{ij} \mathbf{e}^A_i \otimes \mathbf{E}^A_j.
\end{aligned}
$$

This is the point, in which we can perform the QR decomposition of the deformation gradient, as the fibers lie in the direction $\mathbf{E}^C_1$. We get

$$
\begin{aligned}
\mathbb{F}^A &= \mathcal{R}^A \mathcal{U}^A && \text{the QR decomposition of } \mathbb{F}^A, \\
\widetilde{\mathbf{e}}_i &= \mathcal{R}^A \mathbf{e}^A_i && i = 1, 2.
\end{aligned}
$$

As a consequence we see that

$$
\begin{aligned}
\mathcal{R}^A &= R_{ij} \mathbf{e}^A_i \otimes \widetilde{\mathbf{e}}_j, \\
\mathcal{U}^A &= U_{ij} \widetilde{\mathbf{e}}_j \otimes \mathbf{E}^A_j.
\end{aligned}
$$

We call the basis $\{\widetilde{\mathbf{e}}_i\}_{i=1}^2$ the QR basis.

Another way how to obtain the QR basis $\{\widetilde{\mathbf{e}}_i\}_{i=1}^2$ is to apply $\mathbb{F}^A$ and perform the Gram-Schmidt orthogonalization:

$$
\mathbf{f}^A_i = \mathbb{F}^A \mathbf{E}^A_i \qquad i = 1, 2.
$$

This basis is not guaranteed to be orthogonal, so we use the Gram-Schmidt orthogonalization process to get

$$
\begin{aligned}
\widetilde{\mathbf{e}}_1 &= \frac{\mathbf{f}^A_1}{\|\mathbf{f}^A_1\|}, \\
\widetilde{\mathbf{e}}_2 &= \frac{\mathbf{f}^A_2 - \left(\mathbf{f}^A_2 \cdot \widetilde{\mathbf{e}}_1\right) \widetilde{\mathbf{e}}_1}{\|\mathbf{f}^A_2 - \left(\mathbf{f}^A_2 \cdot \widetilde{\mathbf{e}}_1\right) \widetilde{\mathbf{e}}_1\|}.
\end{aligned}
$$

Putting everything together, we obtain

$$
\mathbb{F} = {\mathbb{Q}^A}^\top \mathbb{F}^A \mathbb{Q}^A = {\mathbb{Q}^A}^\top \mathcal{R}^A \mathcal{U}^A \mathbb{Q}^A. \tag{3.1}
$$

This whole procedure in depicted in Diagram 3.1.

3.2 Conjugate stress / strain basis model

In this section we describe and generalize the model presented in Freed et al. [2016] and Erel and Freed [2017]. This model is two dimensional, as it was devised for planar biological materials like membranes. The only change we make is the usage of the matrix of anisotropy $\mathbb{Q}^A$ presented in the previous section. This allows us to work with fibers with arbitrary direction.

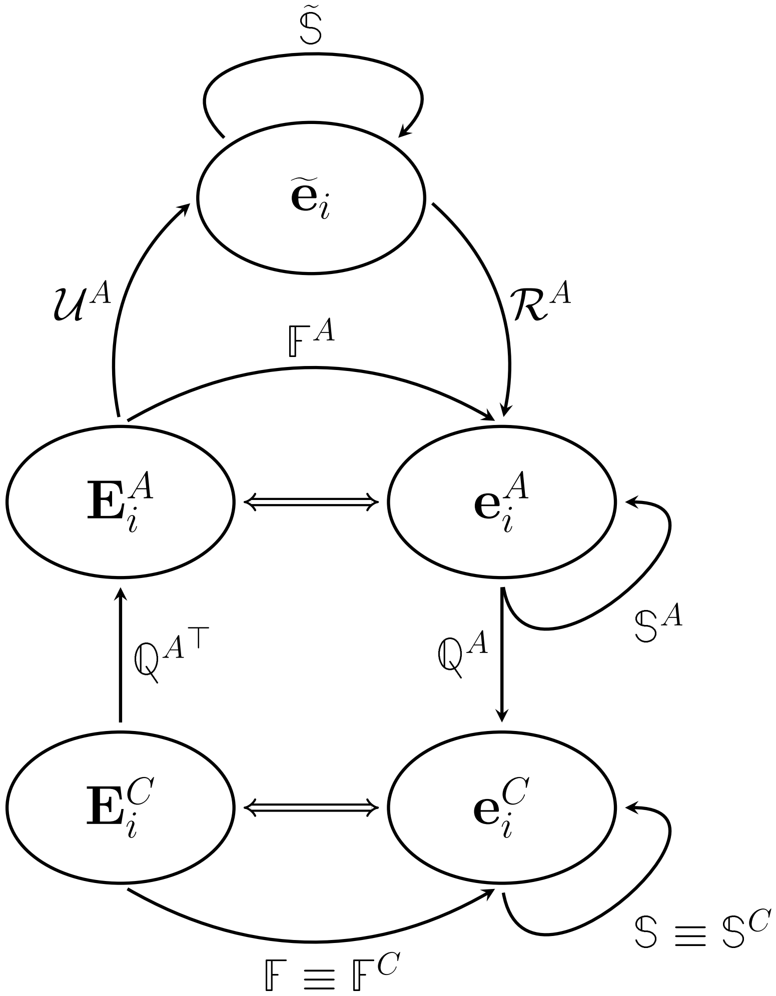


Figure 3.1: A diagram depicting relations between different bases.

We use the Kirchhoff stress tensor $\mathbb{S}$, which is related to the Cauchy stress tensor $\mathbb{T}$ through the following formula:

$$\mathbb{S} = (\det \mathbb{F})\, \mathbb{T}.$$

It is worth mentioning that this formula implies that $\mathbb{S}$ is symmetric. To obtain the Kirchhoff stress tensor in the anisotropy basis, we need to transform it using the matrix $\mathcal{R}^A$. If we want the Kirchhoff stress tensor in the computational basis, we need to transform it further using the matrix of anisotropy $\mathbb{Q}^A$.

$$\begin{aligned} \mathbb{S}^A &= \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top}, \\ \mathbb{S}^C &= \mathbb{Q}^{A^\top} \mathbb{S}^A \mathbb{Q}^A = \mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \mathbb{Q}^A. \end{aligned} \tag{3.2}$$

We usually suppress the superscript C and denote the Kirchhoff stress tensor in computational bases as $\mathbb{S}$ as in the case of the deformation gradient. The formula for the first Piola-Kirchhoff stress tensor $\mathbb{T}_R$ has the following form:

$$\begin{aligned} \mathbb{T}_R =& \ (\det \mathbb{F})\, \mathbb{T} \mathbb{F}^{-\top} = \mathbb{S}\mathbb{F}^{-\top} = \mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \mathbb{Q}^A \left(\mathbb{Q}^{A^\top} \mathcal{R}^A \mathcal{U}^A \mathbb{Q}^A \right)^{-\top} \\ &= \mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \mathbb{Q}^A \mathbb{Q}^{A^\top} \mathcal{R}^A \mathcal{U}^{A^{-\top}} \mathbb{Q}^A = \mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{U}^{A^{-\top}} \mathbb{Q}^A. \end{aligned} \tag{3.3}$$

3.2.1 Stress power

It is well known[2], that

$$\dot{W} = \mathbb{T}_R : \dot{\mathbb{F}} = \mathrm{Tr}\left(\mathbb{T}_R^\top \dot{\mathbb{F}} \right),$$

where $\dot{W}$ is the stress power and $\mathbb{L}$ is the velocity gradient. Since $\mathbb{T}_R = \mathbb{S}\mathbb{F}^{-\top}$ and $\mathbb{L} = \dot{\mathbb{F}}\mathbb{F}^{-1}$, we get

$$\dot{W} = \mathrm{Tr}\left(\mathbb{F} \mathbb{T}_R^\top \dot{\mathbb{F}} \mathbb{F}^{-1} \right) = \mathrm{Tr}\,(\mathbb{S}\mathbb{L}).$$

Transforming $\mathbb{S}$ and $\mathbb{L}$ into the QR basis and using the cyclic property of trace gives

$$\begin{aligned} \dot{W} = & \ \mathrm{Tr}\left(\mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \mathbb{Q}^A \mathbb{Q}^{A^\top} \dot{\mathcal{R}}^A \mathcal{U}^A \mathbb{Q}^A \mathbb{Q}^{A^\top} \mathcal{U}^{A^{-1}} \mathcal{R}^{A^\top} \mathbb{Q}^A \right) \\ & + \mathrm{Tr}\left(\mathbb{Q}^{A^\top} \mathcal{R}^A \widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \mathbb{Q}^A \mathbb{Q}^{A^\top} \mathcal{R}^A \dot{\mathcal{U}}^A \mathbb{Q}^A \mathbb{Q}^{A^\top} \mathcal{U}^{A^{-1}} \mathcal{R}^{A^\top} \mathbb{Q}^A \right) \\ & = \mathrm{Tr}\left(\widetilde{\mathbb{S}} \mathcal{R}^{A^\top} \dot{\mathcal{R}}^A \right) + \mathrm{Tr}\left(\widetilde{\mathbb{S}} \dot{\mathcal{U}}^A \mathcal{U}^{A^{-1}} \right). \end{aligned}$$

Since $\mathbb{0} = \overline{\left(\mathcal{R}^{A^\top} \mathcal{R}^A \right)}^{\,\cdot} = \dot{\mathcal{R}}^{A^\top} \mathcal{R}^A + \mathcal{R}^{A^\top} \dot{\mathcal{R}}^A$, we see that the first trace on the right hand side is zero, as it is the trace of symmetric and skew symmetric tensor. Thus we obtain

$$\dot{W} = \mathrm{Tr}\left(\widetilde{\mathbb{S}} \widetilde{\mathbb{L}} \right) = \widetilde{S}_{11} \widetilde{L}_{11} + \widetilde{S}_{12} \widetilde{L}_{12} + \widetilde{S}_{22} \widetilde{L}_{22}, \tag{3.4}$$

where $\widetilde{\mathbb{L}} = \dot{\mathcal{U}}^A \mathcal{U}^{A^{-1}}$.

[2]See e.g. Ogden [1984]

3.2.2 Decomposition of the Laplace stretch

The Laplace stretch $\mathcal{U}^A$ can be decomposed into a product of three matrices describing dilatation, squeeze and shear:

$$\mathcal{U}^A = \begin{pmatrix} a & a\gamma \\ 0 & b \end{pmatrix} = \underbrace{\begin{pmatrix} \sqrt{ab} & 0 \\ 0 & \sqrt{ab} \end{pmatrix}}_{\text{dilatation}} \underbrace{\begin{pmatrix} \sqrt{a/b} & 0 \\ 0 & \sqrt{b/a} \end{pmatrix}}_{\text{squeeze}} \underbrace{\begin{pmatrix} 1 & \gamma \\ 0 & 1 \end{pmatrix}}_{\text{shear}} = \mathcal{U}^A_d \mathcal{U}^A_{sq} \mathcal{U}^A_{sh}. \tag{3.5}$$

Now we can define the velocity gradient for the dilatation, squeeze and shear.

$$\begin{aligned} \widetilde{\mathbb{L}}_d &= \dot{\mathcal{U}}^A_d {\mathcal{U}^A_d}^{-1} = \frac{1}{2}\left(\frac{\dot{a}}{a} + \frac{\dot{b}}{b}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \widetilde{\mathbb{L}}_{sq} &= \dot{\mathcal{U}}^A_{sq} {\mathcal{U}^A_{sq}}^{-1} = \frac{1}{2}\left(\frac{\dot{a}}{a} - \frac{\dot{b}}{b}\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \widetilde{\mathbb{L}}_{sh} &= \dot{\mathcal{U}}^A_{sh} {\mathcal{U}^A_{sh}}^{-1} = \begin{pmatrix} 0 & \dot{\gamma} \\ 0 & 0 \end{pmatrix}. \end{aligned}$$

Differentiating (3.5) yields

$$\begin{aligned} \dot{\mathcal{U}}^A &= \dot{\mathcal{U}}^A_d \mathcal{U}^A_{sq} \mathcal{U}^A_{sh} + \mathcal{U}^A_d \dot{\mathcal{U}}^A_{sq} \mathcal{U}^A_{sh} + \mathcal{U}^A_d \mathcal{U}^A_{sq} \dot{\mathcal{U}}^A_{sh} \\ &= \dot{\mathcal{U}}^A_d {\mathcal{U}^A_d}^{-1} \mathcal{U}^A + \dot{\mathcal{U}}^A_{sq} {\mathcal{U}^A_{sq}}^{-1} \mathcal{U}^A + \mathcal{U}^A {\mathcal{U}^A_{sh}}^{-1} \dot{\mathcal{U}}^A_{sh} \\ &= \widetilde{\mathbb{L}}_d \mathcal{U}^A + \widetilde{\mathbb{L}}_{sq} \mathcal{U}^A + \mathcal{U}^A \widetilde{\mathbb{L}}_{sh}, \end{aligned}$$

where we used the fact, that $\mathcal{U}^A_d$ and $\mathcal{U}^A_{sq}$ commute. This implies, that

$$\widetilde{\mathbb{L}} = \dot{\mathcal{U}}^A {\mathcal{U}^A}^{-1} = \widetilde{\mathbb{L}}_d + \widetilde{\mathbb{L}}_{sq} + \mathcal{U}^A \widetilde{\mathbb{L}}_{sh} {\mathcal{U}^A}^{-1} = \begin{pmatrix} \frac{\dot{a}}{a} & \frac{a}{b}\dot{\gamma} \\ 0 & \frac{\dot{b}}{b} \end{pmatrix}. \tag{3.6}$$

3.2.3 Stress and strain bases

Plugging (3.6) into (3.4) allows us to decompose the stress power into three parts coming from the dilatation, squeeze and shear:

$$\begin{aligned} \dot{W} &= \dot{W}_d + \dot{W}_{sq} + \dot{W}_{sh}, \\ \dot{W}_d &= \widetilde{\mathbb{S}} : \widetilde{\mathbb{L}}_d = \left(\widetilde{S}_{11} + \widetilde{S}_{22}\right)\frac{1}{2}\left(\frac{\dot{a}}{a} + \frac{\dot{b}}{b}\right), \\ \dot{W}_{sq} &= \widetilde{\mathbb{S}} : \widetilde{\mathbb{L}}_{sq} = \left(\widetilde{S}_{11} - \widetilde{S}_{22}\right)\frac{1}{2}\left(\frac{\dot{a}}{a} - \frac{\dot{b}}{b}\right), \\ \dot{W}_{sh} &= \widetilde{\mathbb{S}} : \left(\mathcal{U}^A \widetilde{\mathbb{L}}_{sh} {\mathcal{U}^A}^{-1}\right) = \frac{a}{b}\widetilde{S}_{12}\dot{\gamma}. \end{aligned}$$

This suggests, that we can express the stress power as

$$\mathrm{d}W = \pi \mathrm{d}\delta + \sigma \mathrm{d}\epsilon + \tau \mathrm{d}\gamma, \tag{3.7}$$

where the conjugate stress / strain pair $\{\pi, \delta\}$ describes uniform dilatation, second pair $\{\sigma, \epsilon\}$ describes squeeze and finally third pair $\{\tau, \gamma\}$ describes shear. The natural stress basis is the following:

$$\pi = \widetilde{S}_{11} + \widetilde{S}_{22},$$
$$\sigma = \widetilde{S}_{11} - \widetilde{S}_{22},$$
$$\tau = \frac{a}{b}\widetilde{S}_{12}.$$

For the strain, we may choose this basis:

$$\delta = \log\sqrt{ab} \qquad \dot{\delta} = \frac{1}{2}\left(\frac{\dot{a}}{a} + \frac{\dot{b}}{b}\right),$$
$$\epsilon = \log\sqrt{a/b} \qquad \dot{\epsilon} = \frac{1}{2}\left(\frac{\dot{a}}{a} - \frac{\dot{b}}{b}\right),$$
$$\gamma \qquad \dot{\gamma}.$$

3.2.4 Constitutive relation

Considering the first law of thermodynamics for a continuum

$$\mathrm{d}S = \frac{1}{T}\left(\mathrm{d}U - \frac{1}{\rho_R}\mathrm{d}W\right),$$

where S is entropy, T is temperature and U is internal energy, and using the free energy $\psi = U - TS$ yields

$$\mathrm{d}T = -\frac{1}{S}\left(\mathrm{d}\psi - \frac{1}{\rho_R}\mathrm{d}W\right).$$

If we assume, that $\psi = \psi(T, \delta, \epsilon, \gamma)$, then, using (3.7), we get

$$\rho_R\left(\frac{\partial\psi}{\partial T}\mathrm{d}T + \frac{\partial\psi}{\partial\delta}\mathrm{d}\delta + \frac{\partial\psi}{\partial\epsilon}\mathrm{d}\epsilon + \frac{\partial\psi}{\partial\gamma}\mathrm{d}\gamma\right) = -\rho_R S\mathrm{d}T + \pi\mathrm{d}\delta + \sigma\mathrm{d}\epsilon + \tau\mathrm{d}\gamma.$$

This implies

$$\begin{aligned} S &= -\frac{\partial\psi}{\partial T} \\ \pi &= \rho_R\frac{\partial\psi}{\partial\delta}, \\ \sigma &= \rho_R\frac{\partial\psi}{\partial\epsilon}, \\ \tau &= \rho_R\frac{\partial\psi}{\partial\gamma}. \end{aligned} \tag{3.8}$$

3.2.5 Bases for anisotropic material

The conjugate stress / strain basis pairs presented in Section 3.2.3 can be generalized to allow fiber-reinforced material. In order to do so, we define the extent of anisotropy n, which describes how much stiffer the fibers are. If $n > 1$, then the fibers are stiffer than the matrix material itself. On the other hand, if $n < 1$, then it is the matrix material, which is stiffer. Even though we would expect an isotropic behaviour for $n = 1$, if the free energy is not isotropic, then we still obtain anisotropy.

We can then define the basis for the stress as follows:

$$\begin{aligned} \pi &= \frac{\widetilde{S}_{11}}{n} + n\widetilde{S}_{22}, \\ \sigma &= \frac{\widetilde{S}_{11}}{n} - n\widetilde{S}_{22}, \\ \tau &= \frac{a}{b}\widetilde{S}_{12}, \end{aligned} \tag{3.9}$$

Inverting this relations we get

$$\widetilde{\mathbb{S}} = \begin{pmatrix} \frac{n}{2}(\pi+\sigma) & \frac{b}{a}\tau \\ \frac{b}{a}\tau & \frac{1}{2n}(\pi-\sigma) \end{pmatrix} \tag{3.10}$$

The conjugate basis for strain is defined by the following way:

$$\begin{aligned} \delta &= \log\sqrt{a^n b^{1/n}}, \\ \epsilon &= \log\sqrt{\frac{a^n}{b^{1/n}}}, \\ \gamma&. \end{aligned} \tag{3.11}$$

For $n = 1$ both conjugate bases have the same form as the bases in the Section 3.2.3.

3.2.6 Simple example

We perform a simple computation to show, how we can use the conjugate stress / strain basis model with the free energy for planar membranes to solve problems. To keep things simple, we assume that

$$\widetilde{\mathbb{S}} = \begin{pmatrix} S & 0 \\ 0 & 0 \end{pmatrix}.$$

Using (3.9), we see that

$$\begin{aligned} \pi &= \frac{S}{n}, \\ \sigma &= \frac{S}{n} \\ \tau &= 0. \end{aligned}$$

from which we can, with the help of (3.12), compute elements of $\mathcal{U}^A$.

$$\begin{aligned} a =& e^{\frac{1}{n}(\delta+\epsilon)}, \\ b =& e^{n(\delta-\epsilon)}. \end{aligned}$$

Thus we see that

$$\mathcal{U}^A = \begin{pmatrix} e^{\frac{1}{n}(\delta+\epsilon)} & 0 \\ 0 & e^{n(\delta-\epsilon)} \end{pmatrix}.$$

If the free energy was given, we could use (3.8) to proceed further with the computation.

3.2.7 Isotropic material

For isotropic free energy we would expect isotropic deformation regardless values of the extent of anisotropy n and the matrix of anisotropy $\mathbb{Q}^A$. However compared to the standard model (2.1), it is not clear, if the presented model for isotropic free energy gives also isotropic stress tensor. In this subsection we answer this question.

In what follows, we show, that if the free energy ψ is isotropic and does not depend on n and $\mathbb{Q}^A$, than also $\mathbb{S}$ is isotropic and does not depend on n and $\mathbb{Q}^A$. First, we show, that $\mathbb{S}$ does not depend on n, then that $\mathbb{S}^A$ is isotropic and finally that $\mathbb{S}$ is also isotropic and does not depend on $\mathbb{Q}^A$.

Let us denote $\mathbb{C}^A = {\mathbb{F}^A}^\top \mathbb{F}^A$ and let ψ depends only on the first and third invariant of $\mathbb{C}^A$. First of all, we need to invert the relations (3.11):

$$\begin{aligned} a =& e^{\frac{1}{n}(\delta+\epsilon)}, \\ b =& e^{n(\delta-\epsilon)}. \end{aligned} \tag{3.12}$$

Using these inverted relations, we can compute derivatives of a and b with respect to δ and ϵ.

$$\begin{aligned} \frac{\partial a}{\partial \delta} &= \frac{1}{n} e^{\frac{1}{n}(\delta+\epsilon)} = \frac{1}{n} a \qquad & \frac{\partial b}{\partial \delta} &= n e^{n(\delta-\epsilon)} = nb \\ \frac{\partial a}{\partial \epsilon} &= \frac{1}{n} e^{\frac{1}{n}(\delta+\epsilon)} = \frac{1}{n} a \qquad & \frac{\partial b}{\partial \epsilon} &= -n e^{n(\delta-\epsilon)} = -nb \end{aligned} \tag{3.13}$$

Using chain rule, (1.6), (3.8), (3.12) and (3.13) we obtain

$$\begin{aligned} \pi = \rho_R \frac{\partial \psi}{\partial \delta} &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(\frac{\partial I_1(\mathbb{C}^A)}{\partial a} \frac{\partial a}{\partial \delta} + \frac{\partial I_1(\mathbb{C}^A)}{\partial b} \frac{\partial b}{\partial \delta} \right) \\ &+ \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(\frac{\partial I_3(\mathbb{C}^A)}{\partial a} \frac{\partial a}{\partial \delta} + \frac{\partial I_3(\mathbb{C}^A)}{\partial b} \frac{\partial b}{\partial \delta} \right) \\ &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2a(1+\gamma^2) \frac{1}{n} a + 2bnb \right) + \rho \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2ab^2 \frac{1}{n} a + 2a^2 bnb \right) \\ &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 (1+\gamma^2) + 2nb^2 \right) + \rho \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 b^2 + 2na^2 b^2 \right), \\ \sigma = \rho_R \frac{\partial \psi}{\partial \epsilon} &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(\frac{\partial I_1(\mathbb{C}^A)}{\partial a} \frac{\partial a}{\partial \epsilon} + \frac{\partial I_1(\mathbb{C}^A)}{\partial b} \frac{\partial b}{\partial \epsilon} \right) \\ &+ \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(\frac{\partial I_3(\mathbb{C}^A)}{\partial a} \frac{\partial a}{\partial \epsilon} + \frac{\partial I_3(\mathbb{C}^A)}{\partial b} \frac{\partial b}{\partial \epsilon} \right) \\ &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2a(1+\gamma^2) \frac{1}{n} a - 2bnb \right) + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2ab^2 \frac{1}{n} a - 2a^2 bnb \right) \\ &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 (1+\gamma^2) - 2nb^2 \right) + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 b^2 - 2na^2 b^2 \right), \\ \tau = \rho_R \frac{\partial \psi}{\partial \gamma} &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \frac{\partial I_1(\mathbb{C}^A)}{\partial \gamma} + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \frac{\partial I_3(\mathbb{C}^A)}{\partial \gamma} = \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2 \gamma. \end{aligned} \tag{3.14}$$

Now we can use (3.10) to get elements of $\widetilde{\mathbb{S}}$:

$$
\begin{aligned}
\widetilde{S}_{11} &= \frac{n}{2}(\pi+\sigma) = \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2(1+\gamma^2) + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2 b^2, \\
\widetilde{S}_{12} &= \frac{b}{a}\tau = \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma, \\
\widetilde{S}_{22} &= \frac{1}{2n}(\pi-\sigma) = \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2b^2 + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2 b^2.
\end{aligned}
\tag{3.15}
$$

Thus $\widetilde{\mathbb{S}}$ does not depend on n, which implies that $\mathbb{S}$ also does not depend on n.

Now we show, that $\mathbb{S}^A$ is isotropic. We verify assumptions of the Representation Theorem 3. To simplify the notation and make the computation easier to follow, we suppress the superscript A in elements of the anisotropic deformation gradient $\mathbb{F}^A$. Instead of F^A_{ij}, we just write F_{ij}. One should keep in mind, that it means the entries of $\mathbb{F}^A$ and not $\mathbb{F} \equiv \mathbb{F}^C$.

Using (1.2b) and (3.2) we obtain

$$
\begin{aligned}
S^A_{11} &= \cos\theta \left(\widetilde{S}^A_{11}\cos\theta + \widetilde{S}^A_{12}\sin\theta\right) + \sin\theta \left(\widetilde{S}^A_{12}\cos\theta + \widetilde{S}^A_{22}\sin\theta\right) \\
S^A_{12} &= -\sin\theta \left(\widetilde{S}^A_{11}\cos\theta + \widetilde{S}^A_{12}\sin\theta\right) + \cos\theta \left(\widetilde{S}^A_{12}\cos\theta + \widetilde{S}^A_{22}\sin\theta\right) \\
S^A_{22} &= -\sin\theta \left(\widetilde{S}^A_{12}\cos\theta - \widetilde{S}^A_{11}\sin\theta\right) + \cos\theta \left(\widetilde{S}^A_{22}\cos\theta - \widetilde{S}^A_{12}\sin\theta\right)
\end{aligned}
$$

Now we can use (1.3a), (1.3b) and (3.15) to get

$$
\begin{aligned}
S^A_{11} = \rho_R &\frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2(1+\gamma^2) + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \right. \\
&\left. + \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right] + \rho_R \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \right. \\
&\left. + \left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2b^2 + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right], \\
S^A_{12} = -\rho_R &\frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2(1+\gamma^2) + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \right. \\
&\left. + \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right] + \rho_R \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \right. \\
&\left. + \left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2b^2 + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right], \\
S^A_{22} = -\rho_R &\frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} - \left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2(1+\gamma^2) \right. \right. \\
&\left. \left. + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right] + \rho_R \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} \left[\left(\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2b^2 \right. \right. \\
&\left. \left. + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right) \frac{F_{11}}{\sqrt{F_{11}^2+F_{21}^2}} - \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma \frac{-F_{21}}{\sqrt{F_{11}^2+F_{21}^2}} \right].
\end{aligned}
$$

After certain manipulations and using (1.6b) we have

$$\begin{aligned}
S^A_{11} &= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{11}^2}{F_{11}^2 + F_{21}^2} a^2(1+\gamma^2) \right. \\
&\quad \left. + \frac{F_{21}^2}{F_{11}^2 + F_{21}^2} b^2 - 2ab\gamma \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} \right], \\
S^A_{12} &= 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} a^2(1+\gamma^2) - \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} b^2 + \frac{F_{11}^2 - F_{21}^2}{F_{11}^2 + F_{21}^2} ab\gamma \right], \\
S^A_{22} &= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{21}^2}{F_{11}^2 + F_{21}^2} a^2(1+\gamma^2) \right. \\
&\quad \left. + \frac{F_{11}^2}{F_{11}^2 + F_{21}^2} b^2 + 2ab\gamma \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} \right].
\end{aligned}$$

Using (1.3c), (1.3d) and (1.3e) leads to

$$\begin{aligned}
S^A_{11} &= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{11}^2}{F_{11}^2 + F_{21}^2} (F_{11}^2 + F_{21}^2) \right. \\
&\quad \left(1 + \left(\frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \right)^2 \right) + \frac{F_{21}^2}{F_{11}^2 + F_{21}^2} \left(\frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \right)^2 \\
&\quad \left. -2\sqrt{F_{11}^2 + F_{21}^2} \frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} \right], \\
S^A_{12} &= 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} (F_{11}^2 + F_{21}^2) \left(1 + \left(\frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \right)^2 \right) \right. \\
&\quad - \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} \left(\frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \right)^2 \\
&\quad \left. + \frac{F_{11}^2 - F_{21}^2}{F_{11}^2 + F_{21}^2} \sqrt{F_{11}^2 + F_{21}^2} \frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \right], \\
S^A_{22} &= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left[\frac{F_{21}^2}{F_{11}^2 + F_{21}^2} (F_{11}^2 + F_{21}^2) \right. \\
&\quad \left(1 + \left(\frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \right)^2 \right) + \frac{F_{11}^2}{F_{11}^2 + F_{21}^2} \left(\frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \right)^2 \\
&\quad \left. +2\sqrt{F_{11}^2 + F_{21}^2} \frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}} \frac{F_{11}F_{12} + F_{21}F_{22}}{F_{11}^2 + F_{21}^2} \frac{F_{11}F_{21}}{F_{11}^2 + F_{21}^2} \right].
\end{aligned}$$

Further manipulations finally give us

$$
\begin{aligned}
S_{11}^A &= 2\rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \det \mathbb{C}^A + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \Big[F_{11}^2 \\
&\quad + \frac{F_{11}^4 F_{12}^2 + 2F_{11}^3 F_{12} F_{21} F_{22} + F_{11}^2 F_{21}^2 F_{22}^2}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad + \frac{F_{11}^2 F_{22}^2 F_{21}^2 - 2F_{11} F_{22} F_{12} F_{21}^3 + F_{12}^2 F_{21}^4}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad - 2\frac{F_{11}^3 F_{12} F_{21} F_{22} + F_{11}^2 F_{21}^2 F_{22}^2 - F_{11}^2 F_{21}^2 F_{12}^2 - F_{11} F_{12} F_{21}^3 F_{22}}{\left(F_{11}^2 + F_{21}^2\right)^2} \Big] \\
&= 2\rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \det \mathbb{C}^A + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C})} \left(F_{11}^2 + F_{12}^2 \right), \\
S_{12}^A &= 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \Big[F_{11} F_{21} + \frac{F_{11}^3 F_{12}^2 F_{21} + 2F_{11}^2 F_{12} F_{21}^2 F_{22} + F_{11} F_{21}^3 F_{22}^2}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad - \frac{F_{11}^2 F_{12} F_{21}^2 F_{22} + F_{11} F_{21}^3 F_{22}^2 - F_{11} F_{12}^2 F_{21}^3 - F_{12} F_{21}^4 F_{22}}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad + \frac{F_{11}^4 F_{12} F_{22} + F_{11}^3 F_{21} F_{22}^2 - F_{11}^3 F_{12}^2 F_{21} - F_{11}^2 F_{12} F_{21}^2 F_{22}}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad - \frac{F_{11}^3 F_{21} F_{22}^2 - 2F_{11}^2 F_{12} F_{21}^2 F_{22} + F_{11} F_{12}^3 F_{21}^2}{\left(F_{11}^2 + F_{21}^2\right)^2} \Big] \\
&= 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(F_{11} F_{21} + F_{12} F_{22} \right), \\
S_{22}^A &= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \Big[F_{21}^2 \\
&\quad + \frac{F_{11}^2 F_{12}^2 F_{21}^2 + 2F_{11} F_{12} F_{21}^3 F_{22} + F_{21}^4 F_{22}^2}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad + \frac{F_{11}^4 F_{22}^2 - 2F_{11}^3 F_{12} F_{21} F_{22} + F_{11}^2 F_{12}^2 F_{21}^2}{\left(F_{11}^2 + F_{21}^2\right)^2} \\
&\quad + \frac{2F_{11}^3 F_{12} F_{21} F_{22} + 2F_{11}^2 F_{21}^2 F_{22}^2 - 2F_{11}^2 F_{12}^2 F_{21}^2 - 2F_{11} F_{12} F_{21}^3 F_{22}}{\left(F_{11}^2 + F_{21}^2\right)^2} \Big] \\
&= 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(F_{21}^2 + F_{22}^2 \right).
\end{aligned}
$$

We no longer omit the superscript A in the elements of $\mathbb{F}^A$ from here. Since

$$
\mathbb{B}^A = \mathbb{F}^A {\mathbb{F}^A}^\top = \begin{pmatrix} {F_{11}^A}^2 + {F_{21}^A}^2 & F_{11}^A F_{21}^A + F_{12}^A F_{22}^A \\ F_{11}^A F_{21}^A + F_{12}^A F_{22}^A & {F_{21}^A}^2 + {F_{22}^A}^2 \end{pmatrix},
$$

we see that $\mathbb{S}^A = 2\rho_R \det \mathbb{C}^A \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \mathbb{I} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \mathbb{B}^A$. This means, that the assumptions of Representation Theorem 3 are satisfied, because $I_i(\mathbb{C}^A) = I_i(\mathbb{B}^A)$ for $i = 1, 3$.

It remains to show that $\mathbb{S}$ is isotropic and does not depend on $\mathbb{Q}^A$. It is easy to see, that we only have to look at the product ${\mathbb{Q}^A}^\top \mathbb{B}^A \mathbb{Q}^A$, because $I_1(\mathbb{B}) = I_1(\mathbb{B}^A)$ and $I_3(\mathbb{B}) = I_3(\mathbb{B}^A)$.

$$
{\mathbb{Q}^A}^\top \mathbb{B}^A \mathbb{Q}^A = {\mathbb{Q}^A}^\top \mathbb{F}^A {\mathbb{F}^A}^\top \mathbb{Q}^A = {\mathbb{Q}^A}^\top \mathbb{Q}^A \mathbb{F} {\mathbb{Q}^A}^\top \mathbb{Q}^A \mathbb{F}^\top {\mathbb{Q}^A}^\top \mathbb{Q}^A = \mathbb{F}\mathbb{F}^\top = \mathbb{B}.
$$

Thus we finally obtain the formula for $\mathbb{S}$:

$$\mathbb{S} = 2\rho_R \det \mathbb{B} \frac{\partial \psi}{\partial I_3(\mathbb{B})} \mathbb{I} + 2\rho_R \frac{\partial \psi}{\partial I_1(\mathbb{B})} \mathbb{B}.$$

This implies that $\mathbb{S}$ is isotropic and does not depend on $\mathbb{Q}^A$. Furthermore we see, that this formula is equivalent to the standard formula (2.1) for the Cauchy stress tensor $\mathbb{T}$, since in two dimensions we assume, that the free energy ψ only depends on I_1 and I_3.

3.2.8 Transversely isotropic material

In the previous section we have shows, that for isotropic materials the conjugate pairs model is equivalent to the standard model of Green elasticity. In this section we take a look at how we can describe transversely isotropic (or fiber-reinforced) materials in terms of QR decomposition.

First of all, we have to write the pseudo-invariants (2.2) in terms a, b and γ. We may assume that the fiber direction $\mathbf{A}$ is equal to $(1,0)^\top$, because this is the direction of fibers in the anisotropy basis. Using (1.1) and (1.5) we obtain:

$$I_4(\mathbb{C}^A, \mathbf{A}) = \mathbf{A} \cdot \mathbb{C}^A \mathbf{A} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} a^2 \\ a^2 + a^2\gamma \end{pmatrix} = a^2 \tag{3.16a}$$

$$I_5(\mathbb{C}^A, \mathbf{A}) = \mathbf{A} \cdot \left(\mathbb{C}^A\right)^2 \mathbf{A} = \mathbb{C}^A \mathbf{A} \cdot \mathbb{C}^A \mathbf{A} = \begin{pmatrix} a^2 \\ a^2 + a\gamma \end{pmatrix} \cdot \begin{pmatrix} a^2 \\ a^2 + a^2\gamma \end{pmatrix} = a^4 + a^4\gamma^2. \tag{3.16b}$$

Now we can extend the result obtained in the previous section and show, that even in the case of transversely isotropic material the Kirchhoff stress tensor $\mathbb{S}$ does not depend on the extent of anisotropy n.

First of all, we have to compute the elements of the stress basis. Extending (3.14) yields

$$\begin{aligned}
\pi &= \rho_R \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 (1+\gamma^2) + 2nb^2 \right) + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 b^2 + 2na^2 b^2 \right) \right. \\
&\quad \left. + \frac{\partial \psi}{\partial I_4(\mathbb{C}^A)} \frac{2}{n} a^2 + \frac{\partial \psi}{\partial I_5(\mathbb{C}^A)} \frac{1}{n} 4a^4 \left(1+\gamma^2\right) \right], \\
\sigma &= \rho_R \left[\cdot \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 (1+\gamma^2) - 2nb^2 \right) + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} \left(2\frac{1}{n} a^2 b^2 - 2na^2 b^2 \right) \right. \\
&\quad \left. + \frac{\partial \psi}{\partial I_4(\mathbb{C}^A)} \frac{2}{n} a^2 + \frac{\partial \psi}{\partial I_5(\mathbb{C}^A)} \frac{1}{n} 4a^4 \left(1+\gamma^2\right) \right], \\
\tau &= \rho_R \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2\gamma + \frac{\partial \psi}{\partial I_5(\mathbb{C}^A)} 2a^4\gamma \right].
\end{aligned}$$

Now we can compute the elements of $\widetilde{\mathbb{S}}$. Using (3.10) we obtain

$$\begin{aligned}
\widetilde{S}_{11} &= \rho_R \left[\frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2a^2(1+\gamma^2) + \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2 \right. \\
&\quad \left. + \frac{\partial \psi}{\partial I_4(\mathbb{C}^A)} 2a^2 + \frac{\partial \psi}{\partial I_5(\mathbb{C}^A)} 4a^4 \left(1+\gamma^2\right) \right], \\
\widetilde{S}_{12} &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2ab\gamma + \rho_R \frac{\partial \psi}{\partial I_5(\mathbb{C}^A)} 2a^3b\gamma, \\
\widetilde{S}_{22} &= \rho_R \frac{\partial \psi}{\partial I_1(\mathbb{C}^A)} 2b^2 + \rho_R \frac{\partial \psi}{\partial I_3(\mathbb{C}^A)} 2a^2b^2.
\end{aligned}$$

We see that $\widetilde{\mathbb{S}}$ does not depend on n, which implies that also $\mathbb{S}$ does not depend on n. Unlike in the previous case, the independence of $\mathbb{S}$ on $\mathbb{Q}^A$ of course cannot be proven. Also it is not possible to show, that this model is equivalent to the standard Spencer's model of fiber-reinforced material.

4. Numerical experiments

In this chapter we perform numerical experiments using the Wolfram Mathematica software and compare the models mentioned in the previous chapter. We start with the description of the so-called standard reinforcing material. Then we proceed with the problem formulation and description of the Wolfram Mathematica including the showcase of a sample code. Then we finally numerically solve several problems with various fiber directions, including curved fibers, and compute norms of the displacement, the Cauchy and the first Piolla-Kirchhoff stress tensors.

4.1 Standard reinforcing material

We assume the Helmholtz free energy of the standard reinforcing material, that is based on neo-Hookean free energy:

$$\begin{aligned}\rho_R\psi = \frac{G}{2}\left(\operatorname{Tr}\mathbb{C} - 2\right) + \frac{\lambda}{2}\left(\log\sqrt{\det\mathbb{C}}\right)^2 - G\log\sqrt{\det\mathbb{C}} \\ + \frac{G}{2}k\left(\mathbf{A}\cdot\mathbb{C}\mathbf{A} - 1\right)^2,\end{aligned} \tag{4.1}$$

where G is shear modulus, λ is Lamé parameter and $k \geq 0$ is a material parameter measuring stiffness of fibers. For $k = 0$ we would obtain the classical neo-Hookean free energy, which is isotropic. This standard reinforcing model is a much-used example of transversely isotropic material used in biomechanics, see e.g. Destrade et al. [2008] or Ning et al. [2006].

Plugging (4.1) into (2.3) yields

$$\mathbb{T} = \frac{1}{\sqrt{\det\mathbb{C}}}\left[\left(\lambda\log\sqrt{\det\mathbb{C}} - G\right)\mathbb{I} + G\mathbb{B} + 2Gk\left(\mathbf{A}\cdot\mathbb{C}\mathbf{A} - 1\right)\mathbf{A}\otimes\mathbf{A}\right]. \tag{4.2}$$

4.1.1 Linearization of the standard reinforcing material

If we want to perform numerical experiments with the standard reinforcing material in the linear elasticity framework, we have to linearize the Cauchy stress tensor. We can assume that $\mathbf{A} = (1,0)^\top$, as we can use the matrix of anisotropy $\mathbb{Q}^A$ to rotate the basis.

Let $\mathbb{F}^A = \mathbb{I} + \nabla\mathbf{u}^A$ and assume, that $\nabla\mathbf{u}^A$ is small. Then, neglecting all terms of second or higher order, we obtain

$$\begin{aligned}\mathbb{B}^A &= \mathbb{F}^A{\mathbb{F}^A}^\top = \left(\mathbb{I} + \nabla\mathbf{u}^A\right)\left(\mathbb{I} + \nabla\mathbf{u}^A\right)^\top \\ &\approx \mathbb{I} + \nabla\mathbf{u}^A + \left(\nabla\mathbf{u}^A\right)^\top = \mathbb{I} + 2\mathbb{e}^A, \\ \det\mathbb{F}^A &= 1 + \nabla\mathbf{u}^A_{11} + \nabla\mathbf{u}^A_{22} + \nabla\mathbf{u}^A_{33} + \mathcal{O}\left(|\nabla\mathbf{u}^A|^2\right) \approx 1 + \operatorname{Tr}\mathbb{e}^A, \\ \frac{1}{\sqrt{\det\mathbb{C}^A}} &\approx \frac{1}{1 + \operatorname{Tr}\mathbb{e}^A} \approx 1 - \frac{\operatorname{Tr}\mathbb{e}^A}{2}, \\ \log\sqrt{\det\mathbb{C}^A} &\approx \log\left(1 + \operatorname{Tr}\mathbb{e}^A\right) \approx \operatorname{Tr}\mathbb{e}^A, \\ \mathbf{A}\cdot\mathbb{C}^A\mathbf{A} &= \left|\left(\mathbb{I} + \nabla\mathbf{u}^A\right)\mathbf{A}\right|^2 = |\mathbf{A}|^2 + 2\mathbb{e}^A\mathbf{A}\cdot\mathbf{A} + \left|\nabla\mathbf{u}^A\mathbf{A}\right| \approx 1 + 2\mathbb{e}^A\mathbf{A}\cdot\mathbf{A}.\end{aligned}$$

Using these yields the following approximation of the Cauchy stress tensor:

$$\begin{aligned}\mathbb{T}^A &\approx \left(1-\frac{\operatorname{Tr}\mathbb{e}^A}{2}\right)\left[\left(\lambda\operatorname{Tr}\mathbb{e}^A - G\right)\mathbb{I} + G\left(\mathbb{I}+2\mathbb{e}^A\right) + 2Gk\left(2\mathbb{e}^A\mathbf{A}\cdot\mathbf{A}\right)\mathbf{A}\otimes\mathbf{A}\right]\\ &\approx \lambda\left(\operatorname{Tr}\mathbb{e}^A\right)\mathbb{I} + 2G\mathbb{e}^A + 4Gk\left(\mathbb{e}^A\mathbf{A}\cdot\mathbf{A}\right)\mathbf{A}\otimes\mathbf{A} =: \mathbb{\tau}^A.\end{aligned}$$

Setting $\mathbf{A} = (1,0)^\top$ and using the Voigt notation, we obtain the following:

$$\begin{pmatrix}\tau_{11}^A\\ \tau_{22}^A\\ \tau_{12}^A\end{pmatrix} = \begin{pmatrix}\lambda+2G+4Gk & \lambda & 0\\ \lambda & \lambda+2G & 0\\ 0 & 0 & G\end{pmatrix}\begin{pmatrix}\epsilon_{11}^A\\ \epsilon_{22}^A\\ 2\epsilon_{12}^A\end{pmatrix},$$

which is the linearized version of the standard reinforcing material.

4.1.2 Standard reinforcing material in conjugate pairs

Using formulas (1.6) and (3.16a), we can write the standard reinforcing material (4.1) in terms of the elements of the Laplace stretch $\mathcal{U}^A$:

$$\begin{aligned}\rho_R\psi = &\frac{G}{2}\left[\left(a^2\left(1+\gamma^2\right)+b^2\right)-2\right] + \frac{\lambda}{2}\left(\log(ab)\right)^2 - G\log(ab)\\ &+\frac{G}{2}k\left(a^2-1\right)^2,\end{aligned} \tag{4.3}$$

To be able to use (3.8), we have to write the free energy in terms of the strain basis δ, ϵ and γ. Using (3.12) we obtain

$$\begin{aligned}\rho_R\psi = &\frac{G}{2}\left[\left(e^{\frac{2}{n}(\delta+\epsilon)}\left(1+\gamma^2\right)+e^{2n(\delta-\epsilon)}\right)-2\right] + \frac{\lambda}{2}\left(\frac{1}{n}(\delta+\epsilon)+n(\delta-\epsilon)\right)^2\\ &- G\left[\frac{1}{n}(\delta+\epsilon)+n(\delta-\epsilon)\right] + \frac{G}{2}k\left(e^{\frac{2}{n}(\delta+\epsilon)}-1\right)^2.\end{aligned}$$

Since according to Section 3.2.8, the resulting stress tensor does not depend on n, we can for simplicity set $n = 1$. Now we can finally use (3.8) to obtain:

$$\begin{aligned}\pi &= G\left[e^{2(\delta+\epsilon)}\left(1+\gamma^2\right)+e^{2(\delta-\epsilon)}\right] + 4\lambda\delta - 2G + 2Gk\left(e^{2(\delta+\epsilon)}-1\right)e^{2(\delta+\epsilon)},\\ \sigma &= G\left[e^{2(\delta+\epsilon)}\left(1+\gamma^2\right)-e^{2(\delta-\epsilon)}\right] + 2Gk\left(e^{2(\delta+\epsilon)}-1\right)e^{2(\delta+\epsilon)}\\ \tau &= Ga^2\gamma.\end{aligned}$$

4.2 Problem description

We assume the following problem for comparison of the models: consider a piece of material, which is fixed on the left hand side and is being pulled to the right on the right hand side. See Figure 4.1.

We consider two different domains. The first domain is just a square $\Omega_1 = (0,1)\times(0,1)$. The second domain Ω_2 is a square $(0,1)\times(0,1)$ from which we subtract an ellipse with center at $(1/2, 1/2)$ and semiaxes with lengths $1/6$ and $1/50$. We consider this domain with both ellipse orientations. This domain can be seen as an approximation of a material with inner crack.

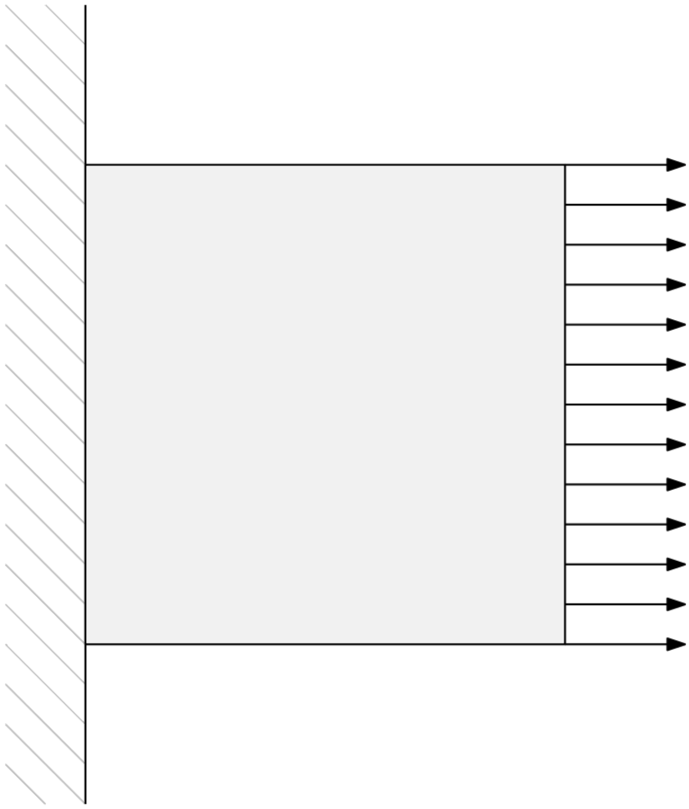


Figure 4.1: An illustration of the problem.

Rigorously, let $\Omega = \Omega_1$ or Ω_2 and $\mathbf{f} = (f, 0)^\top$ be a given function. Then we are looking for a solution of:

$$
\begin{aligned}
\operatorname{div} \mathbb{T}_R &= \mathbf{0} && \text{in } \Omega, \\
\mathbf{u} &= \mathbf{0} && \text{on } \{x = 0\}, \\
\mathbb{T}_R \mathbf{N} &= \mathbf{f} && \text{on } \{x = 1\},
\end{aligned}
$$

where $\mathbf{u}$ is displacement and $\mathbf{N}$ is outer unit normal vector in the reference configuration.

In the case of linear elasticity, we are looking for a solution of an analogous problem:

$$
\begin{aligned}
\operatorname{div} \mathbb{T} &= \mathbf{0} && \text{in } \Omega, \\
\mathbf{u} &= \mathbf{0} && \text{on } \{x = 0\}, \\
\mathbb{T} \mathbf{N} &= \mathbf{f} && \text{on } \{x = 1\}.
\end{aligned}
$$

4.2.1 Material parameters

We have to set a few material parameters in order to be able to perform numerical experiments. The following parameters are required:

- Lamé parameter λ
- shear modulus G

- fiber stiffness k
- fiber direction $\mathbf{A}$
- matrix of anisotropy $\mathbb{Q}^A$
- applied pressure f

We set the Lamé parameter to $\lambda = 10^9$ Pa and the shear modulus to $G = 5 \cdot 10^8$ Pa. We perform the experiments with various fiber stiffness, thus we set $k = 1$ and $k = 100$. The value $k = 100$ represents fibers with very high stiffness, as for example the fiber stiffness of the brainstem of four weeks old piglets is around 20 (Ning et al. [2006]). The matrix of anisotropy $\mathbb{Q}^A$ with the angle α also varies and is specified in the results. The fiber direction $\mathbf{A}$ is simply set as $\mathbf{A} = \mathbb{Q}^{A^\top} \mathbf{e}_1^C = \mathbb{Q}^{A^\top} (1, 0)^\top$.

4.3 Wolfram Mathematica

Wolfram Mathematica is a software for symbolic computations, statistics, data science, optimization as well as machine learning or natural language processing. It contains thousands of built-in functions for all areas of technical computing. Mathematica, firstly released in 1987, is a flagship product of a company Wolfram Research founded by Stephen Wolfram in 1987.

Version 13.0, released on 13th of December 2021, introduced a support of solid and structural mechanics, allowing its users to easily set up and solve complicated problems. Version 13.1, released on 29th of June 2022, further extended the solid mechanics framework and included Green elasticity. The current version 13.2 was released on 14th of December 2022 and polished some flaws and fixed various bugs. For more information about solid Mathematica's solid mechanics framework and Green elasticity, see Mat [c] and Mat [b].

Mathematica uses the finite element method to solve partial differential equations. The default finite element interpolation order is two, but can be specified by the user. More details about the finite element method in Mathematica can be found in Mat [a].

4.3.1 Simple example

Let us take a look at how we can use Mathematica to solve problems arising in solid mechanics. We use the problem described in Section 4.2 as an example.

We start by importing the package for finite elements and by clearing all variables.

```
ClearAll["Global`*"]
Needs["NDSolve`FEM`"]
```

Then we set up parameters `pars`. We want to use neo-Hookean isotropic solid, which is done by setting the `MaterialModel` parameter. Then we set material parameters, in this case Lamé's parameter and shear modulus. We also specify thickness of our sample.

```
pars = <|"MaterialModel" -> "NeoHookeanIsotropic",
        "LameParameter" -> 1000000000, "ShearModulus" -> 5*100000000,
        "Thickness" -> 1|>;
```

Next we set up our variables `vars`. Mathematica computes a displacement, which will have components `u` and `v`. The displacement will depend on coordinates `x` and `y`. What remains is to set our domain Ω (denoted by `\[CapitalOmega]` in the code), which will be a rectangle with vertices at $(0, 0)$ and $(1, 1)$ (or in other words, Ω will be a square at origin with side length equal to 1) and finally create a mesh `mesh` from Ω.

```
vars = {{u[x, y], v[x, y]}, {x, y}};
\[CapitalOmega] = Rectangle[{0, 0}, {1, 1}];
mesh = ToElementMesh[\[CapitalOmega]];
```

Now we set up and solve an equation. `SolidMechanicsPDEComponent` takes our parameters and variables and returns desired equation. To specify boundary conditions we use `SolidBoundaryLoadValue` and `SolidFixedCondition`. We use the first one to specify, that we want pressure `p`[1] acting in acting in direction `x` at $x = 1$. We then use the latter one to set zero displacement at $x = 0$. The equation and boundary conditions are then saved into variable `pde`. If we wanted to prescribe a displacement, we could use `SolidDisplacementCondition`.

```
pde := {SolidMechanicsPDEComponent[vars, pars] ==
        SolidBoundaryLoadValue[x == 1, vars, pars,
           <|"Pressure" -> {p, 0}|>],
        SolidFixedCondition[x == 0, vars, pars]};
```

To solve the equation for displacement, we use `NDSolveValue`. We set the pressure `p`, specify that `u` and `v` are unknowns and that `x` and `y` are in the domain Ω. The `NDSolveValue` function returns computed displacement. To measure computation time, `AbsoluteTiming` is used. ($\in$ is denoted `\[Element]` in the code.)

```
AbsoluteTiming[displacement = NDSolveValue[pde /. p -> 3*100000000,
    {u[x, y], v[x, y]}, {x, y} \[Element] \[CapitalOmega]];]
```

We have computed the displacement, so we can use `VectorDisplacementPlot` to visualize it.

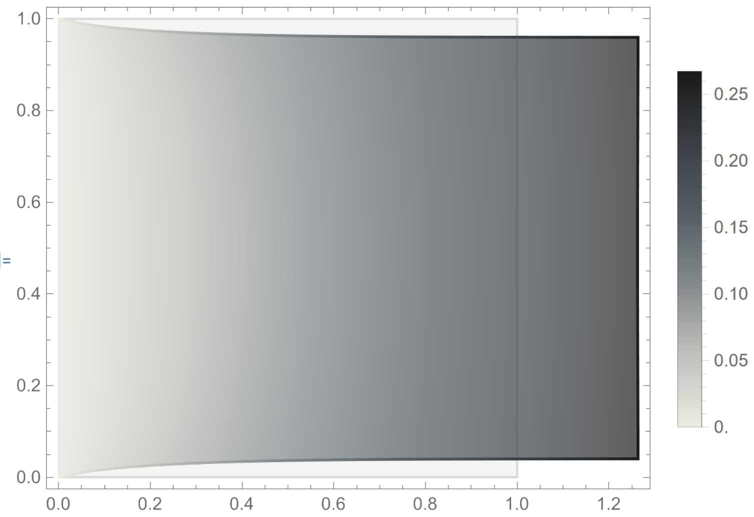
```
VectorDisplacementPlot[displacement,
        {x, y} \[Element] \[CapitalOmega], VectorSizes -> Full,
         ColorFunction -> ColorData[{"GrayTones", "Reverse"}],
         PlotLegends -> Automatic]
```

This is the result. We see that the computation took a little bit more than one second.

[1]It is also possible to prescribe force instead of pressure. Mathematica will automatically convert force to pressure.

Out[128]= {1.19077, Null}

Out[129]=



4.3.2 Stress

We now show, how to compute and visualize stress. First we have to compute `strain` using `SolidMechanicsStrain`.

```
strain = SolidMechanicsStrain[vars, pars, displacement];
```

Now we can easily compute the first Piola-Kirchhoff stress tensor `firstPK`. We use `SolidMechanicsStress`, but we have to specify, that we want the first Piola-Kirchhoff stress tensor using the `OutputStressMeasure` parameter.[2] To do this, we use `Join` to join the parameters together.

```
firstPK = SolidMechanicsStress[vars,
   Join[pars, <|"OutputStressMeasure" -> "FirstPiolaKirchhoff"|>],
   strain, displacement];
```

Since the first Piola-Kirchhoff stress tensor is matrix, its visualization is difficult. Thus we visualize only its norm instead. To compute the norm `firstPKNorm`, we use `Norm`, where we specify, that the desired norm is Frobenius norm.[3]

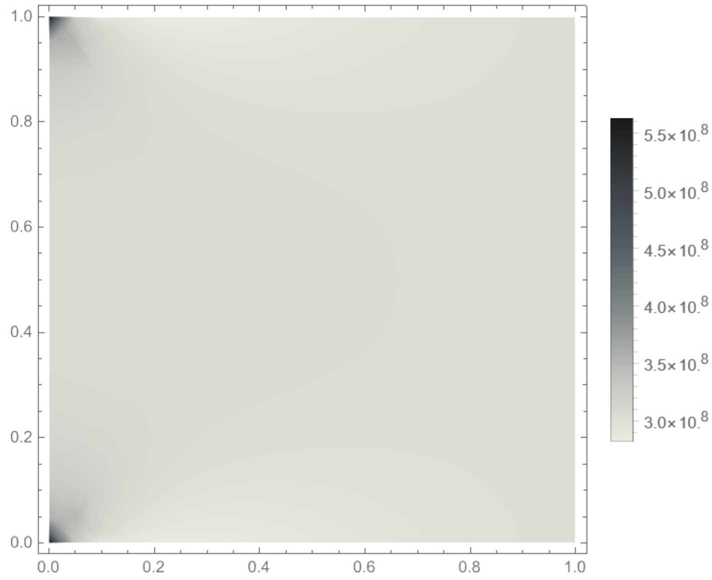
```
firstPKNorm = Norm[firstPK, "Frobenius"];
```

Now we can use `DesnityPlot` to visualize it.

```
DensityPlot[firstPKNorm, {x, y} \[Element] mesh,
        ColorFunction -> ColorData[{"GrayTones", "Reverse"}],
        PlotRange -> Full, PlotLegends -> Automatic]
```

This is the result:

[2]The default option is Cauchy stress tensor.
[3]The default option is spectral norm (largest singular value of matrix).



Visualization of Cauchy stress tensor is more difficult, since Mathematica computes it only in the domain Ω, which is not deformed. Therefore it has to be mapped onto the deformed mesh. First we compute the Cauchy stress tensor `cauchy` using `SolidMechanicsStress`. We do not have to specify the stress measure, since Cauchy stress is the default option.

```
cauchy = SolidMechanicsStress[vars, pars, strain, displacement];
```

Then we compute its Frobenius norm `cauchyNorm` using `Norm`.

```
cauchyNorm = Norm[cauchy, "Frobenius"];
```

Now we use `ElementMeshDeformation` to compute deformed mesh `deformedMesh`.

```
deformedMesh = ElementMeshDeformation[mesh,
               displacement, "ScalingFactor" -> 1];
```

We then evaluate the norm of Cauchy stress tensor on elements of the mesh using `EvaluateOnElementMesh`.

```
evaluatedCauchyNorm = EvaluateOnElementMesh[{x, y}, cauchyNorm, mesh];
```

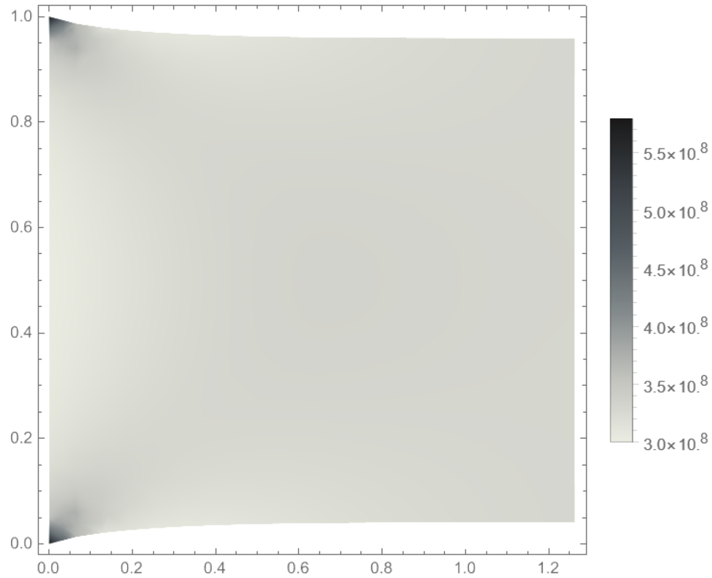
We can finally interpolate the norm of the stress tensor onto the deformed mesh using `ElementMeshInterpolation` to obtain `deformedCauchyNorm`.

```
deformedCauchyNorm = ElementMeshInterpolation[deformedMesh,
                        evaluatedCauchyNorm["ValuesOnGrid"]];
```

Once again we use `DensityPlot` to visualize the result.

```
DensityPlot[deformedCauchyNorm[x, y], {x, y} \[Element] deformedMesh,
        ColorFunction -> ColorData[{"GrayTones", "Reverse"}],
        PlotRange -> Full, PlotLegends -> Automatic]
```

We obtain the following image:



4.3.3 Custom material model

What remains to show is how to implement our custom materials. We present the implementation of the standard reinforced material described in section 4.1, because this is not Mathematica's built-in material model and we use it later.

We need a constitutive equation for some stress tensor to implement custom material. We already have a formula for the Cauchy stress tensor, see 4.2:

$$\mathbb{T} = \frac{1}{\sqrt{\det \mathbb{C}}} \left[\left(\lambda \log \sqrt{\det \mathbb{C}} - G \right) \mathbb{I} + G\mathbb{B} + 2Gk \left(\mathbf{A} \cdot \mathbb{C}\mathbf{A} - 1 \right) \mathbf{A} \otimes \mathbf{A} \right].$$

Now we can write our function, that will implement the standard reinforcing material. We use the `Module` environment, which is used to set up local variables, and create module `StandardReinforcingMaterial`. First, we load variables (displacement `u` and coordinates `x`) and material parameters (shear modulus `G`, Lamé parameter λ (denoted as `\[Lambda]`), fiber strength `k` and fiber direction `A`).

Then we set dimension `dim` as length of `x` and appropriate identity matrix `idm`. Now we can compute gradient of displacement `gradU`, deformation gradient `F` and also determinant of deformation gradient `J` and left Cauchy-Green strain tensor `c`.

Now we have all we need to compute the Cauchy stress tensor `stressMatrix` (tensor product of fiber direction `A` with itself is denoted as `\[TensorProduct]`), which we then simplify using `Simplify` and return.

```
StandardReinforcingMaterial[vars_ , pars_ , data_] :=
 Module[{u, x, dim, G, \[Lambda], k, A, idm, F, J, c, stressMatrix},
  u = vars[[1]];
  x = vars[[-1]];

  G = pars["ShearModulus"];
  \[Lambda] = pars["LameParameter"];
  k = pars["k"];
  A = pars["A"];

  dim = Length[x];
  idm = IdentityMatrix[dim];
  F = Grad[u, x] + idm;
  J = Det[F];
  c = Transpose[F].F;

  stressMatrix = 1/J*((\[Lambda]*Log[J] - G)*idm + G*F.Transpose[F]
                 + 2*G*k*(Transpose[A].c.A - 1)*(A\[TensorProduct]A));
  stressMatrix = Simplify[stressMatrix];
  stressMatrix
 ]
```

Program code 1: Implementation of the standard reinforcing material.

We have successfully implemented standard reinforcing material. We have to slightly modify parameters `pars` in order to use it. We need to set up additional parameters and use `MaterialModelFunction` instead of `MaterialModel`. Also we need to set `ConstitutiveStressMeasure` to Cauchy stress tensor.[4]

```
pars = <|"MaterialModelFunction" -> StandardReinforcingMaterial,
   "ConstitutiveStressMeasure" -> "Cauchy", "LameParameter" -> 270,
   "ShearModulus" -> 400, "k" -> 1, "A" -> {Sqrt[2]/2, Sqrt[2]/2},
   "Thickness" -> 1|>;
```

This is all we have to do. Now we can perform computations with our custom material model.

If we wanted to implement the standard reinforcing material using the conjugate stress / strain basis pairs model, the resulting module could look like this:

[4]Default option is second Piola-Kirchhoff stress tensor.

```
QRStandardReinforcingMaterial[vars_, pars_, data_] :=
 Module[{u, x, dim, idm, k, Q, G, \[Lambda], F, FA, R, sin\[Theta],
   cos\[Theta], a, b, \[Gamma], U, \[Delta], \[Epsilon],
   pi, \[Sigma], \[Tau], STilde11, STilde22, STilde12, STilde,
   stressMatrix},
  u = vars[[1]];
  x = vars[[-1]];
  G = pars["ShearModulus"];
  \[Lambda] = pars["LaméParameter"];
  k = pars["k"];
  Q = pars["Q"];

  dim = Length[x];
  idm = IdentityMatrix[dim];
  F = idm + Grad[u, x];
  FA = Q.F.Transpose[Q];

  sin\[Theta] = -FA[[2, 1]]/Sqrt[FA[[1, 1]]^2 + FA[[2, 1]]^2];
  cos\[Theta] = FA[[1, 1]]/Sqrt[FA[[1, 1]]^2 + FA[[2, 1]]^2];
  R = {{cos\[Theta], sin\[Theta]}, {-sin\[Theta], cos\[Theta]}};

  a = Sqrt[FA[[1, 1]]^2 + FA[[2, 1]]^2];
  b = (FA[[1, 1]] FA[[2, 2]] - FA[[1, 2]] FA[[2, 1]])/
     Sqrt[FA[[1, 1]]^2 + FA[[2, 1]]^2];
  \[Gamma] = (FA[[1, 1]] FA[[1, 2]] +
           FA[[2, 1]] FA[[2, 2]])/(FA[[1, 1]]^2 + FA[[2, 1]]^2);
  U = {{a, a*\[Gamma]}, {0, b}};

  \[Delta] = Log[Sqrt[a*b]];
  \[Epsilon] = Log[Sqrt[a/b]];
  pi = G (Exp[2*(\[Delta] + \[Epsilon])]*(1 + \[Gamma]^2)
      + Exp[2*(\[Delta] - \[Epsilon])]) + 4*\[Lambda]*\[Delta] - 2*G
      + 2*G*k*(Exp[2*(\[Delta] + \[Epsilon])] - 1)
      *Exp[2*(\[Delta] + \[Epsilon])];
  \[Sigma] = G (Exp[2*(\[Delta] + \[Epsilon])]*(1 + \[Gamma]^2)
           - Exp[2*(\[Delta] - \[Epsilon])])
           + 2*G*k*(Exp[2*(\[Delta] + \[Epsilon])] - 1)
           *Exp[2*(\[Delta] + \[Epsilon])];
  \[Tau] = G*a^2*\[Gamma];

  STilde11 = 1./2.*(pi + \[Sigma]);
  STilde22 = 1./2.*(pi - \[Sigma]);
  STilde12 = (b/a)*\[Tau];
  STilde = {{STilde11, STilde12}, {STilde12, STilde22}};

  stressMatrix = 1/Det[F]*Transpose[Q].R.STilde.Transpose[R].Q;
  stressMatrix = Simplify[stressMatrix];
  stressMatrix
 ]
```

Program code 2: Implementation of the standard reinforcing material using the conjugate stress / strain basis model.

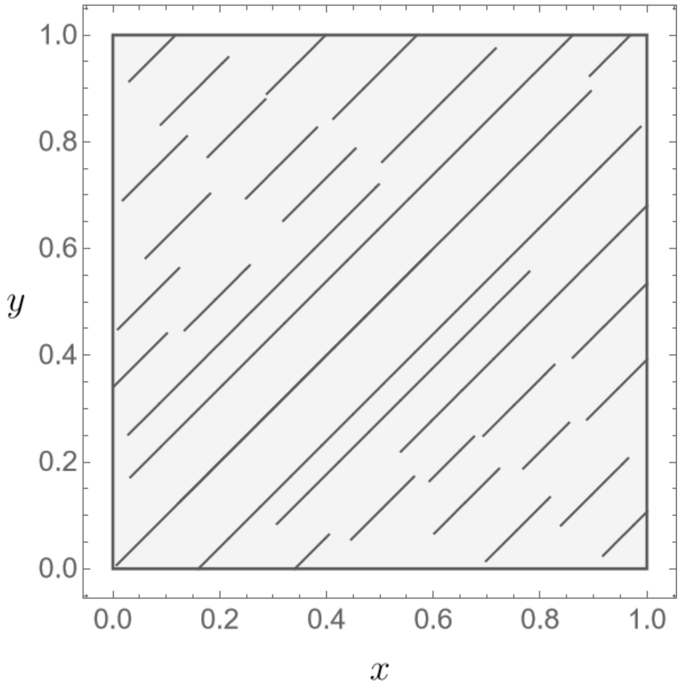


Figure 4.2: Fibers in the reference configuration.

4.4 Results

In this final section we present the results of several numerical experiments. We consider fibers with various directions, which is specified by the anisotropy matrix $\mathbb{Q}^A$ and the angle α:

$$\mathbb{Q}^A = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}.$$

Every experiment is first computed with $k = 1$ and then with $k = 100$. We present the fiber direction in the reference configuration, fiber direction in the current configuration and the norm of the Cauchy stress tensor. For the first experiment we also present the norms of the displacement and the first Piola-Kirchhoff stress tensor. Computation times are also presented.

Computations were performed on six years old laptop Lenovo Ideapad 700-15ISK with the Intel Core i7-6700HQ CPU.

4.4.1 Straight fibers

As the first experiment, we consider fibers with the angle equal to $\alpha = -\pi/4$. The visualization of fibers in the reference configuration can be seen in Figure 4.2. The mesh, that is used, can be seen in Figure 4.3. The mesh has 400 elements and the computational problem has 2562 degrees of freedom.

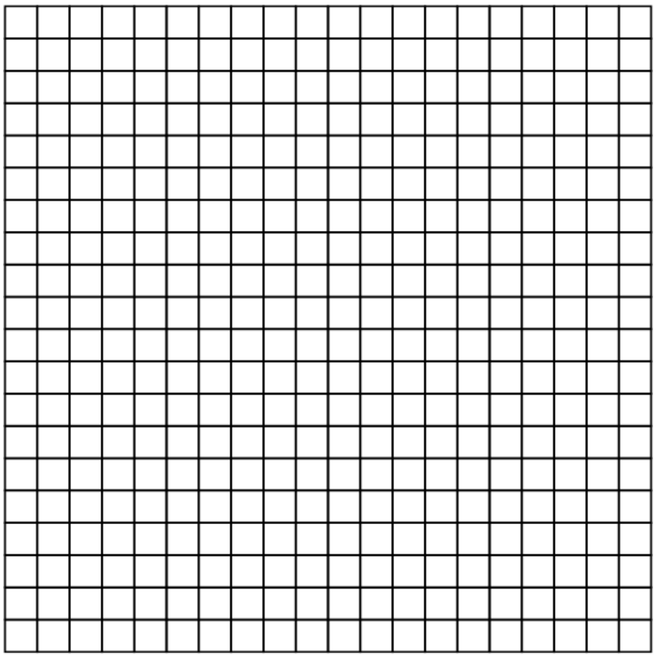


Figure 4.3: The mesh used for the square domain.

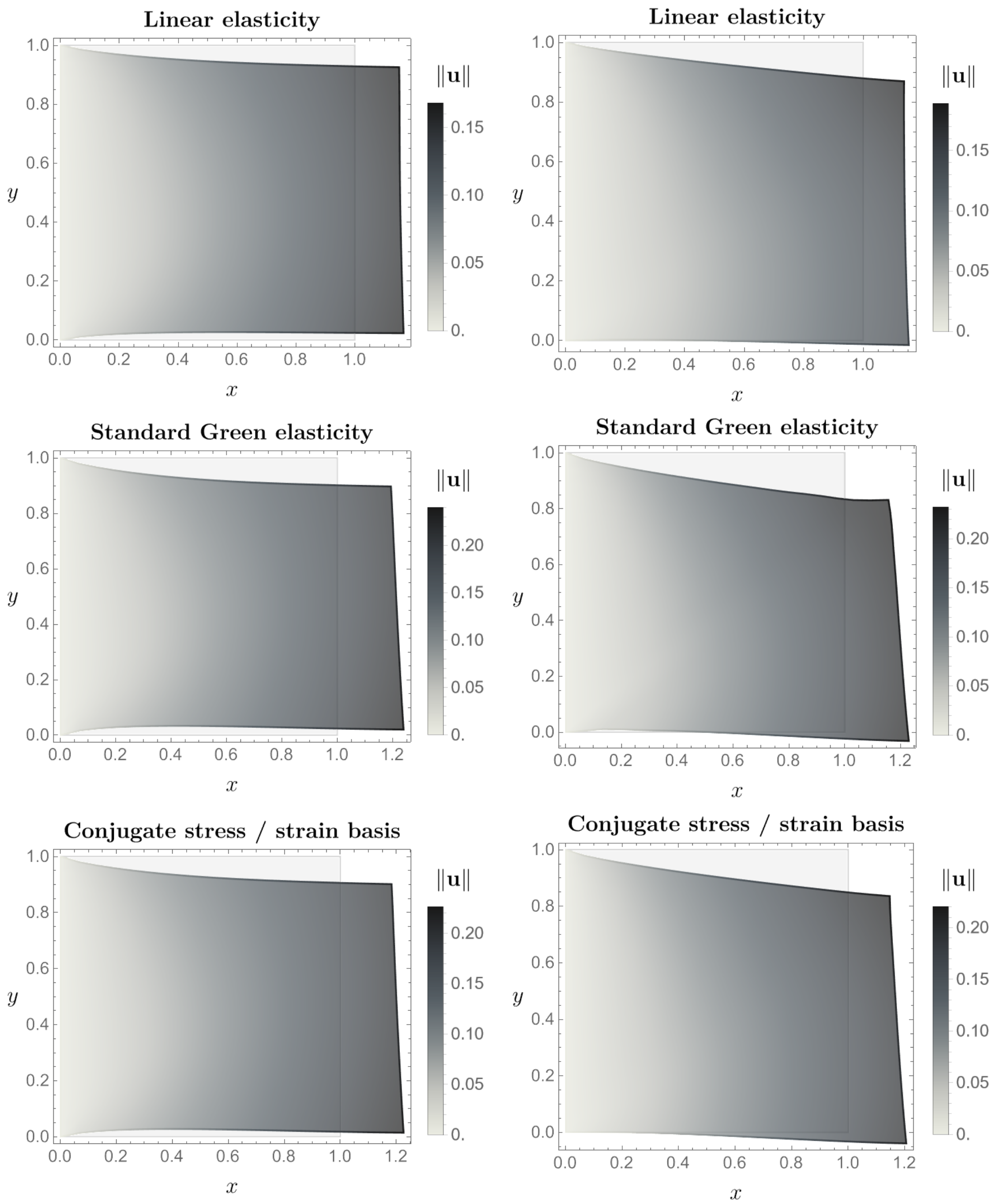


Figure 4.4: Norm of the displacement. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.404	1.399	45.161	1
	0.380	2.411	114.358	100

Table 4.1: Displacement computation time.

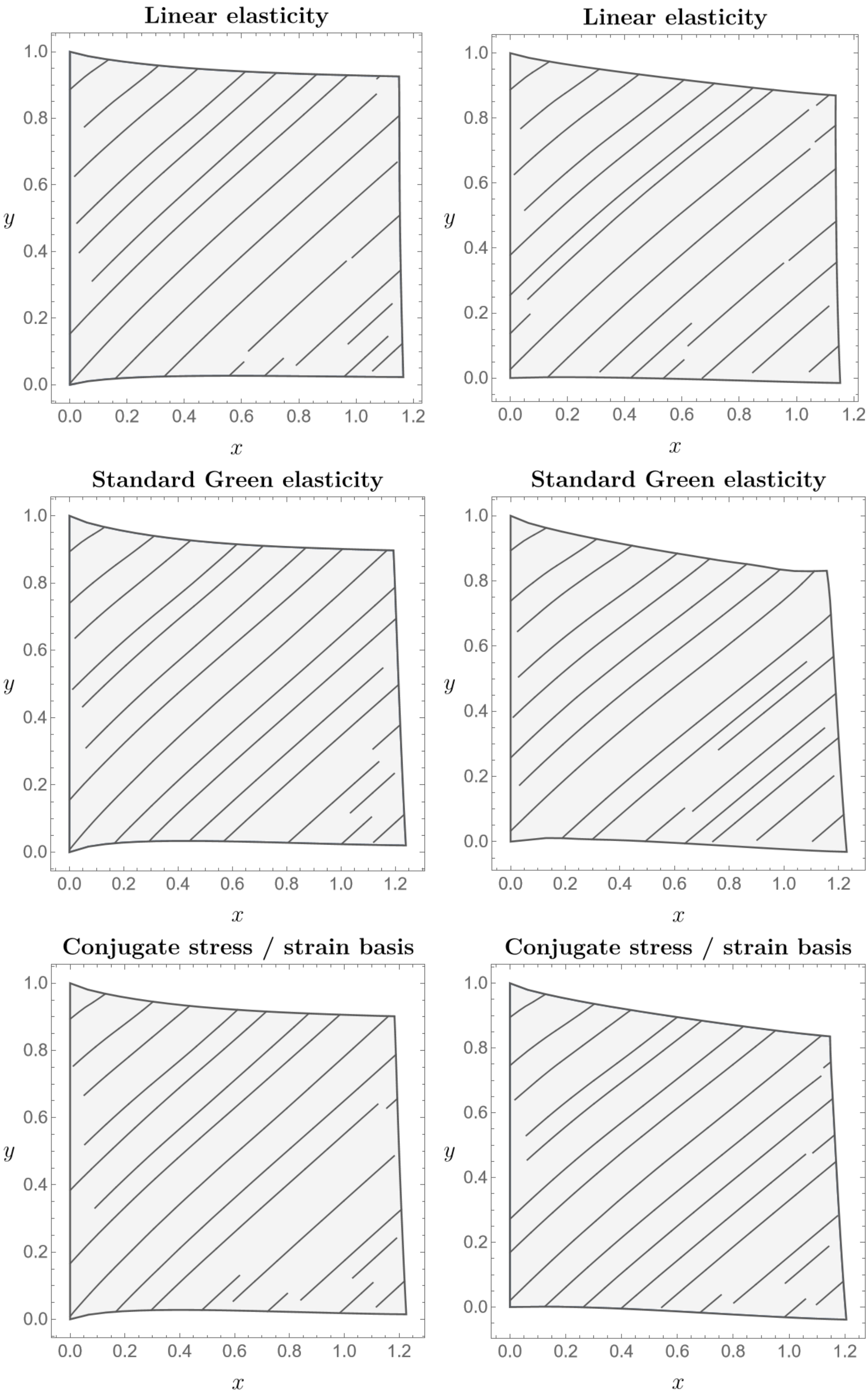


Figure 4.5: Fibers in the current configuration. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

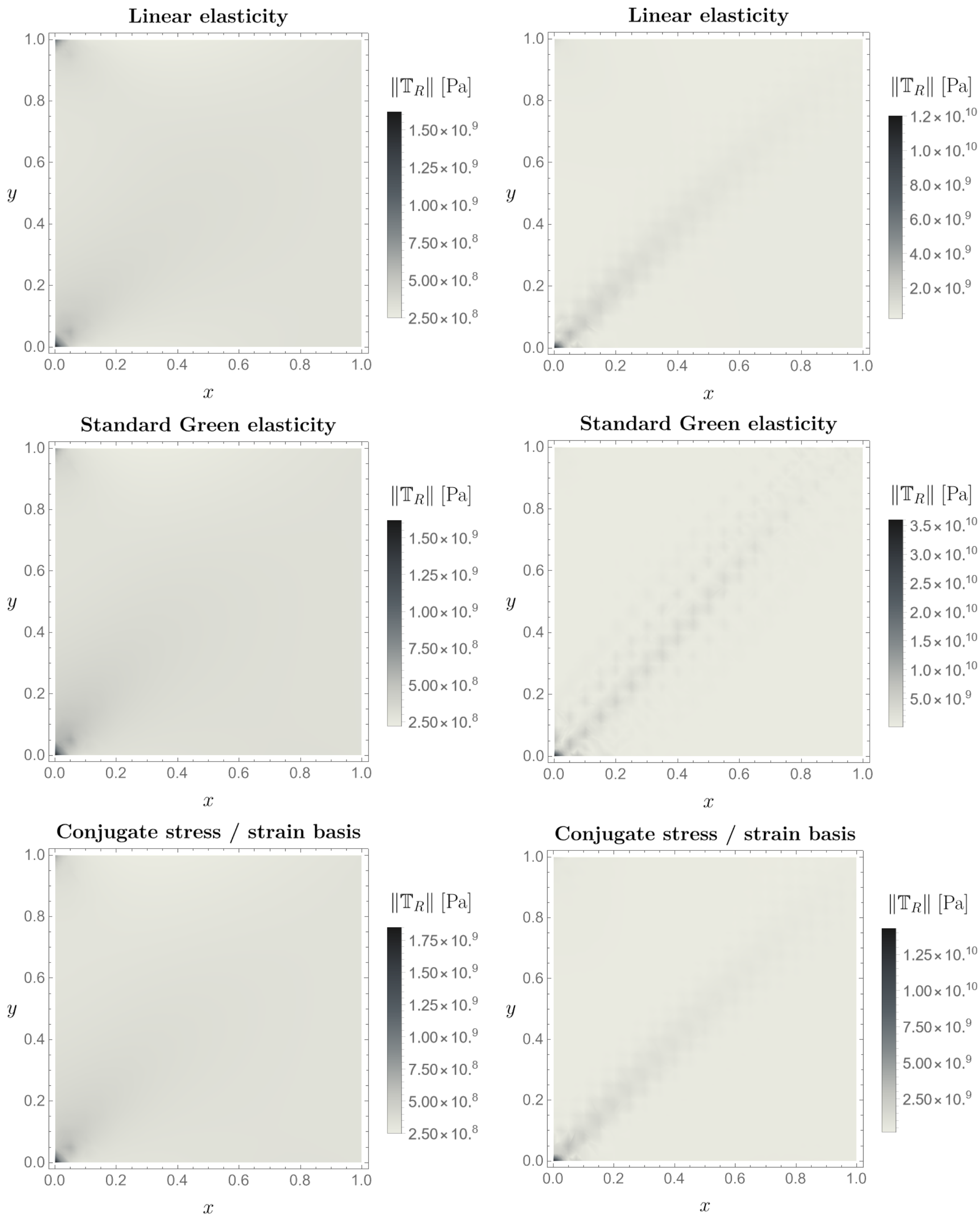


Figure 4.6: Norm of the first Piola-Kirchhoff stress tensor. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.359	1.983	52.091	1
	0.443	1.890	59.807	100

Table 4.2: Norm of the first Piola-Kirchhoff stress tensor computation time

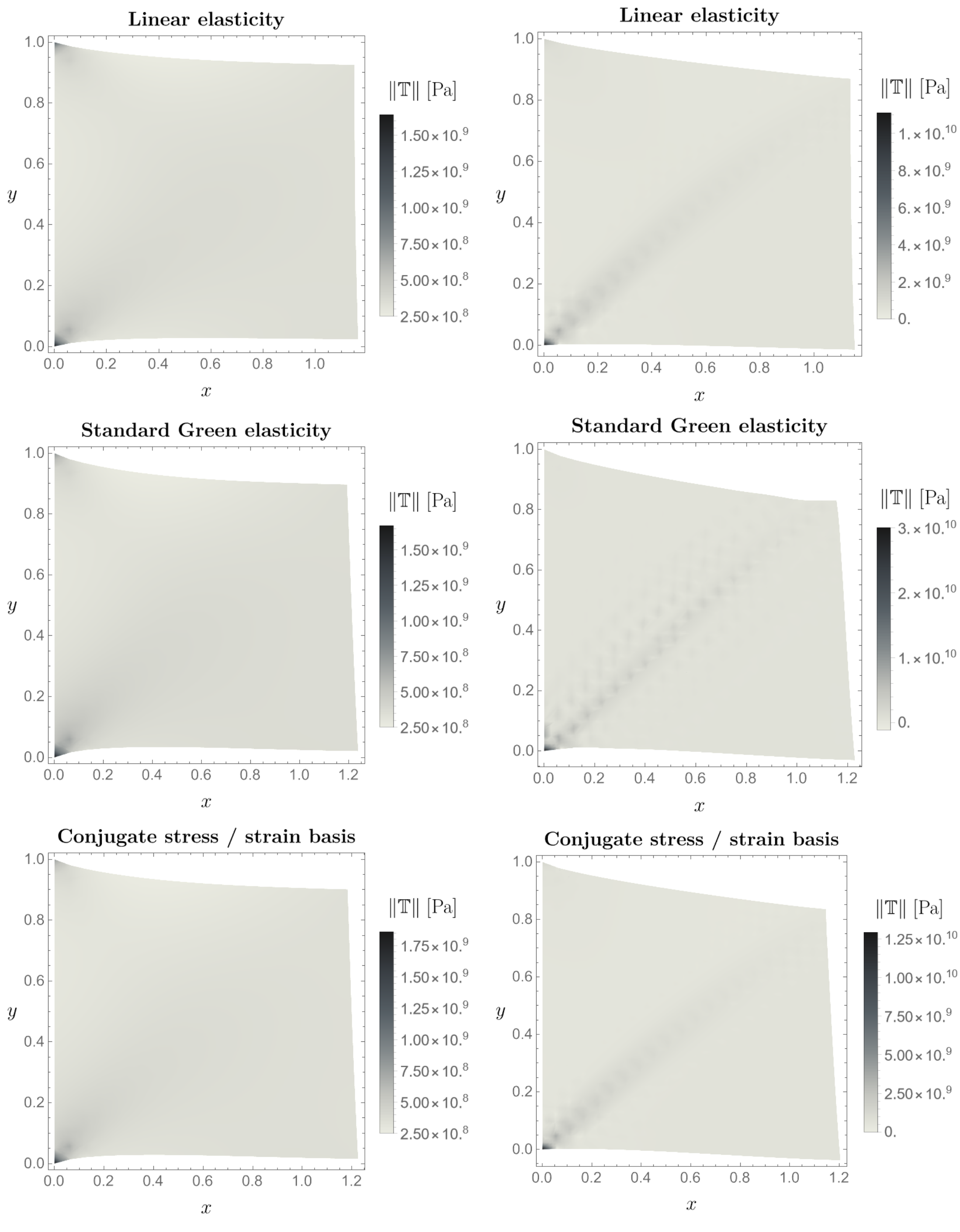


Figure 4.7: Norm of the Cauchy stress tensor. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.896	0.555	27.097	1
	1.159	0.548	33.504	100

Table 4.3: Norm of the Cauchy stress tensor computation time

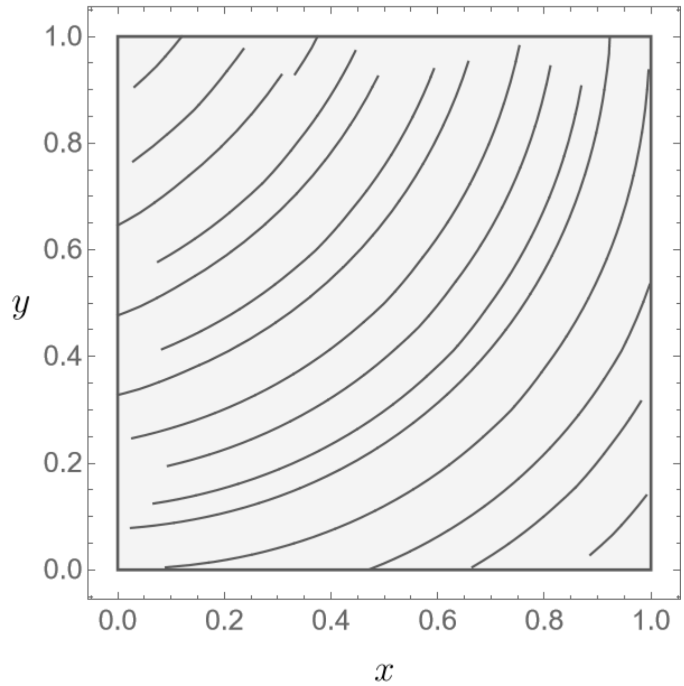
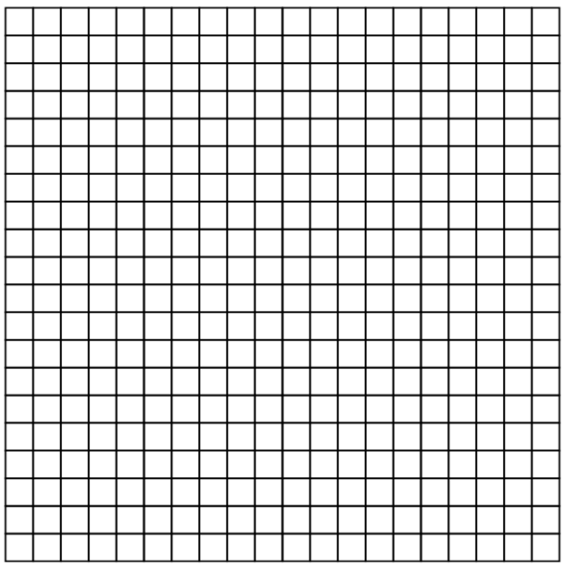


Figure 4.8: Fibers in the reference configuration.

4.4.2 Curved fibers

For the next experiment, we consider fibers with the angle equal to $\alpha = -\frac{\pi}{4}(x+y)$. This results in the fibers, that are not straight. Their visualization can be seen in Figure 4.8. The mesh is the same as in the previous case, that is:



	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.817	4.080	1164.08	1
	0.890	4.964	1235.56	100

Table 4.4: Displacement computation time.

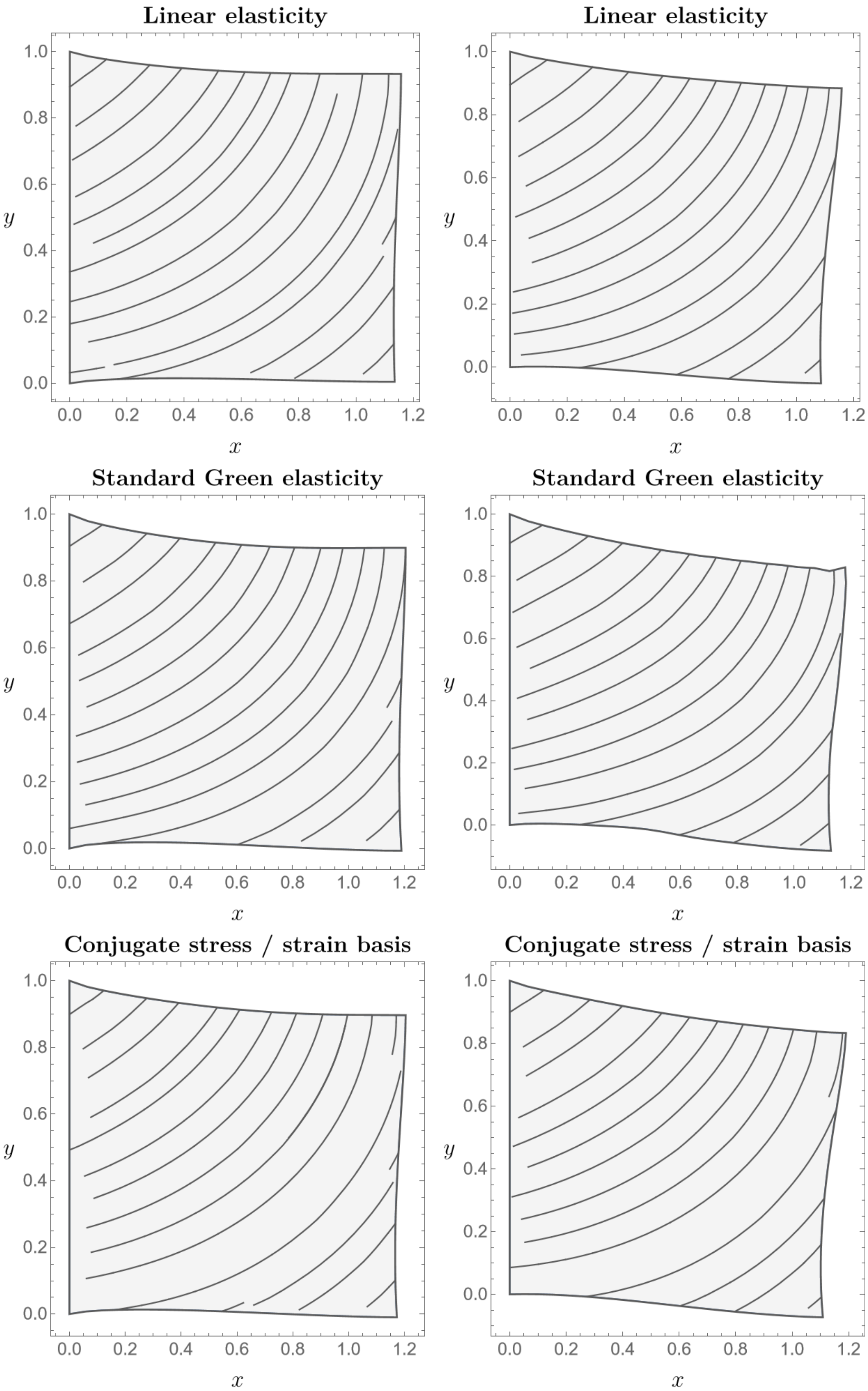


Figure 4.9: Fibers in the current configuration. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

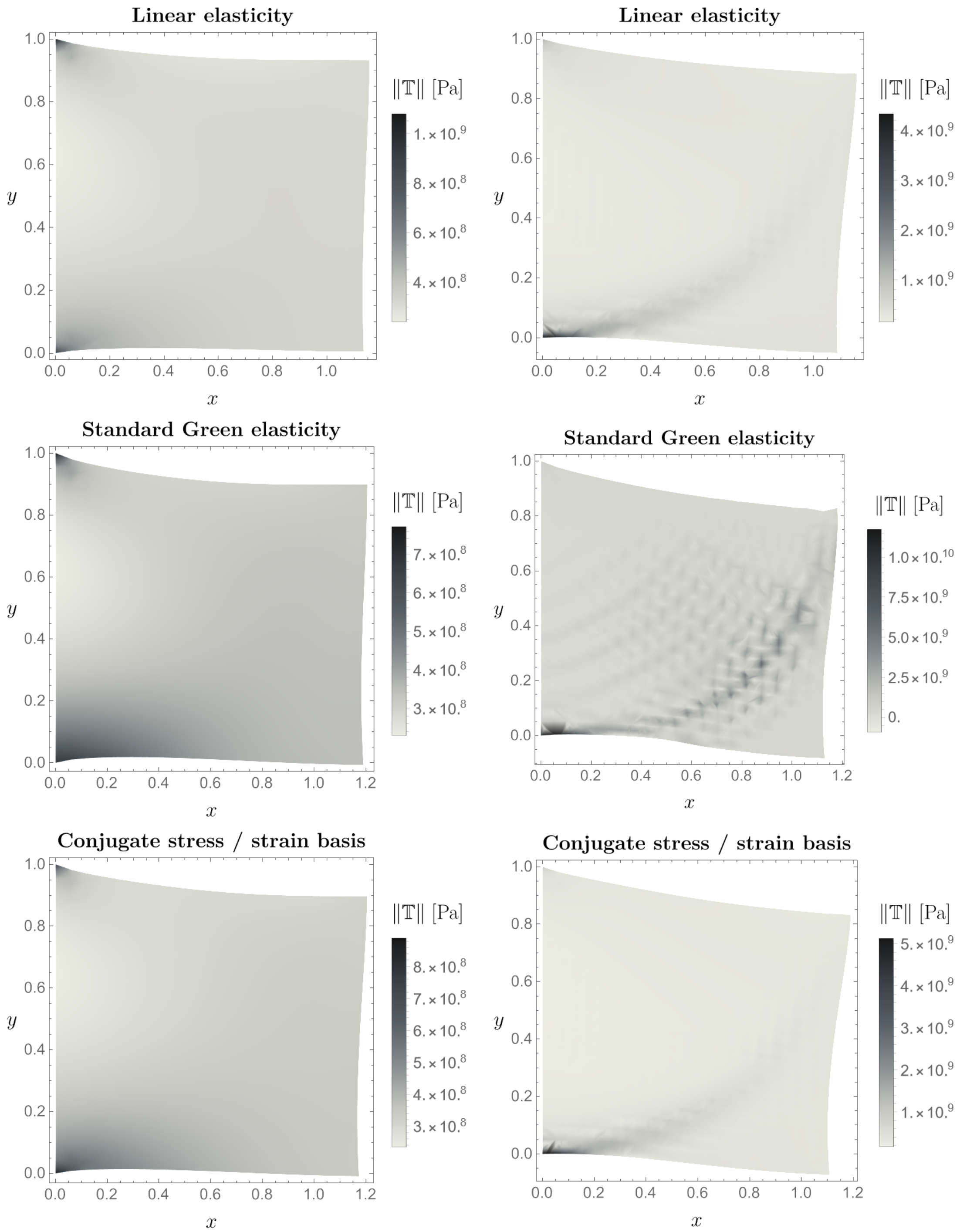


Figure 4.10: Norm of the Cauchy stress tensor. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	1.954	3.000	1084.2	1
	1.960	2.154	1051.78	100

Table 4.5: Norm of the Cauchy stress tensor computation time

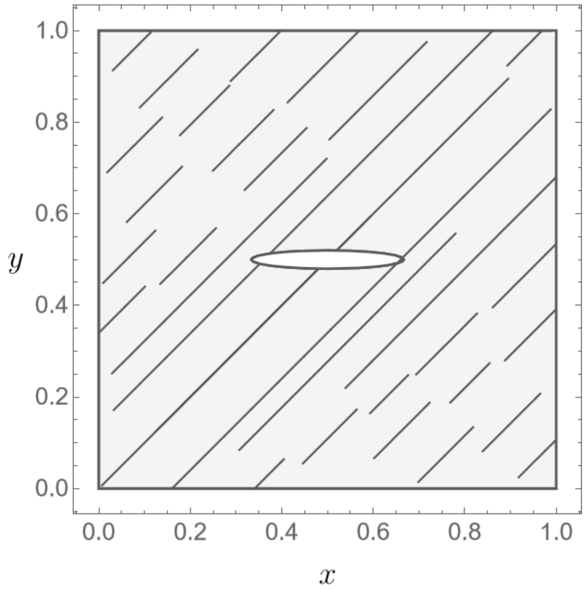


Figure 4.11: Domain shape with fibers.

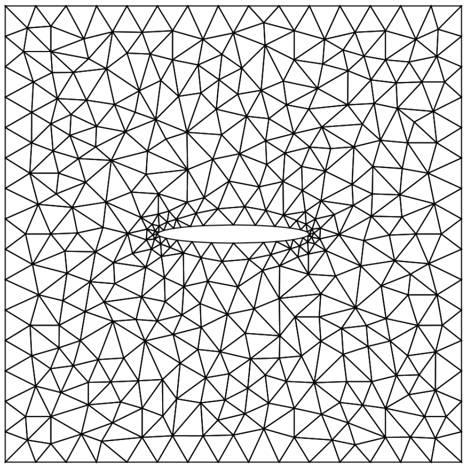


Figure 4.12: The mesh used to approximate a cracked material.

4.4.3 Cracked material I

Now we consider the second domain described in the Section 4.2, which can be seen as an approximation of a cracked material. We for simplicity consider straight fibers angled at $\alpha = -\pi/4$. The domain with the fibers can be seen in Figure 4.11. The used mesh can be seen in Figure 4.12 and has 694 elements. The resulting computational problem has 2948 degrees of freedom.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.529	1.3345	36.314	1
	0.525	2.697	151.372	100

Table 4.6: Displacement computation time.

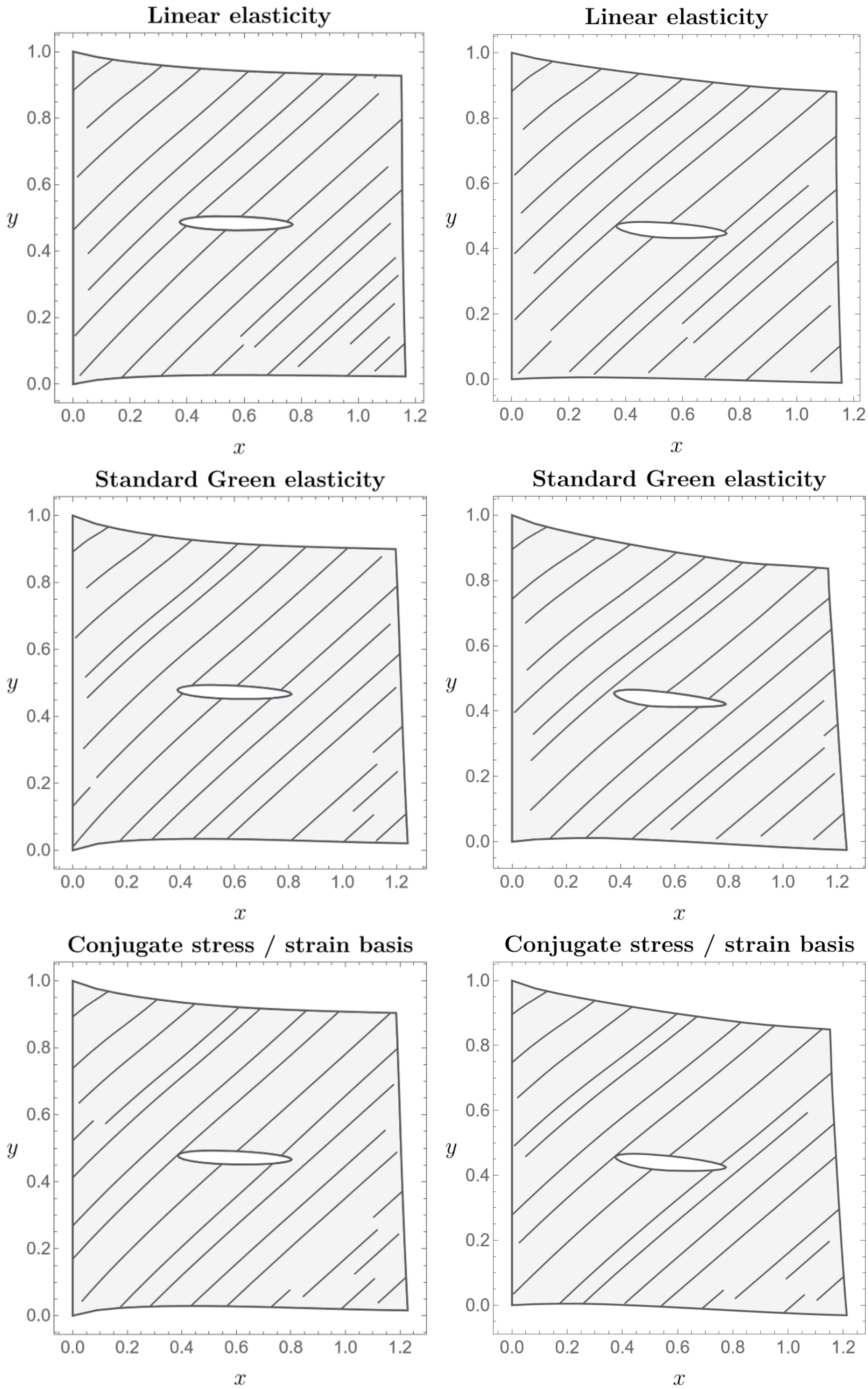


Figure 4.13: Fibers in the current configuration. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

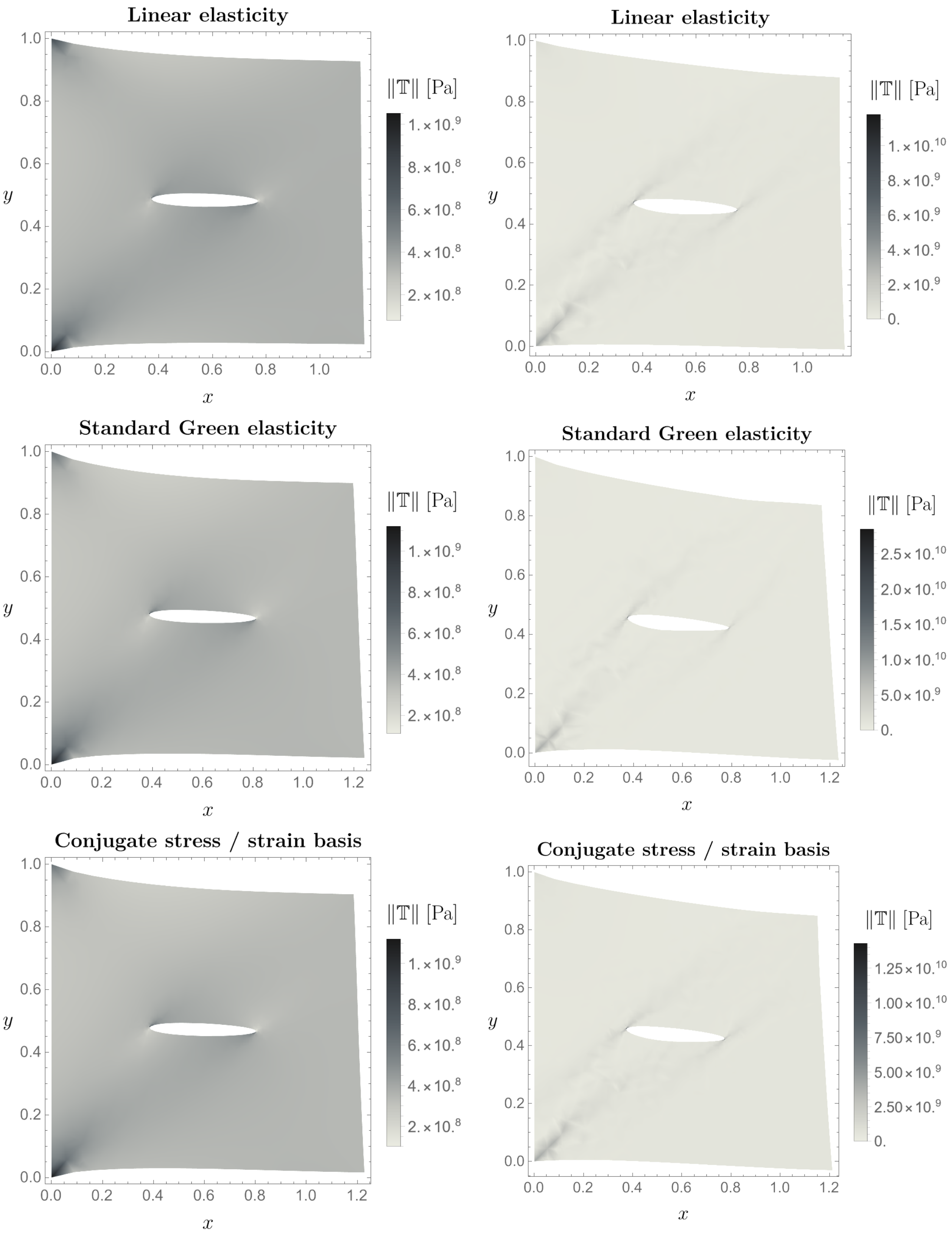


Figure 4.14: Norm of the Cauchy stress tensor. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	1.046	0.644	27.001	1
	1.050	0.761	37.791	100

Table 4.7: Norm of the Cauchy stress tensor computation time

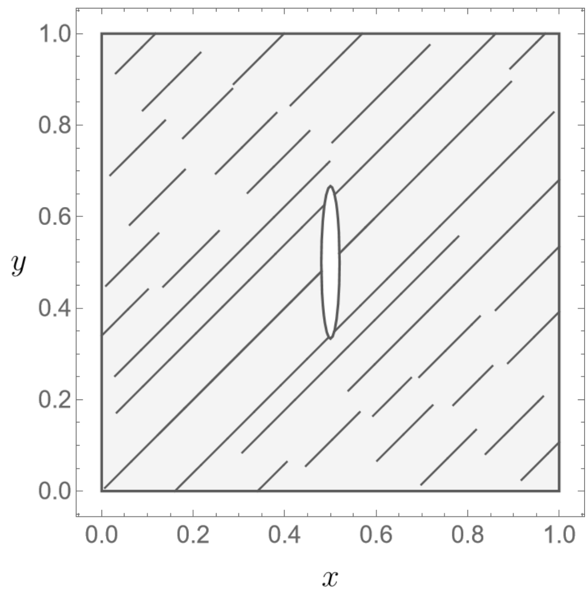


Figure 4.15: Domain shape with fibers.

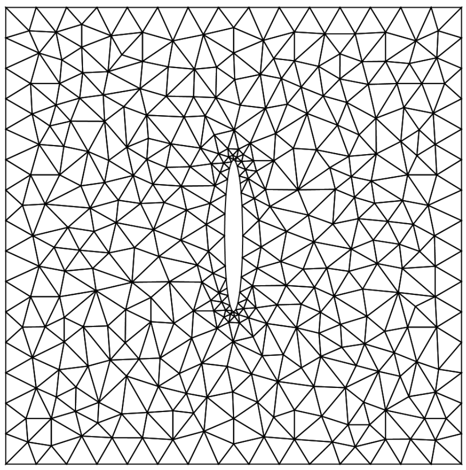


Figure 4.16: The mesh used to approximate a cracked material.

4.4.4 Cracked material II

For the final experiment, we consider the second domain described in the Section 4.2, but now with the ellipse rotated by $\pi/4$. We for simplicity consider straight fibers angled at $\alpha = -\pi/4$. The domain with the fibers can be seen in Figure 4.15 and the mesh, which has 698 elements, in Figure 4.16. The computational problem has 2964 degrees of freedom. The results for the standard Green elastic model with $k = 100$ are not presented, as the computation failed.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	0.708	3.659	59.850	1
	0.509	—	152.578	100

Table 4.8: Displacement computation time.

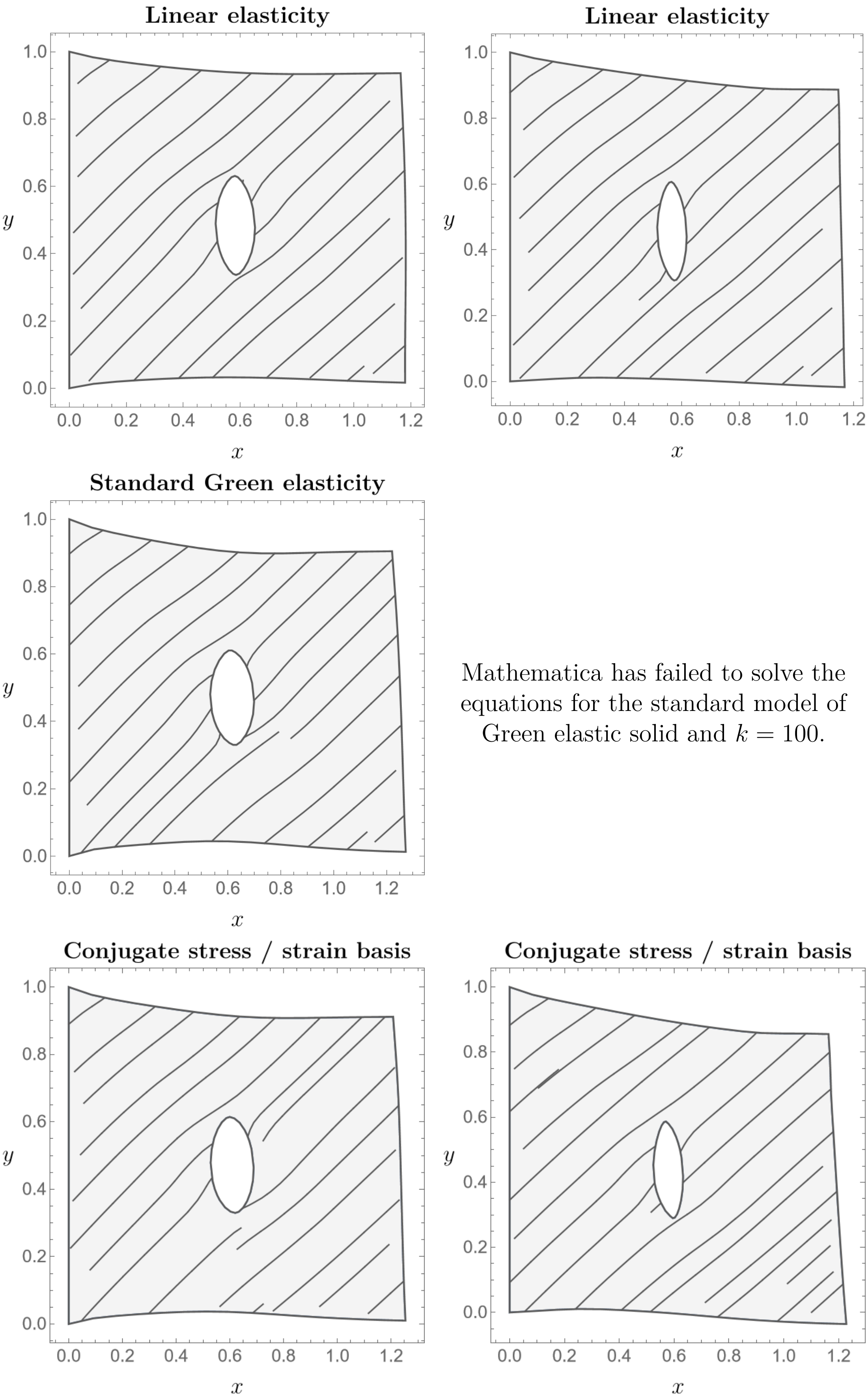


Figure 4.17: Fibers in the current configuration. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

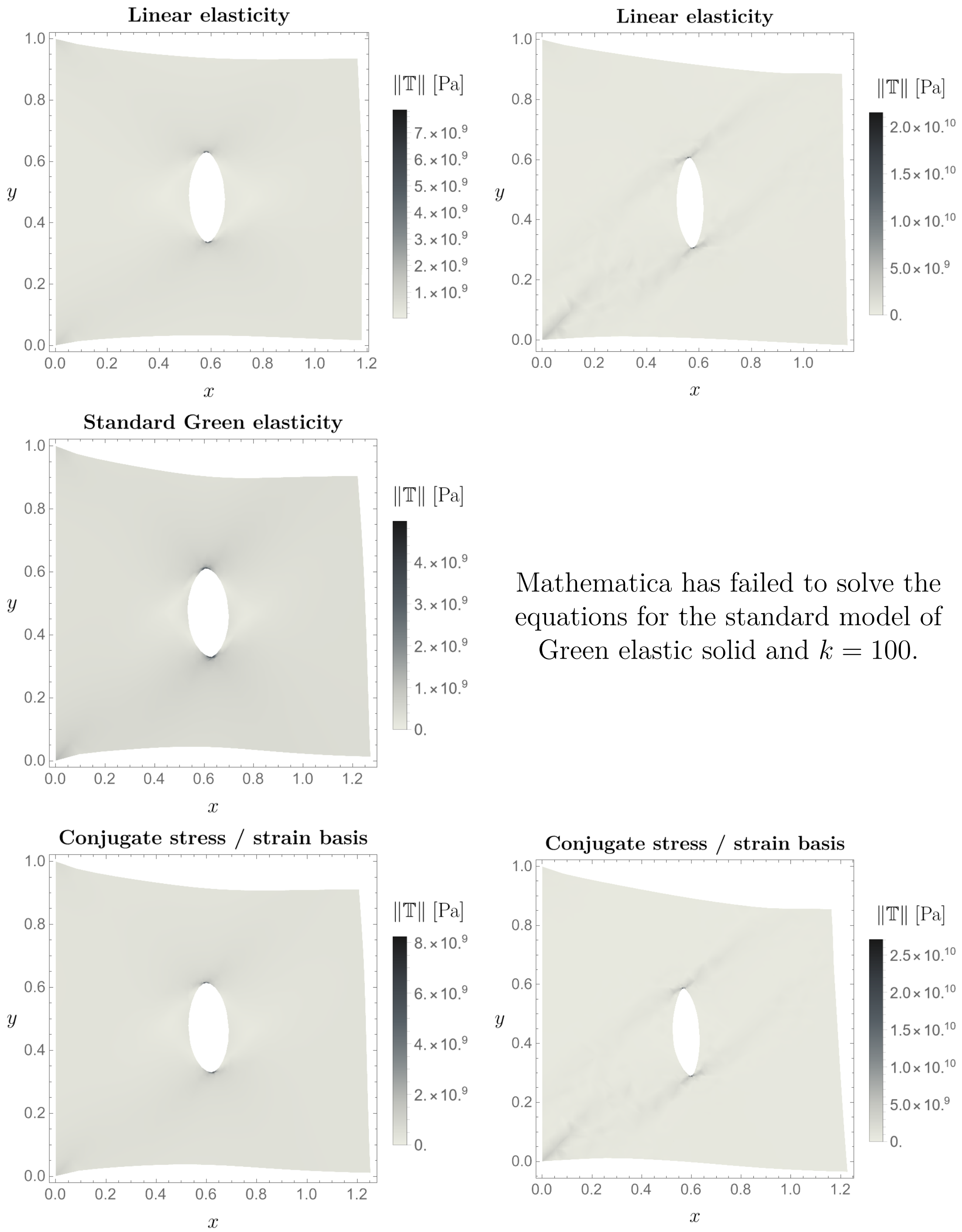


Figure 4.18: Norm of the Cauchy stress tensor. The results for $k = 1$ are on the left hand side, while results for $k = 100$ are on the right hand side.

	Linear elasticity	Green elasticity	Conjugate stress / strain basis	k
Computation time [s]	1.145	0.662	28.081	1
	1.105	—	31.697	100

Table 4.9: Norm of the Cauchy stress tensor computation time

Conclusion

We have studied an alternative approach to constitutive relations for Green elastic solids based on the QR decomposition of the deformation gradient. We focused on the two dimensional conjugate stress / strain model presented in Erel and Freed [2017].

In the first chapter we have compared the polar and QR decompositions. We have introduced both decompositions and shown, how we can interpret them.

In the second chapter we have focused on the standard theory of elasticity. We have started by introducing the principal invariants of matrices. Then we have followed with the description of the theory of Green elastic solids. We have also presented Spencer's model of fiber-reinforced material, which is used to describe transversely isotropic materials. Then we have moved to describe the linear elasticity theory in two dimensions. At the end of the chapter we have briefly discussed potential problems of the standard approach to Green elasticity and we have shown, how the QR decomposition can solve them.

In the third chapter we have studied the elasticity based on the QR decomposition. To overcome the key problem of the necessity of the privileged basis for the QR decomposition, we have introduced the matrix of anisotropy, which allowed us, unlike in Erel and Freed [2017], to work with fibers with arbitrary direction. Then we have presented the conjugate stress / strain model, and we have shown that for isotropic free energy, this model is equivalent to the standard Green elasticity. Even though the three dimensional conjugate bases are known (Freed [2017]), we have decided for simplicity to focus on the two dimensional model. This decision has proven to be a good one, as the conjugate basis pairs model turned out to be computationally expensive even in two-dimensional setting.

In the last chapter we have performed numerical experiments. We have used the standard reinforcing material model to compare the three presented models (standard Green elasticity, linear elasticity and conjugate stress / strain model). We have used Wolfram Mathematica to solve the resulting boundary value problems. We have considered fibers with two different stiffnesses and various directions and three different domains (rectangular block, rectangular block with a horizontally / vertically oriented hole). The results for the linear elasticity are noticeably different from the other two models. This suggests, that the assumption of small displacement gradient does not hold in considered setting.

The conjugate stress / strain model shows results similar to the standard model of Green elastic solid. For fibers with lower stiffness the difference between those two models can be considered negligible. This is because the material is close to being isotropic, and for isotropic material, both models are equivalent. This shows, that at least for almost isotropic materials, the conjugate stress / strain model is consistent with the standard theory of Green elasticity and can be considered as an alternative. For material with stiffer fibers, some differences start to appear. The displacement remains similar, but the magnitude of stress is two or three times lower for the conjugate stress / strain basis model. All three models successfully predict higher stress (stress concentration phenomenon) around the vertices of the ellipse.

For fibers with high stiffness, some noise, which vaguely resembles the underlying mesh structure, starts to appear in the norm of the Cauchy stress tensor plots. This is the most evident in the case of the standard model of Green elasticity if the curved fibers are assumed. The noise in the case of the conjugate stress / strain basis model is much less noticeable. Finer mesh does not solve the problem. In one case the computation of the standard model of Green elastic solid has failed, while the conjugate stress / strain model has been successful. This suggests, that for material with stiff fibers, the conjugate stress / strain basis model might be better.

The downside of the conjugate basis pairs model is, that the model turned out to be computationally expensive. This however might be due to the primitive implementation of the model, and it is possible, that a better implementation could reduce the computation time considerably. However our implementation is the first one, which takes curved fibers into account.

Bibliography

Wolfram Mathematica FEM tutorial, a. URL `https://reference.wolfram.com/language/FEMDocumentation/tutorial/SolvingPDEwithFEM.html`. Last accessed on 2023-04-09.

Wolfram Mathematica hyperelasticity tutorial, b. URL `https://reference.wolfram.com/language/PDEModels/tutorial/StructuralMechanics/Hyperelasticity.html`. Last acessed on 2023-03-11.

Wolfram Mathematica solid mechanics tutorial, c. URL `https://reference.wolfram.com/language/PDEModels/tutorial/StructuralMechanics/SolidMechanics.html`. Last accessed on 2023-03-11.

Encyclopædia Britannica - elasticity, 2022. URL `https://www.britannica.com/science/elasticity-physics`. Last accessed on 2023-04-01.

John C. Criscione. Rivlin's representation formula is ill-conceived for the determination of response functions via biaxial testing. In *The Rational Spirit in Modern Continuum Mechanics*, pages 197–215. Springer, 2004. ISBN 978-1-4020-2308-8. doi: 10.1007/1-4020-2308-1_15.

Michel Destrade, Michael D. Gilchrist, Danila A. Prikazchikov, and Giuseppe Saccomandi. Surface instability of sheared soft tissues. *Journal of Biomechanical Engineering*, 130(6), 10 2008. ISSN 0148-0731. doi: 10.1115/1.2979869.

Veysel Erel and Alan D. Freed. Stress / strain basis pairs for anisotropic materials. *Composites Part B: Engineering*, 120:152–158, 2017. ISSN 1359-8368. doi: 10.1016/j.compositesb.2017.03.065.

Alan D. Freed. A note on stress / strain conjugate pairs: Explicit and implicit theories of thermoelasticity for anisotropic materials. *International Journal of Engineering Science*, 120:155–171, 2017. ISSN 0020-7225. doi: 10.1016/j.ijengsci.2017.08.002.

Alan D. Freed, Veysel Erel, and Michael Moreno. Conjugate stress / strain base pairs for planar analysis of biological tissues. *Journal of Mechanics of Materials and Structures*, 12(2):219–247, 2016.

Alan D. Freed, Jean-Briac le Graverend, and Kumbakonam R. Rajagopal. A decomposition of Laplace stretch with applications in inelasticity. *Acta Mechanica*, 230:3423–3429, 2019. doi: 10.1007/s00707-019-02462-3.

Morton E. Gurtin, Eliot Fried, and Lallit Anand. *The Mechanics and Thermodynamics of Continua*. Cambridge University Press, 2010. doi: 10.1017/CBO9780511762956.

Gerhard A. Holzapfel. *Nonlinear solid mechanics: a continuum approach for engineering science*. Kluwer Academic Publishers Dordrecht, 2000.

Steven J. Leon, Åke Björck, and Walter Gander. Gram-Schmidt orthogonalization: 100 years and more. *Numerical Linear Algebra with Applications*, 20(3): 492–532, 2013. doi: 10.1002/nla.1839.

A. G. McLellan. Finite strain coordinates and the stability of solid phases. *Journal of Physics C: Solid State Physics*, 9(22):4083, 1976. doi: 10.1088/0022-3719/9/22/006.

Xinguo Ning, Qiliang Zhu, Yoram Lanir, and Susan S. Margulies. A transversely isotropic viscoelastic constitutive equation for brainstem undergoing finite deformation. *Journal of Biomechanical Engineering*, 128(6):925–933, 06 2006. ISSN 0148-0731. doi: 10.1115/1.2354208.

Raymond W. Ogden. Nonlinear elastic deformations. 1984.

Sandipan Paul and Alan D. Freed. A simple and practical representation of compatibility condition derived using a QR decomposition of the deformation gradient. *Acta Mechanica*, 231(8):3289–3304, 2020. doi: 10.1007/s00707-020-02702-x.

Ronald Samuel Rivlin and Jerald LaVerne Ericksen. Stress-deformation relations for isotropic materials. *Collected Papers of RS Rivlin*, pages 911–1013, 1997.

Anthony J. M. Spencer. Part III. Theory of invariants. *Continuum physics*, 1: 239–353, 1971.

Anthony J. M. Spencer. Deformations of fibre-reinforced materials. 1972.

Arun R. Srinivasa. On the use of the upper triangular (or QR) decomposition for developing constitutive equations for green-elastic materials. *International Journal of Engineering Science*, 60:1–12, 2012. ISSN 0020-7225. doi: 10.1016/j.ijengsci.2012.05.003.

Clifford Truesdell and Walter Noll. *The non-linear field theories of mechanics.* Springer, 2004.

List of Figures

A. Derivatives of invariants and pseudo-invariants

Sometimes it is useful to take a derivative of an invariant with respect to the matrix. By derivative we mean Gâteaux derivative, which is a generalization of a directional derivative.

Definition (Gâteaux derivative). *Let $f\colon D \subset U \to V$ be a mapping between two Banach spaces U and V, where D is an open subset of U. Then f has a Gâteaux derivative at a point $x \in D$ in the direction y, if and only if there exists a limit*

$$\mathcal{D}f(x)[y] = \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(f(x+\tau y)\right).$$

Remark (Identification of Gâteaux derivative with a matrix). When dealing with a directional derivative of a function f from $\mathbb{R}^n$ to $\mathbb{R}$, it is common to write it as a dot product of a gradient of the function and the directional vector $\mathbf{v}$, i.e. $\frac{\mathrm{d}f}{\mathrm{d}\mathbf{v}} = \nabla f \cdot \mathbf{v}$. In our case we are interested in functions from $\mathbb{R}^{n\times n}$ to $\mathbb{R}$, therefore we can identify the Gâteaux derivative of tensor function f with a matrix in the same way. We then obtain the directional derivative by taking the double dot product.

Due to similarities with partial derivatives and gradient, we will use the following notation for the Gâteaux derivative:

$$\frac{\partial f}{\partial \mathbb{A}}[\mathbb{B}] = \frac{\partial f}{\partial \mathbb{A}} : \mathbb{B} = \mathcal{D}f(\mathbb{A})[\mathbb{B}].$$

Theorem A.1 (Derivatives of invariants). *Let $\mathbb{A}$ be a 3×3 invertible matrix. Then*

$$\begin{aligned}\frac{\partial I_1(\mathbb{A})}{\partial \mathbb{A}} &= \mathbb{I},\\ \frac{\partial I_2(\mathbb{A})}{\partial \mathbb{A}} &= (\mathrm{Tr}\,\mathbb{A})\,\mathbb{I} - \mathbb{A}^\top,\\ \frac{\partial I_3(\mathbb{A})}{\partial \mathbb{A}} &= (\det \mathbb{A})\,\mathbb{A}^{-\top},\end{aligned}$$

where the identification of the derivative with the matrix is in the sense of previous remark.

Proof. Let $\mathbb{B}$ be a fixed 3×3 matrix. Then

$$\begin{aligned}\frac{\partial I_1(\mathbb{A})}{\partial \mathbb{A}}[\mathbb{B}] &= \frac{\partial \mathrm{Tr}\,\mathbb{A}}{\partial \mathbb{A}}[\mathbb{B}] = \lim_{\tau\to 0^+}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\mathrm{Tr}\,(\mathbb{A}+\tau\mathbb{B})\right) = \lim_{\tau\to 0^+}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\mathrm{Tr}\,\mathbb{A}+\tau\mathrm{Tr}\,\mathbb{B}\right)\\ &= \mathrm{Tr}\,\mathbb{B}.\end{aligned}$$

This can be rewritten as $\mathbb{I} : \mathbb{B}$, therefore $\frac{\partial I_1(\mathbb{A})}{\partial \mathbb{A}} = \mathbb{I}$. To prove the second identity, we will use the chain rule.

$$\begin{aligned}
\frac{\partial \mathbb{A}^2}{\partial \mathbb{A}}[\mathbb{B}] &= \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left((\mathbb{A}+\tau\mathbb{B})^2\right) \\
&= \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\mathbb{A}^2+\tau\mathbb{A}\mathbb{B}+\tau\mathbb{B}\mathbb{A}+\tau^2\mathbb{B}^2\right) = \mathbb{A}\mathbb{B}+\mathbb{B}\mathbb{A}, \\
\frac{\partial \mathrm{Tr}\ (\mathbb{A}^2)}{\partial \mathbb{A}}[\mathbb{B}] &= \left.\frac{\partial \mathrm{Tr}\,\mathbb{C}}{\partial \mathbb{C}}\right|_{\mathbb{C}=\mathbb{A}} \left[\frac{\partial \mathbb{A}^2}{\partial \mathbb{A}}[\mathbb{B}]\right] = \mathrm{Tr}\,(\mathbb{A}\mathbb{B}+\mathbb{B}\mathbb{A}) = 2\mathrm{Tr}\,(\mathbb{A}\mathbb{B}), \\
\frac{\partial\,(\mathrm{Tr}\,\mathbb{A})^2}{\partial \mathbb{A}}[\mathbb{B}] &= 2\mathrm{Tr}\,\mathbb{A}\,\mathrm{Tr}\,\mathbb{B}.
\end{aligned}$$

Thus we see, that

$$\frac{\partial}{\partial \mathbb{A}}\left(\frac{1}{2}(\mathrm{Tr}\,\mathbb{A})^2 - \frac{1}{2}\mathrm{Tr}\,(\mathbb{A}^2)\right)[\mathbb{B}] = \mathrm{Tr}\,\mathbb{A}\,\mathrm{Tr}\,\mathbb{B} - \mathrm{Tr}\,(\mathbb{A}\mathbb{B}).$$

We can rewrite it as $\left[(\mathrm{Tr}\,\mathbb{A})\,\mathbb{I} - \mathbb{A}^\top\right] : \mathbb{B}$. This proves the second identity. Now only the derivative of determinant remains.

$$\begin{aligned}
\frac{\partial \det \mathbb{A}}{\partial \mathbb{A}}[\mathbb{B}] &= \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\det(\mathbb{A}+\tau\mathbb{B})\right) = \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\det(\mathbb{A}(\mathbb{I}+\tau\mathbb{A}^{-1}\mathbb{B}))\right) \\
&= \det \mathbb{A} \lim_{\tau\to 0^+} \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\det(\mathbb{I}+\tau\mathbb{A}^{-1}\mathbb{B})\right)
\end{aligned}$$

Now we expand the determinant of $\mathbb{I}+\tau\mathbb{A}^{-1}\mathbb{B}$ in terms of powers of τ:

$$\begin{aligned}
\det(\mathbb{I}+\tau\mathbb{A}^{-1}\mathbb{B}) &= 1 + \tau\left((\mathbb{A}^{-1}\mathbb{B})_{11} + (\mathbb{A}^{-1}\mathbb{B})_{22} + (\mathbb{A}^{-1}\mathbb{B})_{33}\right) + \mathcal{O}(\tau^2) \\
&= 1 + \tau\mathrm{Tr}\,\left(\mathbb{A}^{-1}\mathbb{B}\right) + \mathcal{O}(\tau^2).
\end{aligned}$$

From this we see, that $\frac{\partial \det \mathbb{A}}{\partial \mathbb{A}}[\mathbb{B}] = (\det \mathbb{A})\mathrm{Tr}\,(\mathbb{A}^{-1}\mathbb{B})$. Rewriting it as $(\det \mathbb{A})\mathbb{A}^{-\top} : \mathbb{B}$ finishes the proof. ☐

Theorem A.2 (Derivatives of pseudo-invariants)**.** *Let* $I_4(\mathbb{C}, \mathbf{A}) = \mathbf{A} \cdot \mathbb{C}\mathbf{A}$ *and* $I_5(\mathbb{C}, \mathbf{A}) = \mathbf{A} \cdot \mathbb{C}^2\mathbf{A}$. *Then*

$$\begin{aligned}
\frac{\partial I_4}{\partial \mathbb{C}} &= \mathbf{A} \otimes \mathbf{A}, \\
\frac{\partial I_5}{\partial \mathbb{C}} &= \mathbf{A} \otimes \mathbb{C}\mathbf{A} + \mathbb{C}\mathbf{A} \otimes \mathbf{A}.
\end{aligned}$$

Proof. By direct computation.

$$\begin{aligned}
\left(\frac{\partial I_4}{\partial \mathbb{C}}\right)_{ij} &= \frac{\partial A_k C_{kl} A_l}{\partial C_{ij}} = A_i A_j \implies \frac{\partial I_4}{\partial \mathbb{C}} = \mathbf{A} \otimes \mathbf{A}, \\
\left(\frac{\partial I_5}{\partial \mathbb{C}}\right)_{ij} &= \frac{\partial C_{km} A_m C_{kl} A_l}{\partial C_{ij}} = A_j C_{il} A_l + C_{im} A_m A_j \\
&\implies \frac{\partial I_5}{\partial \mathbb{C}} = \mathbf{A} \otimes \mathbb{C}\mathbf{A} + \mathbb{C}\mathbf{A} \otimes \mathbf{A}.
\end{aligned}$$

☐