University of South Bohemia, České Budějovice

Faculty of Science

An introduction to mathematical modelling in continuum mechanics

Bachelor's thesis

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Annotation:

The objective of the bachelor's thesis is to introduce the basic notation in mechanics of continuum. Key concepts are deformation mappings, strains in materials, density models in elasticity, and the corresponding energy functional. Practical examples of various mappings are presented with elaborate computations and visualizations. Some MATLAB codes used to illustrate the examples are listed.

I declare that I am the author of this qualification thesis and that in writing it I have used the sources and literature displayed in the list of used sources only.

České Budějovice, 11. 4. 2022

Lucie Pelikánová

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Contents

Chapter 1

Introduction

The main focus of this work is the introduction of the basic concepts of continuum mechanics and their mathematical description. We are primarily interested in mechanics of solids. The key concepts are deformation mapping, strain in materials, density models in elasticity and the corresponding energy functional. The three density models that are implemented are:

1. The Neo-Hookean density model

2. The Saint Venant-Kirchhoff density model

3. The linear elasticity or the Hookean density model

Furthermore, the goal is to demonstrate the key aspects of mechanics of solids using practical examples. Therefore, various examples of deformation mappings are created and are extensively supported by elaborate computations and various visualizations. The deformation mappings are based on a cuboid reference configuration and include the following.

1. The deformation into a partial and a whole toroid

2. The deformation into a twist

3. The deformations into two types of hourglass

All computations are calculated in an analytical manner and namely the evaluations of the energy functional are compared to a numeric solution.

The given mappings are completely prescribed in the whole reference domain and are not obtained by any energy minimizations or equivalent boundary value problems. Thus, they might serve as testing benchmarks for various computing tools, for example, by using the finite element method [5]. Some important concepts such as stress in materials and practical computations of energy minimizer might be added in forthcoming works.

The basic theoretical concepts of continuum mechanics are partially taken from the works [1, 2, 3], and are described in Chapter 2. Chapter 3 includes above mentioned examples, their visualization, and corresponding analytical computations and their comparison to a numeric solution. The codes used for visualizations and numeric computations were performed in MATLAB numeric computing environment [4] utilizing the codes specifically developed for the purpose of this thesis and the partially adjusted codes of [5]. The codes and the changes in the codes are listed in the Appendix.

This work was written completely in LaTeX, a document preparation system.

Chapter 2

Basics of continuum mechanics

Continuum mechanics studies mathematical models of continuous materials and their mechanical behavior when the material undergoes geometrical changes: deformations. The material is represented by a domain and its deformation is given by a deformation mapping. Furthermore, continuum mechanics focuses on describing the material changes by means of the deformation gradient, strain tensors, density models and corresponding energy functional.

2.1 Deformation mapping

Assume that Ω is a domain in $\mathbb{R}^n$, where $n \in \mathbb{R}$ is the dimension of the space.

Remark 1 *Throughout this thesis, we consider $n = 3$, therefore, a three-dimensional space $\mathbb{R}^3$. Thus, all aspects in this chapter and in the following chapters are described in $\mathbb{R}^3$.*

A deformation of Ω describes the relocation of any point $\mathbf{x} \in \Omega$ during the *deformation process* and is given by the mapping

$$\mathbf{v}(\mathbf{x}) : \Omega \to \mathbb{R}^3, \qquad \mathbf{v}(\mathbf{x}) = \left(v^{(1)}(\mathbf{x}), v^{(2)}(\mathbf{x}), v^{(3)}(\mathbf{x}) \right),$$

and $\mathbf{x} = (x, y, z)$ represents the material coordinates.

Similarly, a displacement can be described in terms of $\mathbf{v}(\mathbf{x})$ and the *displacement function* $\mathbf{w}(\mathbf{x}) : \Omega \to \mathbb{R}^3$ is defined as

$$\mathbf{w}(\mathbf{x}) = \mathbf{v}(\mathbf{x}) - \mathbf{id}(\mathbf{x}), \qquad \mathbf{w}(\mathbf{x}) = \left(w^{(1)}(\mathbf{x}), w^{(2)}(\mathbf{x}), w^{(3)}(\mathbf{x}) \right),$$

where $\mathbf{id}(\mathbf{x})$ is the identity operator.

Remark 2 *We will focus on describing material changes by the deformation mapping in Chapter 3. The displacement mapping is listed for illustrative purposes.*

Remark 3 *The material before a deformation is represented by* Ω *and is referred to as the* reference configuration, *after it is deformed it is called the* current configuration.

Furthermore, the Lagrangian description, *also known as the material description, is used, which means that the material is described in terms of the material coordinates.*
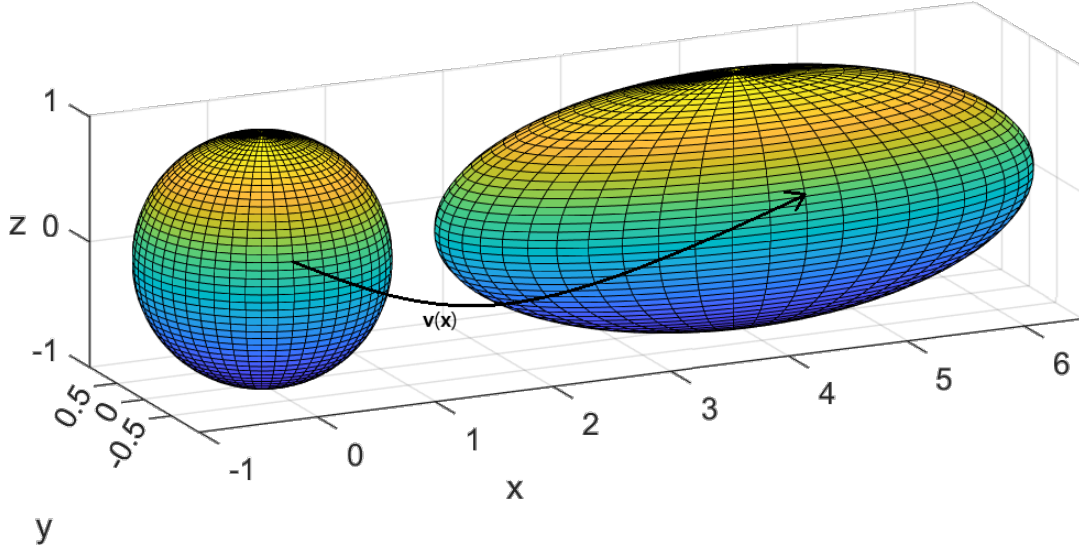

Figure 2.1: Example of a deformation mapping: deformation of a sphere into an ellipsoid.

Example 1 *A deformation mapping* $\mathbf{v}(\mathbf{x})$ *of a sphere into an ellipsoid. The spherical domain* Ω *is parametrized by spherical coordinates* (r, ϕ, θ) *as follows:*

$$
\begin{aligned}
x &= x_0 + r\cos(\phi)\sin(\theta), \\
y &= y_0 + r\sin(\phi)\sin(\theta), \\
z &= z_0 + r\cos(\theta),
\end{aligned}
$$

where (x_0, y_0, z_0) *represents the centre of the sphere,* $r \in (0, 1]$ *is the radius, and* $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$. *The deformation is given by the following mapping* $\mathbf{v}(\mathbf{x})$:

$$
\begin{aligned}
v^{(1)}(x, y, z) &= x_1 + l_x(x - x_0), \\
v^{(2)}(x, y, z) &= y_1 + l_y(y - y_0), \\
v^{(3)}(x, y, z) &= z_1 + l_z(z - z_0),
\end{aligned}
$$

where (x_1, y_1, z_1) *represents the center of the ellipsoid and* l_x, l_y, l_z *are the lengths of the semi-axes.*

The deformation in Fig. 2.1 *is visualized for* $(x_0, y_0, z_0) = (0, 0, 0)$, $(x_1, y_1, z_1) = (4, 0, 0)$ *and* $l_x = 2.5$, $l_y = l_z = 1$ *with the help of* Code - Matlab 1.

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2.2   Deformation gradient

The *deformation gradient* is one of the main elements in continuum mechanic. It brings together the reference configuration and the current configuration and creates a relationship between them. The deformation gradient is defined as

$$\mathbf{F}(\mathbf{v}) := \nabla\mathbf{v} = \begin{pmatrix} \frac{\partial v^{(1)}}{\partial x} & \frac{\partial v^{(1)}}{\partial y} & \frac{\partial v^{(1)}}{\partial z} \\ \frac{\partial v^{(2)}}{\partial x} & \frac{\partial v^{(2)}}{\partial y} & \frac{\partial v^{(2)}}{\partial z} \\ \frac{\partial v^{(3)}}{\partial x} & \frac{\partial v^{(3)}}{\partial y} & \frac{\partial v^{(3)}}{\partial z} \end{pmatrix}. \tag{2.1}$$

The *displacement gradient* can be written as

$$\nabla\mathbf{w} = \nabla\mathbf{v} - \mathbf{I},$$

where $\mathbf{I} \in \mathbb{R}^{3\times 3}$ is the identity matrix. Thus, the deformation gradient can also be written in terms of $\mathbf{w}$ as follows:

$$\mathbf{F}(\mathbf{w}) = \nabla\mathbf{w} + \mathbf{I} = \begin{pmatrix} \frac{\partial w^{(1)}}{\partial x} & \frac{\partial w^{(1)}}{\partial y} & \frac{\partial w^{(1)}}{\partial z} \\ \frac{\partial w^{(2)}}{\partial x} & \frac{\partial w^{(2)}}{\partial y} & \frac{\partial w^{(2)}}{\partial z} \\ \frac{\partial w^{(3)}}{\partial x} & \frac{\partial w^{(3)}}{\partial y} & \frac{\partial w^{(3)}}{\partial z} \end{pmatrix} + \mathbf{I}.$$

Remark 4 *Similarly to the displacement mapping, the displacement gradient is used for illustrative purposes.*

2.3   Types of deformations

The deformation is said to be *homogeneous*, if $\mathbf{F}$ is independent of $\mathbf{x}$, therefore the deformation mapping $\mathbf{v}(\mathbf{x})$ can be expressed as

$$\mathbf{v}(\mathbf{x}) = \mathbf{F}\mathbf{x} + \mathbf{c},$$

here $\mathbf{c} \in \mathbb{R}^3$. Furthermore, if $\mathbf{F} = \mathbf{I}$ the material does not deform.

If the deformation gradient is a function of $\mathbf{x}$, the deformation is called *nonhomogeneous*. Examples of nonhomogeneous deformations are illustrated in Chapter 3.

Example 2 *An illustration of a simple homogeneous deformation can be, for example, the mapping $\mathbf{v}(\mathbf{x})$:*
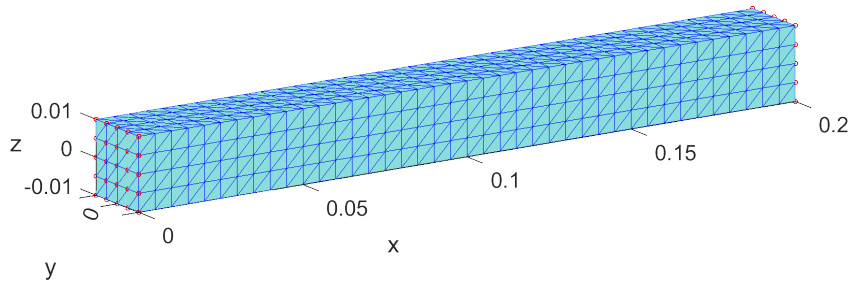
$$v^{(1)}(x, y, z) = s_x x + x_2,$$
$$v^{(2)}(x, y, z) = s_y y + y_2,$$
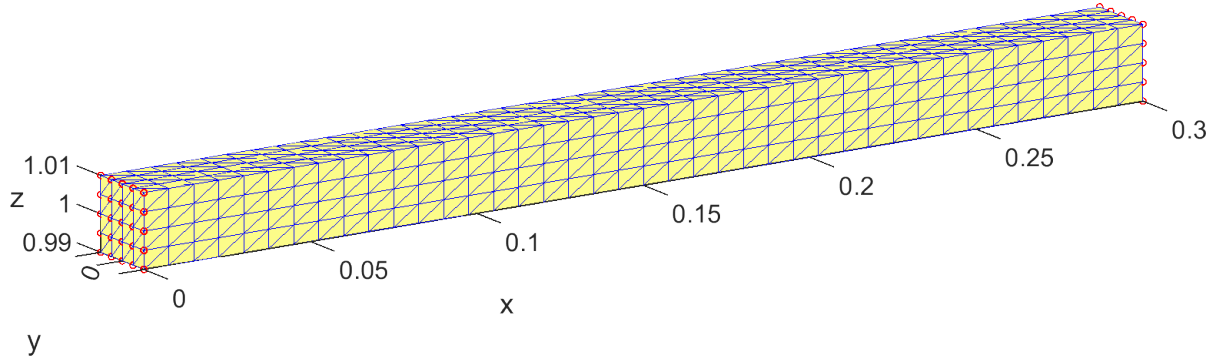
$$v^{(3)}(x, y, z) = s_z z + z_2,$$

where $s_x, s_y, s_z, x_2, y_2, z_2 \in \mathbb{R}$. The specific example in Fig. 2.2 *is shown for $x_2, y_2 = 0$ and $z_2 = 1$ $s_x = \frac{3}{2}$ and $s_y, s_z = 1$, in $\Omega = (0, 0.2) \times (-0.01, 0.01) \times (-0.01, 0.01)$. In this case the deformation gradient is*

$$\mathbf{F}(\mathbf{v}) = \begin{pmatrix} x_2 & 0 & 0 \\ 0 & y_2 & 0 \\ 0 & 0 & z_2 \end{pmatrix} = \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Here $\mathbf{F}(\mathbf{v})$ is indeed independent of $\mathbf{x}$.

(a) Reference configuration

(b) Current configuration

Figure 2.2: Example: a homogeneous deformation of a cuboid.

The determinant of $\mathbf{F}$ is extensively used in the calculations in the examples in the following chapters. Suppose that $\det(\mathbf{F})$ signifies the determinant of the deformation gradient, also known as the *Jacobian determinant*.

$$\det(\mathbf{F}) = F_{11}F_{22}F_{33} + F_{12}F_{23}F_{31} + F_{13}F_{21}F_{32} - F_{13}F_{22}F_{31} - F_{12}F_{21}F_{33} - F_{11}F_{23}F_{32}.$$

The Jacobian determinant indicates local changes in volume of Ω, more explicitly the local ratio between the volumes denoted by the current and the reference configurations of a material. We distinguish the following cases:

- $\det(\mathbf{F}) > 0$ - Volumes are naturally considered positive values; thus, the volume ratio is also locally positive.

- $\det(\mathbf{F}) = 1$ - The deformation locally preserves the volume. The deformation is called *isochoric*, if the volume does not change.

More specifically:

- $0 < \det(\mathbf{F}) < 1$ - The volume decreases.

- $\det(\mathbf{F}) > 1$ - The volume increases.

Furthermore, we also demonstrate two other cases that are physically unrealistic:

- $\det(\mathbf{F}) = 0$ signifies that the material is locally compressed into a single point, line or surface.

- $\det(\mathbf{F}) < 0$ means that the deformation does not preserves the orientation of the material.

Remark 5 *To simplify the notation of $\mathbf{F}(\mathbf{v})$ for forthcoming computations, we establish that its elements can be written as*

$$
\begin{pmatrix}
\frac{\partial v^{(1)}}{\partial x} & \frac{\partial v^{(1)}}{\partial y} & \frac{\partial v^{(1)}}{\partial z} \\
\frac{\partial v^{(2)}}{\partial x} & \frac{\partial v^{(2)}}{\partial y} & \frac{\partial v^{(2)}}{\partial z} \\
\frac{\partial v^{(3)}}{\partial x} & \frac{\partial v^{(3)}}{\partial y} & \frac{\partial v^{(3)}}{\partial z}
\end{pmatrix}
=
\begin{pmatrix}
F_{11} & F_{12} & F_{13} \\
F_{21} & F_{22} & F_{23} \\
F_{31} & F_{32} & F_{33}
\end{pmatrix}.
\tag{2.2}
$$

2.4 Strain tensors

Strain tensors indicate how much the reference configuration differs locally from the current configuration.

The *large strain tensor*, also called the *Green-Lagrange strain tensor* is defined as

$$
\mathbf{E}(\mathbf{F}) := \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}),
$$

where the element $\mathbf{F}^T\mathbf{F}$ is defined as the right *Cauchy-Green deformation tensor* $\mathbf{C}$

$$
\mathbf{C}(\mathbf{F}) := \mathbf{F}^T\mathbf{F}.
$$

The *small strain tensor* is defined as

$$
\mathbf{e}(\mathbf{F}) := \frac{1}{2}(\mathbf{F} + \mathbf{F}^T) - \mathbf{I}.
$$

Remark 6 *The small strain tensor is best used to describe deformations, where $\mathbf{F} \to \mathbf{I}$.*

Remark 7 *It holds*

$$\mathbf{e}(\mathbf{F}) \approx \mathbf{E}(\mathbf{F}) \quad for \quad \mathbf{F} \to \mathbf{I}.$$

To show it, the large strain tensor $\mathbf{E}(\mathbf{F})$ is linearized by the Taylor series as

$$\mathbf{E}(\mathbf{F}) \approx \mathbf{E}(\mathbf{I}) + \frac{\partial \mathbf{E}}{\partial \mathbf{F}}(\mathbf{I})(\mathbf{F} - \mathbf{I}),$$

where $\mathbf{E}(\mathbf{I}) = \frac{1}{2}(\mathbf{I}^T \mathbf{I} - \mathbf{I})$ is a zero matrix. The derivative $\frac{\partial \mathbf{E}}{\partial \mathbf{F}}$ denotes the derivative of the matrix with respect to a different matrix, so it actually represents a fourth-order tensor. To compute it efficiently, we take advantage of the Einstein summation notation, where the indices $i, j, k, l, m \in \{1, 2, 3\}$ are used. It holds

$$E_{ij}(\mathbf{F}) = \frac{1}{2}(F_{im}^T F_{mj} - I_{ij}),$$

$$e_{ij}(\mathbf{F}) = \frac{1}{2}(F_{ij} + F_{ji} - 2I_{ij}).$$

Furthermore, the above equations can be written using the Kronecker delta symbol, which is defined as

$$\delta_{ij} = \begin{cases} 1 & if \quad i = j, \\ 0 & if \quad i \neq j. \end{cases}$$

Thus,

$$E_{ij}(\mathbf{F}) = \frac{1}{2}(F_{im}^T F_{mj} - \delta_{ij}),$$

$$e_{ij}(\mathbf{F}) = \frac{1}{2}(F_{ij} + F_{ji} - 2\delta_{ij}). \tag{2.3}$$

Moreover,

$$\frac{\partial \mathbf{E}}{\partial \mathbf{F}}(\mathbf{I})(\mathbf{F} - \mathbf{I}) \simeq \frac{\partial E_{ij}}{\partial F_{kl}}(\mathbf{I})(F_{kl} - \delta_{kl}),$$

where the symbol $\simeq$ denotes the relation of the tensor object and its components. In the following computations, the Kronecker delta is also used. Therefore,

$$
\begin{aligned}
\frac{\partial E_{ij}}{\partial F_{kl}}(\mathbf{F}) &= \frac{1}{2}\frac{\partial(F_{im}^T F_{mj} - \delta_{ij})}{\partial F_{kl}} = \frac{1}{2}\frac{\partial(F_{mi} F_{mj} - \delta_{ij})}{\partial F_{kl}} = \\
&= \frac{1}{2}\left(\frac{\partial F_{mi}}{\partial F_{kl}}F_{mj} + F_{mi}\frac{\partial F_{mj}}{\partial F_{kl}}\right) = \\
&= \frac{1}{2}\left(\delta_{mk}\delta_{il}F_{mj} + F_{mi}\delta_{mk}\delta_{jl}\right) = \\
&= \frac{1}{2}\left(\delta_{il}F_{kj} + F_{ki}\delta_{jl}\right),
\end{aligned}
$$

Therefore we obtain

$$\frac{\partial E_{ij}}{\partial F_{kl}}(\mathbf{I}) = \frac{1}{2}\left(\delta_{il}\delta_{kj} + \delta_{ki}\delta_{jl}\right).$$

Thus,

$$\mathbf{E}(\mathbf{F}) \simeq E_{ij}(\mathbf{F}) \approx \frac{1}{2} \left(\delta_{il}\delta_{kj} + \delta_{ki}\delta_{jl} \right) \left(F_{kl} - \delta_{kl} \right) =$$

$$= \frac{1}{2} (\delta_{il}\delta_{kj}F_{kl} - \delta_{il}\delta_{kj}\delta_{kl} + \delta_{ki}\delta_{jl}F_{kl} - \delta_{ki}\delta_{jl}\delta_{kl}) =$$

$$= \frac{1}{2} (F_{ij} + F_{ji} - 2\delta_{ij}) = e_{ij}(\mathbf{F}) \simeq \mathbf{e}(\mathbf{F}).$$

It concludes (2.3) *and the final formula, where* $\mathbf{E}(\mathbf{F}) \approx \mathbf{e}(\mathbf{F})$ *for* $\mathbf{F} \to \mathbf{I}$.

In practical computations, $\mathbf{E}$ and $\mathbf{e}$ can be expressed from (2.2) as

$$\mathbf{E} = \frac{1}{2} \begin{pmatrix} F_{11}^2 + F_{21}^2 + F_{31}^2 - 1 & F_{11}F_{12} + F_{21}F_{22} + F_{31}F_{32} & F_{11}F_{13} + F_{21}F_{23} + F_{31}F_{33} \\ F_{11}F_{12} + F_{21}F_{22} + F_{31}F_{32} & F_{12}^2 + F_{22}^2 + F_{32}^2 - 1 & F_{12}F_{13} + F_{22}F_{23} + F_{32}F_{33} \\ F_{11}F_{13} + F_{21}F_{23} + F_{31}F_{33} & F_{12}F_{13} + F_{22}F_{23} + F_{32}F_{33} & F_{13}^2 + F_{23}^2 + F_{33}^2 - 1 \end{pmatrix},$$

$$\mathbf{e} = \frac{1}{2} \begin{pmatrix} 2(F_{11} - 1) & F_{12} + F_{21} & F_{13} + F_{31} \\ F_{12} + F_{21} & 2(F_{22} - 1) & F_{23} + F_{32} \\ F_{13} + F_{31} & F_{23} + F_{32} & 2(F_{33} - 1) \end{pmatrix}.$$

2.5 Elastic energy functional

Materials for which there exists a stored energy are called *hyperelastic materials*. Therefore, the *energy functional* of a hyperelastic material is assumed in the form

$$J(\mathbf{v}) = \int_{\Omega} W(\mathbf{F}(\mathbf{v}(\mathbf{x}))) \, \mathrm{d}\mathbf{x},$$

where the density $W(\mathbf{F})$ of the elastic energy is specified for different material models. As examples we consider the following density models:

(i) *The Neo-Hookean density model*

$$W_{NH}(\mathbf{F}) = C_1 \left(||\mathbf{F}||^2 - 3 - 2\ln(\det(\mathbf{F})) \right) + D_1(\det(\mathbf{F}) - 1)^2$$

is used to describe densities for neo-Hookean materials, which have nonlinear behavior.

(ii) *The Saint Venant-Kirchhoff density model*

$$W_{SVK}(\mathbf{F}) = \mu ||\mathbf{E}(\mathbf{F})||^2 + \frac{\lambda}{2} (\mathrm{tr}(\mathbf{E}(\mathbf{F})))^2$$

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is one of the simplest nonlinear models to describe hyperelastic materials. And is the generalization of the following density model.

(iii) *The linear elasticity density model* or *the Hookean density model*

$$W_H(\mathbf{F}) = \mu||\mathbf{e}(\mathbf{F})||^2 + \frac{\lambda}{2}(\mathrm{tr}(\mathbf{e}(\mathbf{F})))^2.$$

Here $|| \cdot ||$ is the Frobenius norm and $\mathrm{tr}(\cdot)$ is the trace. To evaluate the above given symbols we utilize their elementwise forms. These formulas are used mainly for numeric evaluations.

$$||\mathbf{F}||^2 = F_{11}^2 + F_{12}^2 + F_{13}^2 + F_{21}^2 + F_{22}^2 + F_{23}^2 + F_{31}^2 + F_{32}^2 + F_{33}^2,$$

$$\begin{aligned}
||\mathbf{E}||^2 = &\frac{1}{4}\left(F_{11}^2 + F_{21}^2 + F_{31}^2 - 1\right)^2 + \frac{1}{4}\left(F_{12}^2 + F_{22}^2 + F_{32}^2 - 1\right)^2 + \\
&+ \frac{1}{4}\left(F_{13}^2 + F_{23}^2 + F_{33}^2 - 1\right)^2 + \\
&+ \frac{1}{2}\left(F_{11}F_{12} + F_{21}F_{22} + F_{31}F_{32}\right)^2 + \frac{1}{2}\left(F_{11}F_{13} + F_{21}F_{23} + F_{31}F_{33}\right)^2 + \\
&+ \frac{1}{2}\left(F_{12}F_{13} + F_{22}F_{23} + F_{32}F_{33}\right)^2,
\end{aligned}$$

$$(\mathrm{tr}(\mathbf{E}))^2 = \left(F_{11}^2 + F_{12}^2 + F_{13}^2 + F_{21}^2 + F_{22}^2 + F_{23}^2 + F_{31}^2 + F_{32}^2 + F_{33}^2 - 3\right)^2,$$

$$\begin{aligned}
||\mathbf{e}||^2 = &(F_{11} - 1)^2 + (F_{22} - 1)^2 + (F_{33} - 1)^2 + \\
&+ \frac{1}{2}\left((F_{12} + F_{21})^2 + (F_{13} + F_{31})^2 + (F_{23} + F_{32})^2\right),
\end{aligned}$$

$$(\mathrm{tr}(\mathbf{e}))^2 = (F_{11} + F_{22} + F_{33} - 3)^2.$$

2.5.1 Material parameters

We deal with isotropic materials, which are materials whose properties are the same regardless of the direction in which they are oriented. Various pairs of material parameters can be used to describe isotropic materials. In this work, we will describe materials in terms of *Young's modulus E* and *Poisson's ratio ν*. The *Lamé parameters λ and μ*, referred to as *Lamé's first parameter* and *Lamé's second parameter*, respectively, can be expressed as

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \qquad \mu = \frac{E}{2(1+\nu)}.$$

Furthermore, the *bulk modulus* K is introduces as

$$K = \frac{E}{3(1 - 2\nu)}.$$

The material constants C_1, D_1 in the Neo-Hookean density $W_{NH}(\mathbf{F})$ are expressed as

$$C_1 = \frac{\mu}{2}, \qquad D_1 = \frac{K}{2}.$$

Poisson's ratio represents the ratio of the change in width to the change of length of a material. The values of Poisson's ratio range from *0* to *0.5*. If $\nu = 0.5$, the material is considered incompressible. Young's modulus represents the stiffness of a material when a force is applied.

Example 3 *Values of the Poisson's ratio ν and the Young's modulus for various materials* [6] *are provided in the table below:*

Material	E [GPa]	ν
Steel	190-210	0.27-0.3
Aluminum alloys	70-79	0.33
Rubber	0.0007-0.004	0.45-0.49
Polyethylene	0.7-1.4	0.4

In examples in Chapter 3, we consider Young's modulus and Poisson's ratio of steel:

$$E = 190 \text{ GPa}, \qquad \nu = 0.27. \tag{2.4}$$

Chapter 3

Examples of deformations

In this chapter, there are shown practical examples of different deformations which use the concepts of Chapter 2. All deformations and corresponding computations consider a general cuboid domain:

$$\Omega = (0, l_x) \times (-\frac{l_y}{2}, \frac{l_y}{2}) \times (-\frac{l_z}{2}, \frac{l_z}{2}), \quad l_x, l_y, l_z > 0.$$

The following figures and graphs are, however, visualized for specific values of l_x, l_y, l_z. We assume that $l_x = 0.2$, $l_y = l_z = 0.01$, therefore, the cuboid domain Ω (see Fig. 3.1) is

$$\Omega = (0, 0.2) \times (-0.005, 0.005) \times (-0.005, 0.005).$$

Furthermore, the material parameters of steel (2.4) are considered in the following computations.

Figure 3.1: The cuboid domain Ω.
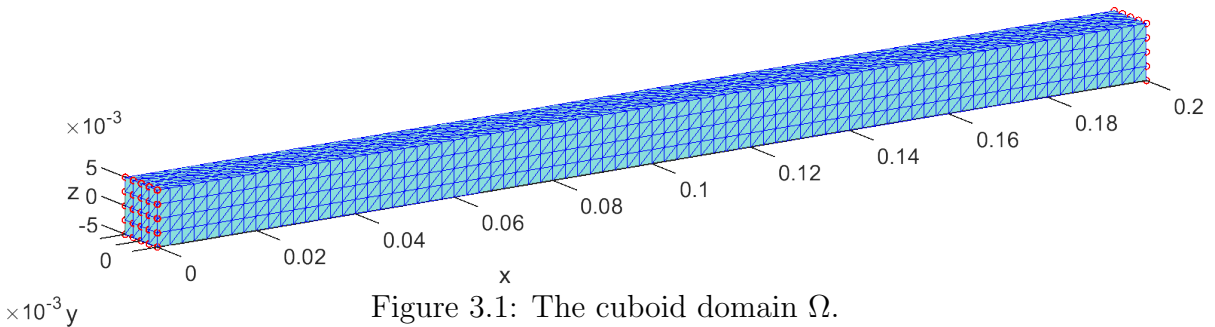
3.1 Deformation into a partial and a whole toroid

The deformation of a cuboid domain Ω is prescribed by the deformation mapping $\mathbf{v}(\mathbf{x}) = \left(v^{(1)}(\mathbf{x}), v^{(2)}(\mathbf{x}), v^{(3)}(\mathbf{x})\right)$, where

$$v^{(1)}(x, y, z) = (z + \frac{l_x}{\alpha}) \sin(\frac{\alpha}{l_x} x),$$

$$v^{(2)}(x, y, z) = y,$$

$$v^{(3)}(x, y, z) = (z + \frac{l_x}{\alpha}) \cos(\frac{\alpha}{l_x} x) - \frac{l_x}{\alpha}.$$

This deformation preserves the length l_x of the axis that is on the x-axes of the original cuboid domain (see Fig. 3.1), and depends on the angle $\alpha \in (0, 2\pi]$. For $\alpha \in (0, 2\pi)$ the cuboid deforms into a partial toroid, e.g. in Fig. 3.2 (a), and for $\alpha = 2\pi$ the cuboid becomes a whole toroid, e.g. in Fig. 3.2 (b).
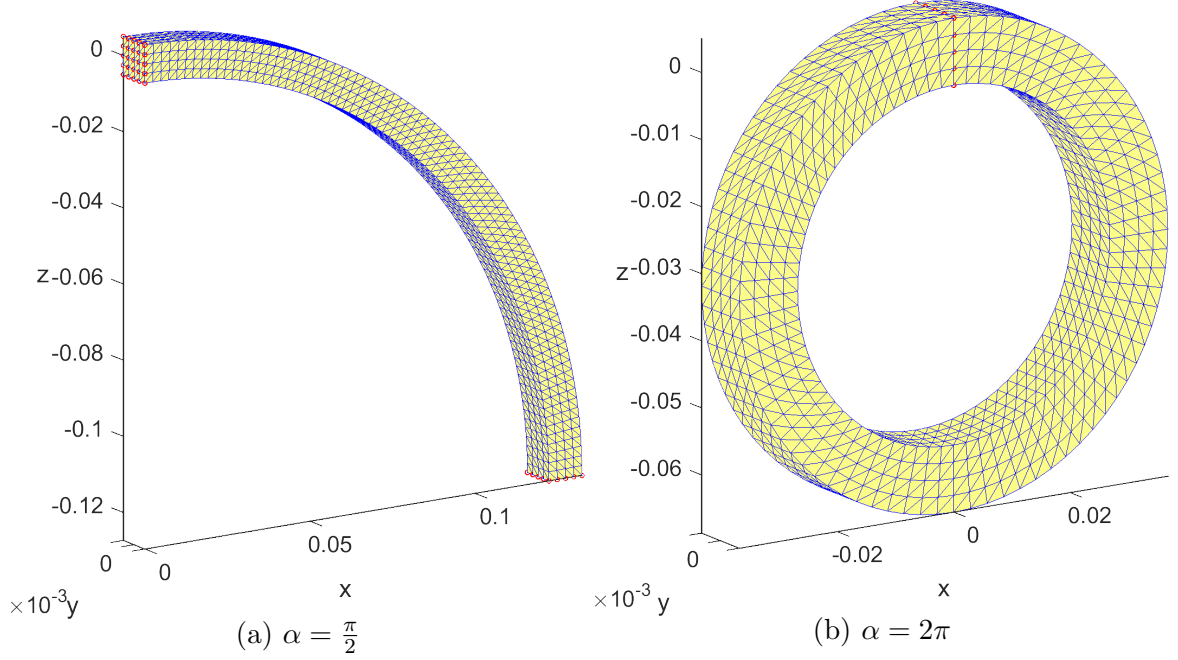

(a) $\alpha = \frac{\pi}{2}$ (b) $\alpha = 2\pi$

Figure 3.2: Deformation into a partial toroid and a whole toroid for different angles α.

3.1.1 Deformation gradient and determinant

Using the definition (2.1), the deformation gradient for this deformation is

$$\mathbf{F}(\mathbf{v}) = \begin{pmatrix} (z\frac{\alpha}{l_x} + 1) \cos(\frac{\alpha}{l_x} x) & 0 & \sin(\frac{\alpha}{l_x} x) \\ 0 & 1 & 0 \\ -(z\frac{\alpha}{l_x} + 1) \sin(\frac{\alpha}{l_x} x) & 0 & \cos(\frac{\alpha}{l_x} x) \end{pmatrix}.$$

This deformation is nonhomogeneous, since the deformation gradient is dependent on the variables x and z. Furthermore, for $\alpha \to 0$, $\mathbf{F} = \mathbf{I}$, indicating that the cuboid domain does not deform. The determinant is expressed as

$$\det(\mathbf{F}) = (z\frac{\alpha}{l_x} + 1) \cos^2(\frac{\alpha}{l_x} x) + (z\frac{\alpha}{l_x} + 1) \sin^2(\frac{\alpha}{l_x} x) = z\frac{\alpha}{l_x} + 1$$

and is dependent on z. Therefore, the volume change depends on z. In this case, the natural condition of the locally positive volume change is met:

$$\det(\mathbf{F}) = z\frac{\alpha}{l_x} + 1 > 0 \quad \forall z, \alpha, l_x.$$

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- ○ The volume increases for $z > 0$.

- ○ The volume is preserved for $z = 0$.

- ○ The volume decreases for $z < 0$.

The values of the determinant are depicted in Fig. 3.3 (a) for $\alpha = \frac{\pi}{2}$ and in Fig. 3.3 (b) for $\alpha = 2\pi$.
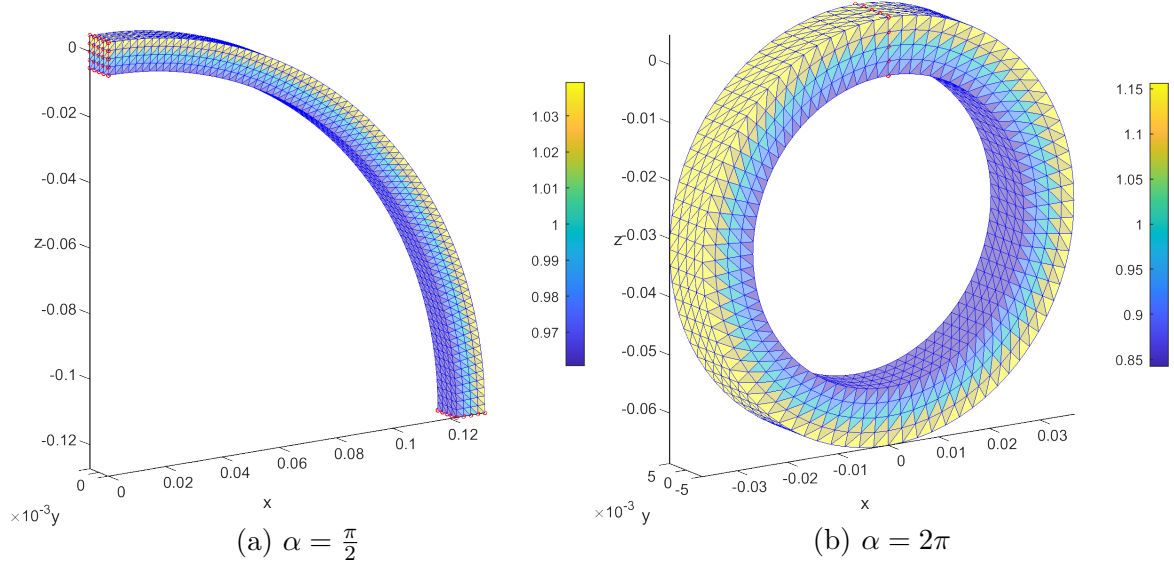

(a) $\alpha = \frac{\pi}{2}$ (b) $\alpha = 2\pi$

Figure 3.3: The determinant for different angles α.

Next, we use the deformation gradient to compute $||\mathbf{F}||^2$, which is used to evaluate the Neo-Hookean density:

$$||\mathbf{F}||^2 = 2 + \left(z\frac{\alpha}{l_x} + 1 \right)^2.$$

3.1.2 Strain tensors

The large and the small strain tensors and their corresponding $|| \cdot ||^2$ and $(\mathrm{tr}(\cdot))^2$ are expressed as

$$\mathbf{E} = \frac{1}{2} \begin{pmatrix} (z\frac{\alpha}{l_x} + 1)^2 - 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad ||\mathbf{E}||^2 = (\mathrm{tr}(\mathbf{E}))^2 = \frac{1}{4} \left((z\frac{\alpha}{l_x} + 1)^2 - 1 \right)^2,$$

$$\mathbf{e} = \frac{1}{2} \begin{pmatrix} 2\left((z\frac{\alpha}{l_x} + 1)\cos(\frac{\alpha}{l_x}x) - 1 \right) & 0 & -z\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x) \\ 0 & 0 & 0 \\ -z\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x) & 0 & 2\left(\cos(\frac{\alpha}{l_x}x) - 1 \right) \end{pmatrix},$$

$$||\mathbf{e}||^2 = \left((z\frac{\alpha}{l_x}+1)\cos(\frac{\alpha}{l_x}x)-1\right)^2 + \left(\cos(\frac{\alpha}{l_x}x)-1\right)^2 + \frac{1}{2}\left(z\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x)\right)^2,$$

$$(\mathrm{tr}(\mathbf{e}))^2 = \left((z\frac{\alpha}{l_x}+2)\cos(\frac{\alpha}{l_x}x)-2\right)^2.$$

3.1.3 Energy densities

The different density models can be expressed as

$$W_{NH}(\mathbf{F}) = C_1\left(\left(z\frac{\alpha}{l_x}+1\right)^2-1-2\log(z\frac{\alpha}{l_x}+1)\right)+D_1\left(z\frac{\alpha}{l_x}\right)^2, \tag{3.1}$$

$$W_{SVK}(\mathbf{F}) = \frac{1}{4}(\mu+\frac{\lambda}{2})\left((z\frac{\alpha}{l_x}+1)^2-1\right)^2, \tag{3.2}$$

$$W_H(\mathbf{F}) = \mu\left(\left((z\frac{\alpha}{l_x}+1)\cos(\frac{\alpha}{l_x}x)-1\right)^2+\left(\cos(\frac{\alpha}{l_x}x)-1\right)^2+\frac{1}{2}\left(z\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x)\right)^2\right)+$$
$$+\frac{\lambda}{2}\left((z\frac{\alpha}{l_x}+2)\cos(\frac{\alpha}{l_x}x)-2\right)^2. \tag{3.3}$$

For the density models, similarly to for the deformation gradient, $\alpha \to 0$ should indicate that the cuboid domain does not deform. This is reflected in the values of densities which satisfy $W_{NH} \to 0, W_{SVK} \to 0, W_H \to 0$ for $\alpha \to 0$.

The density values are visualized for the angles $\alpha = \frac{\pi}{2}$ and $\alpha = 2\pi$ in Fig. 3.4. Furthermore, the values of the Neo-Hookean model and the Saint Venant-Kirchhoff model reach similar values. However, the linear elasticity model shows an unrealistic distribution of densities.

The value of the energy functional for different density models reads (detailed evaluations of integrals are omitted):

$$J_{NH}(\mathbf{v}) = \int_\Omega W_{NH}(\mathbf{F})\,\mathrm{d}\mathbf{x} =$$

$$= \int_{-\frac{l_z}{2}}^{\frac{l_z}{2}}\int_{-\frac{l_y}{2}}^{\frac{l_y}{2}}\int_0^{l_x}\left(C_1\left(\left(z\frac{\alpha}{l_x}+1\right)^2-1-2\ln(z\frac{\alpha}{l_x}+1)\right)+D_1\left(z\frac{\alpha}{l_x}\right)^2\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z =$$

$$= C_1 l_x l_y\left(\frac{\alpha^2 l_z^3}{12 l_x^2}+2l_z-2(\frac{l_x}{\alpha}+\frac{l_z}{2})\ln(1+\frac{\alpha l_z}{2l_x})+2(\frac{l_x}{\alpha}-\frac{l_z}{2})\ln(1-\frac{\alpha l_z}{2l_x})\right)+D_1\frac{\alpha^2 l_y l_z^3}{12 l_x},$$
$$\tag{3.4}$$

(a) NH density for $\alpha = \frac{\pi}{2}$

(b) NH density for $\alpha = 2\pi$

(c) SVK density for $\alpha = \frac{\pi}{2}$

(d) SVK density for $\alpha = 2\pi$

(e) H density for $\alpha = \frac{\pi}{2}$
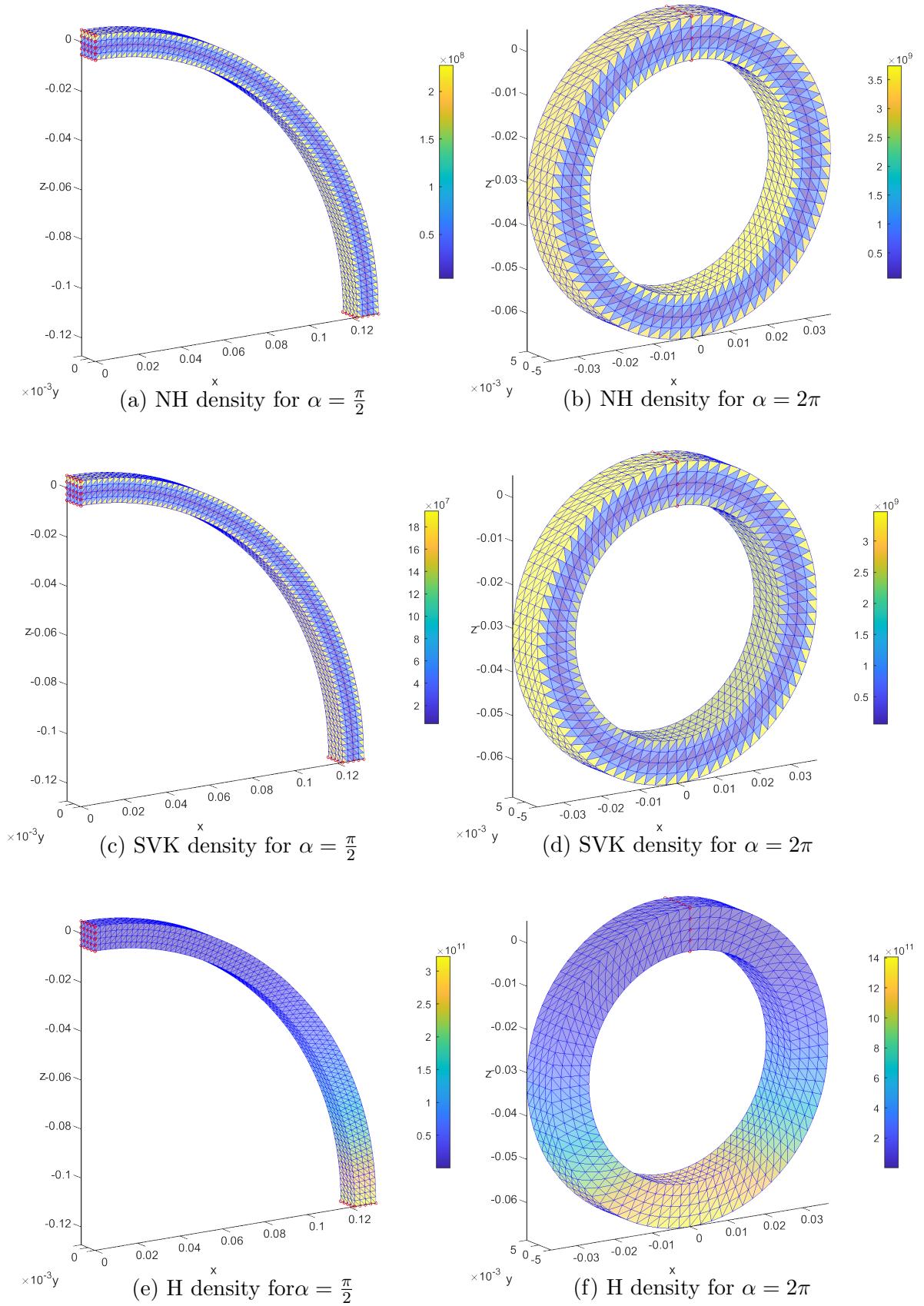
(f) H density for $\alpha = 2\pi$

Figure 3.4: The values of the Neo-Hookean densities, the Saint Venant-Kirchhoff densities and the linear elasticity densities visualized for the angles $\alpha = \frac{\pi}{2}$ and $\alpha = 2\pi$.

$$J_{SVK}(\mathbf{v}) = \frac{1}{4}(\mu + \frac{\lambda}{2}) \int_\Omega \left((z\frac{\alpha}{l_x} + 1)^2 - 1 \right)^2 \mathrm{d}\mathbf{x} = \frac{l_y}{4}(\mu + \frac{\lambda}{2}) \left(\frac{\alpha^4 l_z^5}{80 l_x^3} + \frac{\alpha^2 l_z^3}{3 l_x} \right), \quad (3.5)$$

$$J_H(\mathbf{v}) = \int_{-\frac{l_z}{2}}^{\frac{l_z}{2}} \int_{-\frac{l_y}{2}}^{\frac{l_y}{2}} \int_0^{l_x} \left(\mu \left(\left((z\frac{\alpha}{l_x} + 1) \cos(\frac{\alpha}{l_x}x) - 1 \right)^2 + \left(\cos(\frac{\alpha}{l_x}x) - 1 \right)^2 + \right. \right.$$

$$\left. \left. + \frac{1}{2} \left(z\frac{\alpha}{l_x} \sin(\frac{\alpha}{l_x}x) \right)^2 \right) + \frac{\lambda}{2} \left((z\frac{\alpha}{l_x} + 2) \cos(\frac{\alpha}{l_x}x) - 2 \right)^2 \right) \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z =$$

$$= \mu l_x l_y l_z \left(\left(\frac{\alpha^2 l_z^2}{48 l_x^2} + \frac{1}{4} \right) \left(\frac{1}{\alpha} \sin(2\alpha) + 2 \right) - \frac{4}{\alpha} \sin(\alpha) + \frac{5}{2} + \quad (3.6)\right.$$

$$+ \frac{1}{4\alpha} \sin(2\alpha) + \frac{\alpha^2 l_z^2}{48 l_x^2} \left(1 - \frac{1}{2\alpha} \sin(2\alpha) \right) \right) +$$

$$+ \frac{\lambda}{2} l_x l_y l_z \left(\left(\frac{\alpha^2 l_z^2}{48 l_x^2} + 1 \right) \left(\frac{1}{\alpha} \sin(2\alpha) + 2 \right) - \frac{8}{\alpha} \sin(\alpha) + 4 \right).$$

3.1.4 Evaluation of exact and approximate energies

The approximate values of the energy functional can be alternatively computed numerically using [5] for various levels of uniform mesh refinements in the finite element discretization of the cuboid domain. The higher the mesh level, the finer mesh is applied.

mesh level	number of nodes	number of elements
1	369	960
2	2,025	7,680
3	13,041	61,440
4	92,769	491,520
5	698,049	3,932,160

By the choice level=∞, we denote the exact value of the energy functional computed independently in (3.4), (3.5) and (3.6) with the help of Code - Matlab 4. In the following tables, we can clearly see how the numeric values converge to the exact solution. The convergence is used to verify the results of the solution.

∘ The energy functional values for the Neo-Hookean density model.

mesh level	$\alpha = \frac{\pi}{2}$	$\alpha = 2\pi$
1	2,503.497615	40,044.019563
2	1,733.613962	27,772.705833
3	1,541.121847	24,699.438950
4	1,492.997492	23,930.780059
5	1,480.966321	23,738.592914
∞	1,476.955923	23,674.529961

∘ The energy functional values for the Saint Venant-Kirchhoff density model.

mesh level	$\alpha = \frac{\pi}{2}$	$\alpha = 2\pi$
1	2,119.312486	33,974.529251
2	1,445.407271	23,204.270785
3	1,276.889944	20,501.154260
4	1,234.758049	19,824.714483
5	1,224.224915	19,655.563230
∞	1,220.713856	19,599.175807

∘ The energy functional values for the linear elasticity density model.

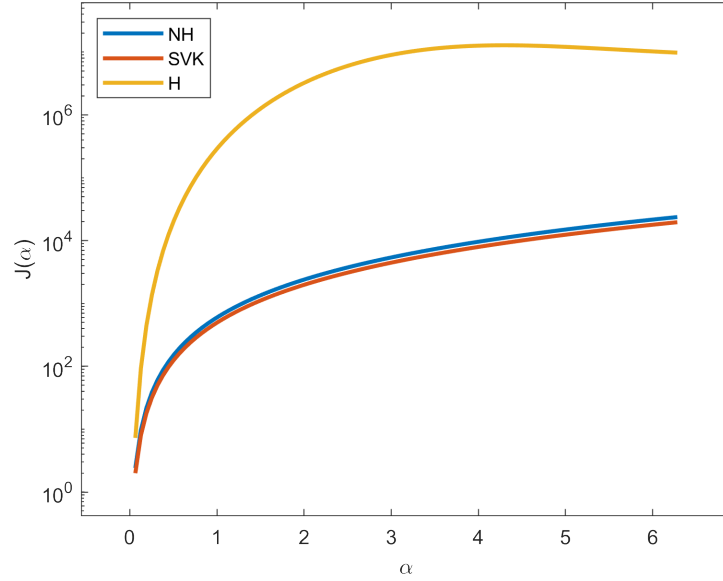| mesh level	$\alpha = \frac{\pi}{2}$	$\alpha = 2\pi$
1	1,476,891.836962	9,772,410.814876
2	1,476,068.045306	9,770,433.678206
3	1,475,862.102017	9,769,937.659739
4	1,475,810.616484	9,769,813.546628
5	1,475,797.745119	9,769,782.511568
∞	1,475,793.454665	9,769,772.165945

Figure 3.5: The comparison of exact energies.

The comparison of exact energy densities is illustrated in Fig. 3.5 for angles $\alpha \in (0, 2\pi]$ with the help of Code - Matlab 2. The values of $J(\mathbf{v})$ are shown on a logarithmic scale for better visualization, since the values of the linear elasticity energy reach high values compared to the other energies.

Remark 8 *The linear elasticity model is shown only for illustrative purposes, since the deformation is very different from the identity deformation. In this case, it causes an unrealistic distribution of densities (see Fig. 3.4 (e), (f)) and reaches unrealistically high values of energies (see Fig. 3.5).*

3.2 Deformation into a twist

The deformation of a cuboid domain Ω is prescribed by the deformation mapping $\mathbf{v}(\mathbf{x})$:

$$v^{(1)}(x, y, z) = x,$$
$$v^{(2)}(x, y, z) = y\cos(\frac{\alpha}{l_x}x) + z\sin(\frac{\alpha}{l_x}x),$$
$$v^{(3)}(x, y, z) = -y\sin(\frac{\alpha}{l_x}x) + z\cos(\frac{\alpha}{l_x}x).$$

The deformation mapping determines how much Ω (see Fig. 3.1) twists around the x-axis depending on the angle α. The deformation is visualized for $\alpha = 2\pi$ in Fig. 3.6 (a) and for $\alpha = 4\pi$ in Fig. 3.6 (b).
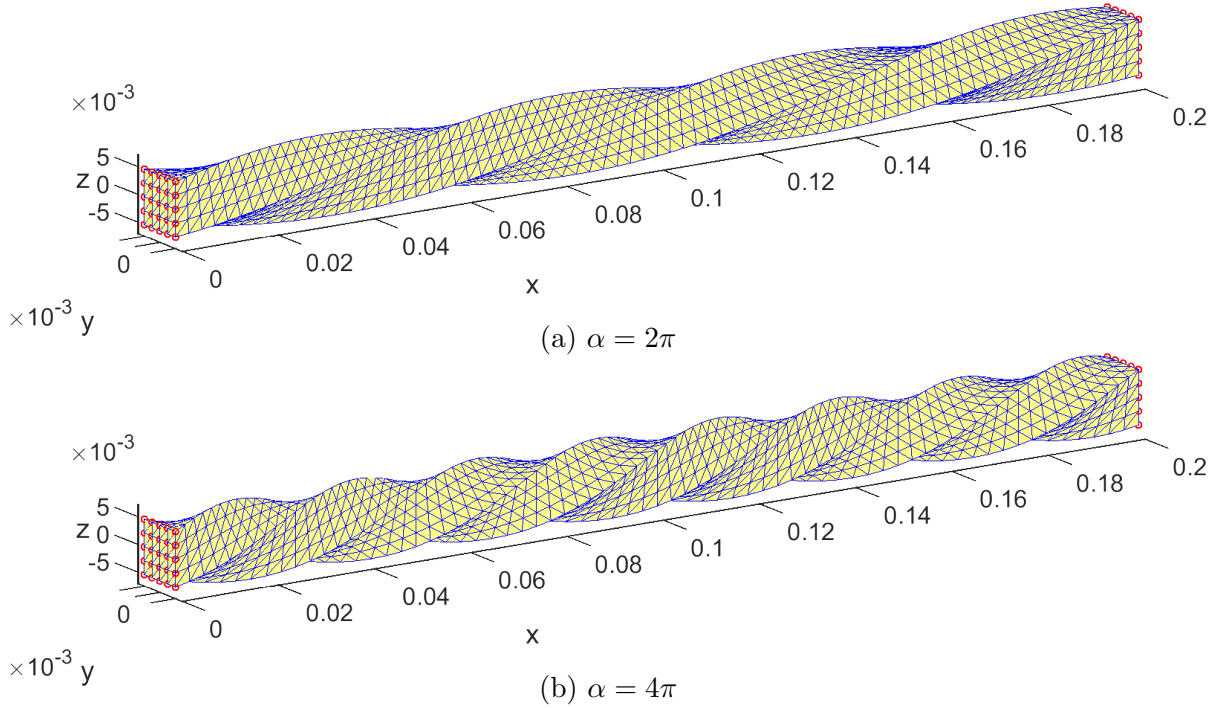

(a) $\alpha = 2\pi$

(b) $\alpha = 4\pi$

Figure 3.6: Deformation into a twist for different angles α.

3.2.1 Deformation gradient and determinant

$$\mathbf{F}(\mathbf{v}) = \begin{pmatrix} 1 & 0 & 0 \\ -y\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x) + z\frac{\alpha}{l_x}\cos(\frac{\alpha}{l_x}x) & \cos(\frac{\alpha}{l_x}x) & \sin(\frac{\alpha}{l_x}x) \\ -y\frac{\alpha}{l_x}\cos(\frac{\alpha}{l_x}x) - z\frac{\alpha}{l_x}\sin(\frac{\alpha}{l_x}x) & -\sin(\frac{\alpha}{l_x}x) & \cos(\frac{\alpha}{l_x}x) \end{pmatrix}.$$

The deformation gradient $\mathbf{F}(\mathbf{v})$ is a function of $\mathbf{x}$, therefore, the deformation is nonhomogeneous. The cuboid domain Ω does not deform, if the deformation gradient $\mathbf{F} = \mathbf{I}$, which is met for $\alpha = 0$. Furthermore, the determinant $\det(\mathbf{F}) = 1$, which signifies that the volume is preserved. Therefore, the deformation is isochoric in Ω.

$$\det(\mathbf{F}) = \cos^2(\frac{\alpha}{l_x}x) + \sin^2(\frac{\alpha}{l_x}x) = 1.$$

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From the deformation gradient $||\mathbf{F}||^2$ is expressed as

$$||\mathbf{F}||^2 = 3 + \frac{\alpha^2}{l_x^2}(y^2 + z^2).$$

3.2.2 Strain tensors

The large and the small strain tensors and their corresponding $||\cdot||^2$ and $(\mathrm{tr}(\cdot))^2$ are expressed as

$$\mathbf{E} = \frac{1}{2}\begin{pmatrix} \frac{\alpha^2}{l_x^2}(y^2 + z^2) & z\frac{\alpha}{l_x} & -y\frac{\alpha}{l_x} \\ z\frac{\alpha}{l_x} & 0 & 0 \\ -y\frac{\alpha}{l_x} & 0 & 0 \end{pmatrix},$$

$$||\mathbf{E}||^2 = \frac{1}{4}\frac{\alpha^4}{l_x^4}(y^2 + z^2)^2 + \frac{1}{2}\frac{\alpha^2}{l_x^2}(y^2 + z^2), \qquad (\mathrm{tr}(\mathbf{E}))^2 = \frac{1}{4}\frac{\alpha^4}{l_x^4}(y^2 + z^2)^2,$$

$$\mathbf{e} = \frac{1}{2}\begin{pmatrix} 0 & \frac{\alpha}{l_x}(z\cos(\frac{\alpha}{l_x}x) - y\sin(\frac{\alpha}{l_x}x)) & \frac{\alpha}{l_x}(-y\cos(\frac{\alpha}{l_x}x) - z\sin(\frac{\alpha}{l_x}x)) \\ \frac{\alpha}{l_x}(z\cos(\frac{\alpha}{l_x}x) - y\sin(\frac{\alpha}{l_x}x)) & 2(\cos(\frac{\alpha}{l_x}x) - 1) & 0 \\ \frac{\alpha}{l_x}(-y\cos(\frac{\alpha}{l_x}x) - z\sin(\frac{\alpha}{l_x}x)) & 0 & 2(\cos(\frac{\alpha}{l_x}x) - 1) \end{pmatrix},$$

$$||\mathbf{e}||^2 = 2(\cos(\frac{\alpha}{l_x}x) - 1)^2 + \frac{\alpha^2}{2l_x^2}(y^2 + z^2), \qquad (\mathrm{tr}(\mathbf{e}))^2 = 4(\cos(\frac{\alpha}{l_x}x) - 1)^2.$$
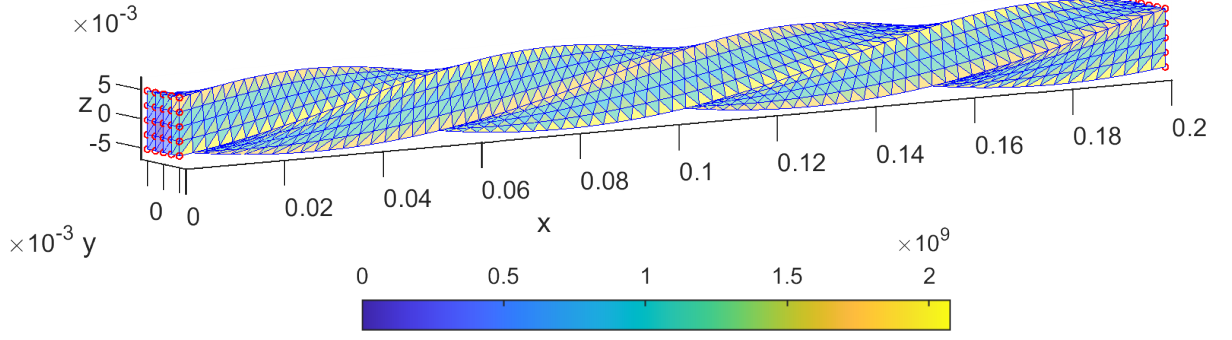
3.2.3 Energy densities

The different density models can be expressed as

$$W_{NH}(\mathbf{F}) = C_1 \frac{\alpha^2}{l_x^2}(y^2 + z^2), \tag{3.7}$$

$$W_{SVK}(\mathbf{F}) = (\mu + \frac{\lambda}{2})\frac{\alpha^4}{4l_x^4}(y^2 + z^2)^2 + \mu\frac{\alpha^2}{2l_x^2}(y^2 + z^2), \tag{3.8}$$

$$W_H(\mathbf{F}) = (2\mu + 2\lambda)(\cos(\frac{\alpha}{l_x}x) - 1)^2 + \mu\frac{\alpha^2}{2l_x^2}(y^2 + z^2). \tag{3.9}$$
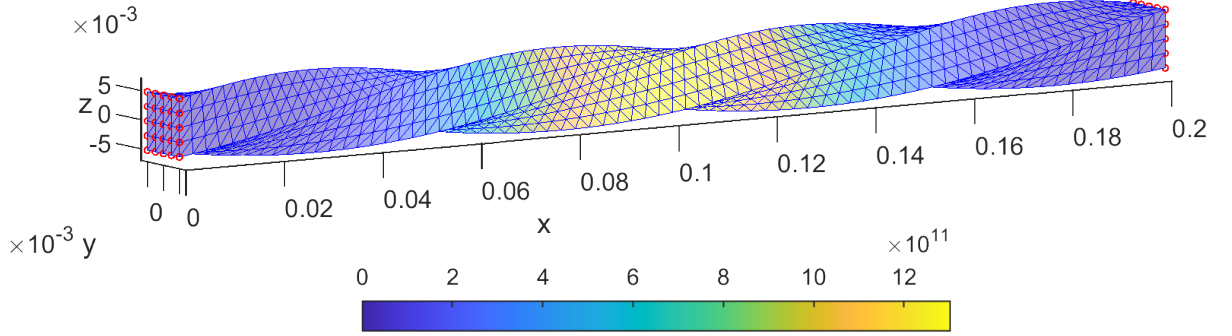
For the density models, similarly as for the deformation gradient, $\alpha \to 0$ should indicate that the cuboid domain Ω does not deform. This is reflected in the values of densities which satisfy $W_{NH} \to 0, W_{SVK} \to 0, W_H \to 0$ for $\alpha \to 0$. The density values are visualized for angles $\alpha = 2\pi$ in Fig. 3.7 and $\alpha = 4\pi$ in Fig. 3.8.

(a) NH density for $\alpha = 2\pi$
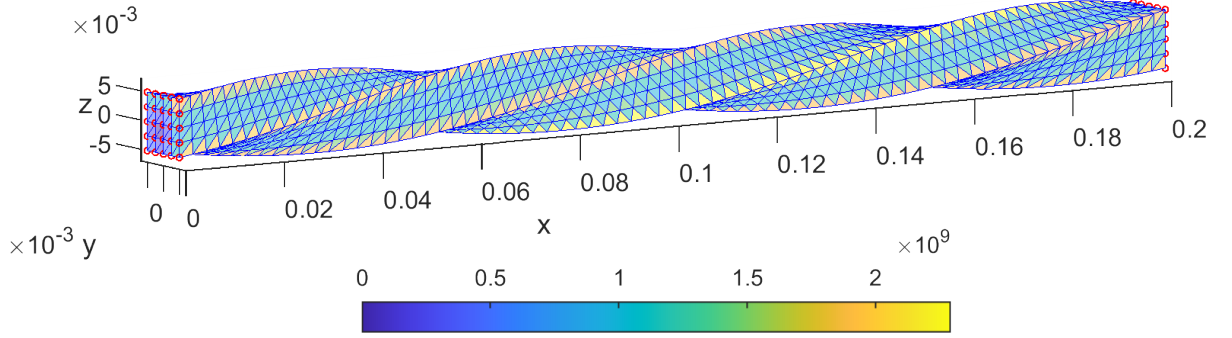
(b) SVK density for $\alpha = 2\pi$

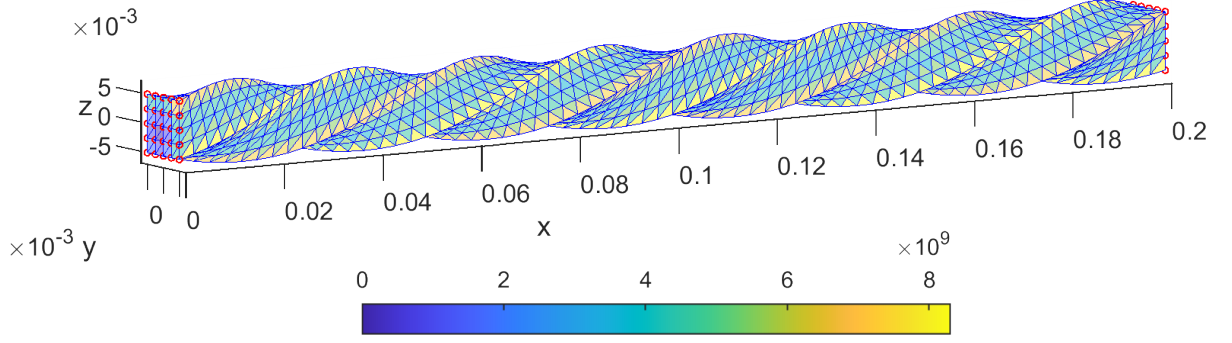(c) H density for $\alpha = 2\pi$

Figure 3.7: The values of the Neo-Hookean densities, the Saint Venant-Kirchhoff densities and the linear elasticity densities visualized for the angle $\alpha = 2\pi$.

The energy functional for different density models reads (detailed evaluations of integrals are omitted):

$$J_{NH}(\mathbf{v}) = C_1 (\frac{\alpha}{l_x})^2 \int_\Omega (y^2 + z^2)\,\mathrm{d}\mathbf{x} = \frac{C_1 \alpha^2}{12 l_x}(l_y^3 l_z + l_y l_z^3), \qquad (3.10)$$

$$J_{SVK}(\mathbf{v}) = (\mu + \frac{\lambda}{2})\frac{\alpha^4}{4 l_x^4}\int_\Omega (y^2 + z^2)^2\,\mathrm{d}\mathbf{x} + \frac{\mu\alpha^2}{2 l_x^2}\int_\Omega (y^2 + z^2)\,\mathrm{d}\mathbf{x} =$$

$$= (\mu + \frac{\lambda}{2})\frac{\alpha^4 l_y l_z}{4 l_x^3}(\frac{l_y^4}{80} + \frac{l_y^2 l_z^2}{72} + \frac{l_z^4}{80}) + \mu\frac{\alpha^2 l_y l_z}{24 l_x}(l_y^2 + l_z^2), \qquad (3.11)$$

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$$J_H(\mathbf{v}) = (2\mu + 2\lambda) \int_\Omega (\cos(\frac{\alpha}{l_x}x) - 1)^2 \, d\mathbf{x} + \mu \frac{\alpha^2}{2l_x^2} \int_\Omega (y^2 + z^2) \, d\mathbf{x} =$$

$$= (2\mu + 2\lambda) l_x l_y l_z (\frac{1}{4\alpha} \sin(2\alpha) - \frac{2}{\alpha} \sin(\alpha) + \frac{3}{2}) + \mu \frac{\alpha^2 l_y l_z}{24 l_x} (l_y^2 + l_z^2).$$

(3.12)

(a) NH density for $\alpha = 4\pi$
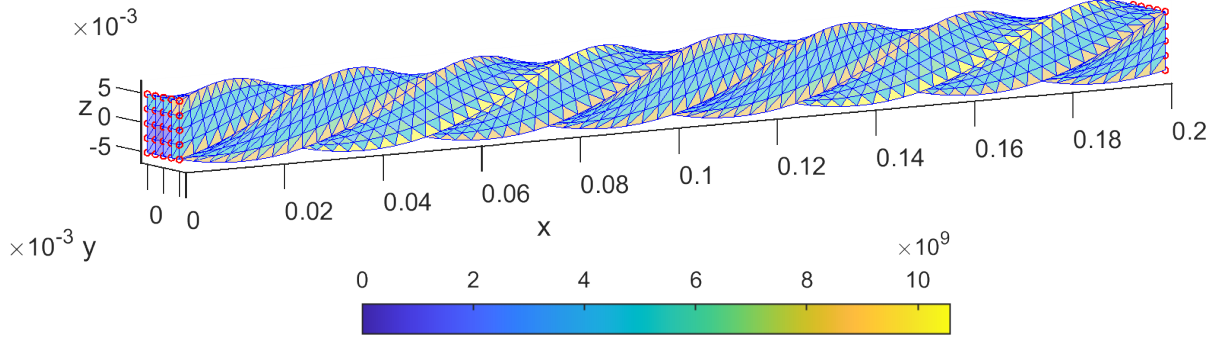
(b) SVK density for $\alpha = 4\pi$
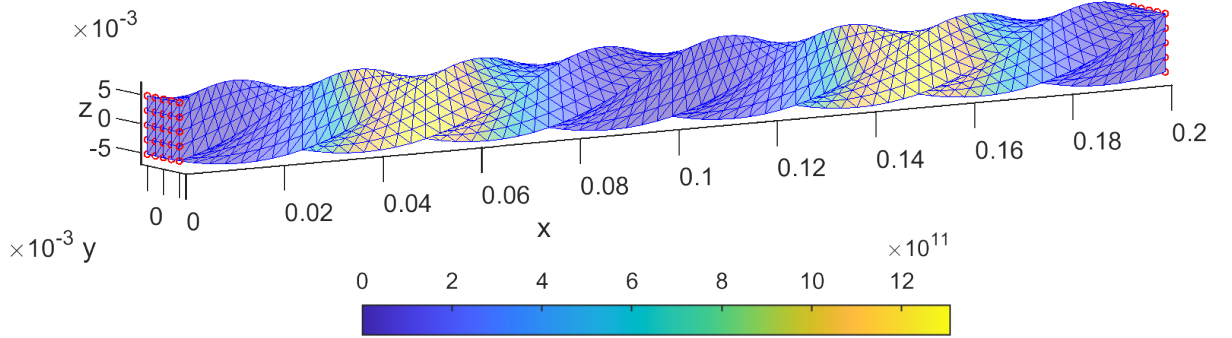
(c) H density for $\alpha = 4\pi$

Figure 3.8: The values of the Neo-Hookean densities, the Saint Venant-Kirchhoff densities and the linear elasticity densities visualized for the angle $\alpha = 4\pi$.

3.2.4 Evaluation of exact and approximate energies

The approximate values of energy functional can be computed numerically using [5] and the exact values are computed in (3.10), (3.11) and (3.12) with the help of Code - Matlab 4 and 5.

○ The energy functional values for the Neo-Hookean density model.

mesh level	$\alpha = 2\pi$	$\alpha = 4\pi$
1	24,666.362864	99,346.942080
2	15,379.611952	61,504.398878
3	13,072.405018	52,274.515304
4	12,496.509502	49,981.536171
5	12,352.592280	49,409.198291
∞	12,304.624909	49,218.499638

○ The energy functional values for the Saint Venant-Kirchhoff density model.

mesh level	$\alpha = 2\pi$	$\alpha = 4\pi$
1	25,060.703942	105,563.672992
2	15,675.087145	66,217.204313
3	13,316.675712	56,179.830149
4	12,726.320289	53,657.799967
5	12,578.684365	53,026.497315
∞	12,529.468205	52,815.992372

○ The energy functional values for the linear elasticity density model.

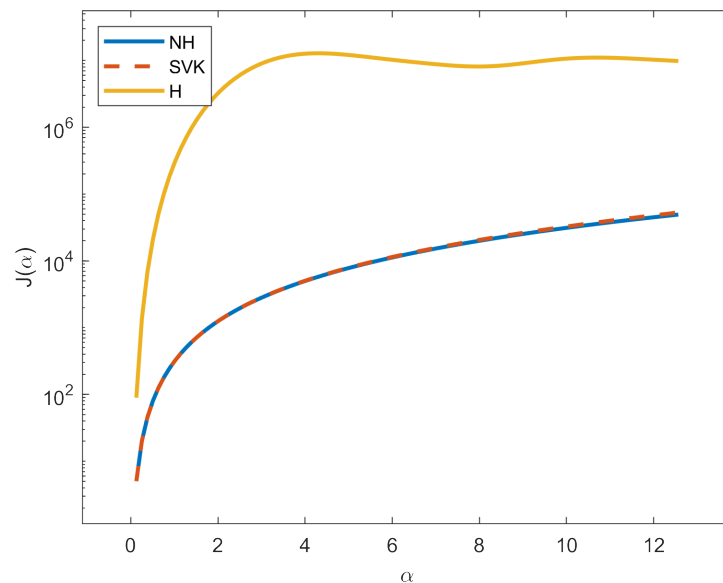| mesh level	$\alpha = 2\pi$	$\alpha = 4\pi$
1	9,774,817.690771	9,828,032.699710
2	9,770,634.468914	9,811,655.726785
3	9,769,586.638993	9,807,529.372266
4	9,769,324.554882	9,80,6495.770146
5	9,769,259.025938	9,806,237.243671
∞	9,769,237.182253	9,806,151.056981

Figure 3.9: The comparison of exact energies.

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The comparison of exact energy densities is illustrated in Fig. 3.9 for angles $\alpha \in (0, 4\pi]$ with the help of Code - Matlab 2 and 3. The values of $J(\mathbf{v})$ are shown on a logarithmic scale, since the values of the linear elasticity energy reach high values in comparison to the other energies.

Remark 9 *Similarly as in the previous example, the linear elasticity model is shown only for illustrative purposes.*

3.3   Deformation into a hourglass

This section focuses on examples of physically unrealistic deformations, therefore the computation of strain tensors, densities and the evaluation of exact and approximate energies are omitted. The deformation gradient and the determinant of the deformation gradient and their significance is discussed.

The layers of the cuboid domain Ω are colored to illustrate how the material deforms (see Fig. 3.10).

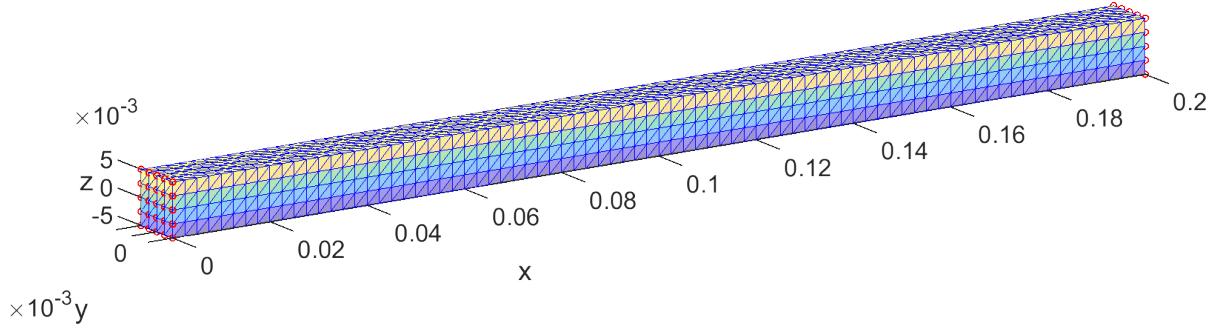Figure 3.10: The coloured cuboid domain to show how the material deforms.

3.3.1   Hourglass: type 1

The deformation of a cuboid domain Ω is prescribed by the deformation mapping $\mathbf{v}(\mathbf{x})$:

$$
\begin{aligned}
v^{(1)}(x, y, z) &= x, \\
v^{(2)}(x, y, z) &= y, \\
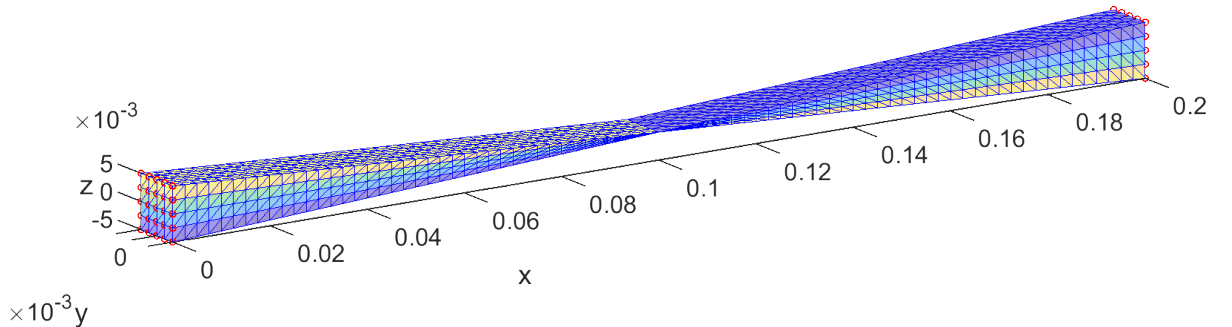v^{(3)}(x, y, z) &= (-\frac{2x}{l_x} + 1)z.
\end{aligned}
$$

Figure 3.11: Deformation into hourglass: type 1.

The deformation represents an unrealistic deformation, where the material changes its orientation at $x = \frac{l_x}{2}$ (see Fig. 3.11).

Deformation gradient and determinant

The deformation gradient is expressed as

$$
\mathbf{F}(\mathbf{v}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{2z}{l_x} & 0 & -\frac{2x}{l_x} + 1 \end{pmatrix}.
$$

The determinant of the deformation gradient is

$$
\det(\mathbf{F}) = -\frac{2x}{l_x} + 1.
$$

The determinant changes the sign for $x = \frac{l_x}{2}$, therefore the deformation for $x > \frac{l_x}{2}$ does not preserve the orientation of the material. Furthermore, for $x = \frac{l_x}{2}$

$$
\det(\mathbf{F}) = 0,
$$

which signifies that the material is compressed to a single line (see Fig. 3.12).
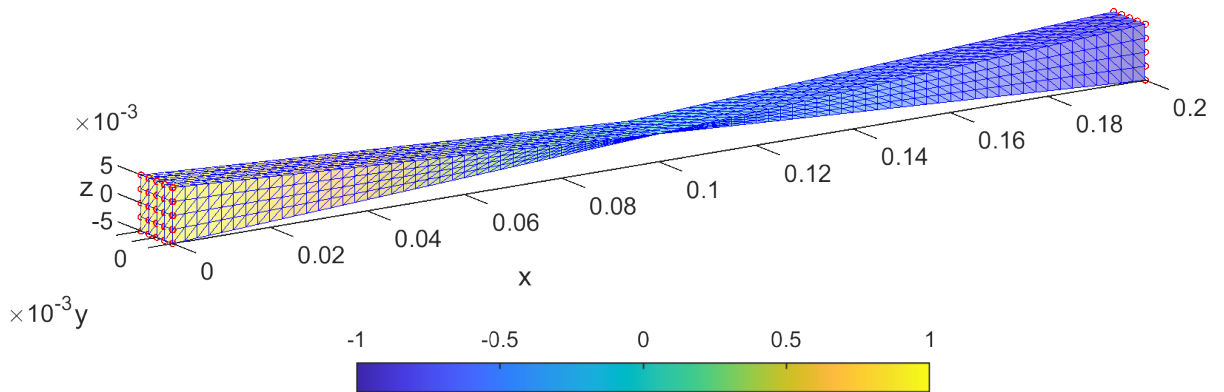
Figure 3.12: Values of determinant.

3.3.2   Hourglass: type 2

The deformation of a cuboid domain Ω is prescribed by the following deformation mapping $\mathbf{v}(\mathbf{x})$:

$$
\begin{aligned}
v^{(1)}(x, y, z) &= x, \\
v^{(2)}(x, y, z) &= (-\frac{2x}{l_x} + 1)y, \\
v^{(3)}(x, y, z) &= (-\frac{2x}{l_x} + 1)z.
\end{aligned}
$$

Deformation gradient and determinant

The deformation gradient can be expressed as

$$\mathbf{F}(\mathbf{v}) = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{2y}{l_x} & -\frac{2x}{l_x} + 1 & 0 \\ -\frac{2z}{l_x} & 0 & -\frac{2x}{l_x} + 1 \end{pmatrix}$$

The determinant of the deformation gradient is

$$\det(\mathbf{F}) = (-\frac{2x}{l_x} + 1)^2 \geq 0 \quad \forall x, l_x.$$

For $x = \frac{l_x}{2}$

$$\det(\mathbf{F}) = 0,$$

which signifies a case of an unrealistic deformation, where the material is compressed to a single point (see Fig. 3.13).
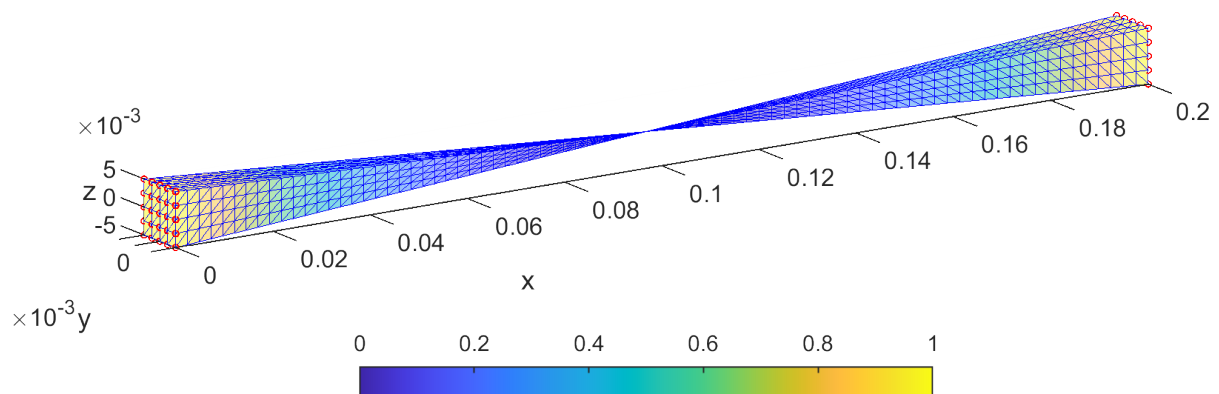
Figure 3.13: The values of determinant.

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Chapter 4

Conclusion

Within the thesis we introduced the key concepts of continuum mechanics and successfully demonstrated them in practical examples that were specifically developed to support the aspects of the theoretical part from Chapter 2. The examples were extensively provided with elaborate computations and visualizations. All computations were calculated in an analytical manner and the values of elastic energy functional were compared to the corresponding numeric solution.

Own Matlab codes were developed and used for visualizations and computations. Also other Matlab codes [5] were used and adjusted for the same purposes. The codes were listed and described in the Appendix.

Forthcoming works might also incorporate the concepts and calculations of stress and energy minimizers of materials.

Appendix

In this part we will show and describe the codes used in Chapter 2 and Chapter 3 to visualize deformations, corresponding values of deformation gradients, density models and energy functionals. As well the codes to numerically evaluate the values are listed.

Some own codes were developed specifically for the thesis and are shown in the Section A. The other codes in Section B represent parts of codes that replace corresponding parts of codes provided in [5].

All codes were performed in MATLAB numeric computing environment [4]

A   New own codes

The following Code - Matlab 1 illustrates the deformation of a sphere into an ellipsoid seen in Chapter 2, Example 1.

Code - Matlab 1: A deformation of a sphere into an ellipsoid.

```matlab
close all
theta=linspace(0,pi,40); phi=linspace(0,2*pi,40);
[theta,phi]=meshgrid(theta,phi);
x0=0; y0=0; z0=0; r=1;
X=x0+r.*cos(phi).*sin(theta);          %spherical coordinates
Y=y0+r.*sin(phi).*sin(theta);
Z=z0+r.*cos(theta);
surf(X,Y,Z)
axis on; axis tight;
xlabel('x'); ylabel('y'); zlabel('z'); axis image;
set(get(gca,'zlabel'),'rotation',0)
hold on
x1=4; y1=0; z1=0; rx = 2.5; ry = 1; rz = 1;
X= x1+rx*(X-x0);                        %mapping into an ellipsoid
Y = y1+ry*(Y-y0);
Z = z1+rz*(Z-z0);
surf(X,Y,Z)
hold off
view(-25,16)
```

The values of energies to graphically compare the Neo-Hookean, the Saint Venant-Kirchhoff and the linear elasticity density models of the deformation into a partial and a whole toroid are computed by using the trapezoidal rule in Code - Matlab 2

Code - Matlab 2: A comparison of the energy values - a toroid deformation.

```matlab
close all
lx=0.2; ly=0.01; lz=ly;                    % cuboid geometry
E = 190e9; nu = 0.27;                      % material parameters for steel
mu=E/(2*(1+nu)); lambda=E*nu/((1+nu)*(1-2*nu));
K= E/(3*(1-2*nu)); C_1=mu/2; D_1=K/2;
nx=50; ny=50; nz=ny;                       % discretization
xx=linspace(0,lx,nx); yy=linspace(-ly/2,ly/2,ny); zz=yy;
[XX,YY,ZZ]=meshgrid(xx,yy,zz);
alphas=linspace(0,2*pi,100);               % sequence of alpha parameters
for i=1:numel(alphas)
    alpha=alphas(i);
    al=alpha/lx;                           % new variable
    % densities - formulas (3.1), (3.2), (3.3) from bc thesis
    W_NH=@(x,y,z) C_1*((z*al+1).^2-1-2*log(z*al+1))+D_1*(z*al).^2;
    W_SVK=@(x,y,z) (mu+lambda/2)/4*((z*al+1).^2-1).^2;
    W_H=@(x,y,z) mu*(((z*al+1).*cos(al*x)-1).^2 ...
                 +(cos(x*al)-1).^2+1/2*(z*al.*sin(x*al)).^2)...
                 +lambda/2*((z*al+2).*cos(al*x)-2).^2;
    % numerical integrals using trapezoidal rule in 3 dimensions
    J_NH(i)=trapz(zz,trapz(yy,trapz(xx,W_NH(XX,YY,ZZ))));
    J_SVK(i)=trapz(zz,trapz(yy,trapz(xx,W_SVK(XX,YY,ZZ))));
    J_H(i)=trapz(zz,trapz(yy,trapz(xx,W_H(XX,YY,ZZ))));
end
semilogy(alphas,J_NH,'-',alphas,J_SVK,'-',alphas,J_H,'-','LineWidth',2)
xlabel('\alpha'); ylabel('J(\alpha)');
legend('NH','SVK','H','Location','northwest')
```

To graphically compare the energies for the deformation into a twist the line 9 from the previous code:

'**alphas=linspace(0,2*pi,100);**' is changed to '**alphas=linspace(0,4*pi,100);**', and the lines $13 - 18$ are substituted by Code - Matlab 3.

Code - Matlab 3: Densities for a twist.

```matlab
% densities - formulas (3.7), (3.8), (3.9) from bc thesis
W_NH=@(x,y,z) C_1*al^2*(y.^2+z.^2);
W_SVK=@(x,y,z)(mu+lambda/2)/4*al^4*(y.^2+z.^2).^2+mu/2*al^2*(y.^2+z.^2);
W_H=@(x,y,z) (2*mu+2*lambda)*(cos(al*x)-1).^2+mu/2*al^2*(y.^2+z.^2);
```

To evaluate the exact energy values for a deformation into a toroid Code - Matlab 4 is used, where the values are further verified by using the symbolic computing. The line 6: '**alpha=2*pi;**' can be replaced by a different choice of the angle α, e.g. '**alpha=pi/2;**'.

Code - Matlab 4: Exact energy values for a toroid.

```matlab
1  close all
2  lx=0.2; ly=0.01; lz=ly;                    % cuboid geometry
3  E = 190e9; nu = 0.27;                       % material parameters for steel
4  mu=E/(2*(1+nu)); lambda=E*nu/((1+nu)*(1-2*nu));
5  K= E/(3*(1-2*nu)); C_1=mu/2; D_1=K/2;
6  alpha=2*pi;                                 % angle of deflection - given
7  al=alpha/lx;                                % abbreviation
8  % derived energies (3.4), (3.5), (3.6)
9  J_NH=C_1*lx*ly*(al^2*lz^3/12+2*lz-2*(lx/alpha+lz/2)*log(1+lz*al/2) ...
10          +2*(lx/alpha-lz/2)*log(1-lz*al/2))+D_1*alpha^2*ly*lz^3/12/lx
11 J_SVK=ly/4*(mu+lambda/2)*((alpha)^4*lz^5/(80*lx^3)+(alpha)^2*lz^3/(3*lx))
12 J_H=mu*lx*ly*lz*((al^2*lz^2/48+1/4)*(1/alpha*sin(2*alpha)+2) ...
13          -4/alpha*sin(alpha)+5/2+1/4/alpha*sin(2*alpha) ...
14          +al^2*lz^2/48*(1-1/2/alpha*sin(2*alpha))) ...
15          +lambda/2*lx*ly*lz*((al^2*lz^2/48+1)*(1/alpha*sin(2*alpha)+2) ...
16          -8/alpha*sin(alpha)+4)
17 %verification of energies above using formulas (3.1), (3.2), (3.3)
18 W_NH=@(x,y,z)  C_1*((z*al+1).^2-1-2*log(z*al+1))+D_1*(z*al).^2;
19 W_SVK=@(x,y,z)  (mu+lambda/2)/4*((z*al+1).^2-1).^2;
20 W_H=@(x,y,z)  mu*(((z*al+1).*cos(al*x)-1).^2  ...
21                  +(cos(x*al)-1).^2+1/2*(z*al.*sin(x*al)).^2) ...
22                  +lambda/2*((z*al+2).*cos(al*x)-2).^2;
23 %symbolic computing
24 syms x y z
25 expr_NH=W_NH(x,y,z);
26 expr_SVK=W_SVK(x,y,z);
27 expr_H=W_H(x,y,z);
28 J_NH_comp=double(int(int(int(expr_NH,z,[-lz/2 lz/2]),y,[-ly/2 ly/2]),...
29              x,[0 lx]))
30 J_SVK_comp=double(int(int(int(expr_SVK,z,[-lz/2 lz/2]),y,[-ly/2 ly/2]),...
31              x,[0 lx]))
32 J_H_comp=double(int(int(int(expr_H,z,[-lz/2 lz/2]),y,[-ly/2 ly/2]),...
33              x,[0 lx]))
```

To evaluate the exact energy values for a deformation into a twist the following changes are made in Code - Matlab 4. The lines 8-16 are replaced by Code - Matlab 5 and the lines 17-22 by Code - Matlab 3.

Code - Matlab 5: Derived energies for a twist.

```matlab
1  % derived energies (3.10), (3.11), (3.12)
2  J_NH=C_1*alpha^2/12/lx*(ly^3*lz+ly*lz^3)
3  J_SVK=(mu+lambda/2)*alpha^4*ly*lz/4/lx^3*(ly^4/80+ly^2*lz^2/72+lz^4/80) ...
4          +mu*alpha^2*ly*lz/24/lx*(ly^2+lz^2)
5  J_H=(2*mu+2*lambda)*lx*ly*lz*(1/4/alpha*sin(2*alpha) ...
6          -2/alpha*sin(alpha)+3/2)+mu*alpha^2*ly*lz/24/lx*(ly^2+lz^2)
```

B Interpreted codes

The codes in this subsection represent the adjustments which were made in codes provided in [5], more specifically only the folder '**benchmark2_3D_elasticity**' is used.

The values of the material parameters E and ν are changed to the values corresponding to steel. The change is made in the code '**benchmark2_setup.m**'.

Code - Matlab 6: Material parameters.

```
1  E = 190e9; nu = 0.27;
```

The examples use a different reference configuration Ω than the configuration used in [5], thus the proportions of Ω are adjusted in '**setup_project_and_subproject_3D.m**' from the subfolder '**setups**' (see Code - Matlab 7).

Code - Matlab 7: Proportions of Ω.

```
1  params.lx = 0.2; params.ly = 0.01; params.lz = 0.01;
```

B.1 Codes for deformations

In the Matlab codes the angle α is represented by '**alpha_max**'. For example, suppose that '**alpha_max=pi/2∗turning**' and '**alpha_max=2∗pi∗turning**' correspond to $\alpha = \frac{\pi}{2}$ and $\alpha = 2\pi$, respectively. The following codes represent the changed parts in '**benchmark2.m**', which replace the lines in Code - Matlab 8.

Code - Matlab 8: A deformation into a twist.

```
1  turning = 1;   alpha_max = pi/2*turning;   lx = params.lx;
2  f1 = @(x,y,z)   x;
3  f2 = @(x,y,z)   cos(alpha_max*x/lx).*y + sin(alpha_max*x/lx).*z;
4  f3 = @(x,y,z)  -sin(alpha_max*x/lx).*y + cos(alpha_max*x/lx).*z;
```

The homogeneous deformation from Chapter 2, Example 2 can be depicted with Code - Matlab 9.

Code - Matlab 9: A homogeneous deformation.

```
1  sx=3/2; sy=1; sz=1; x2=0; y2=0; z2=1;
2  f1 = @(x,y,z)   sx*x+x2;
3  f2 = @(x,y,z)   sy*y+y2;
4  f3 = @(x,y,z)   sz*z+z2;
```

The deformation into a partial toroid, e.g. for '**alpha_max=pi/2∗turning**', and a whole toroid, for '**alpha_max=2∗pi∗turning**', is defined in Code - Matlab 10.

Code - Matlab 10: A deformation into a partial and a whole toroid.

```
1  turning = 1;   alpha_max = pi/2*turning;   lx = params.lx;
2  f1 = @(x,y,z)   (z+lx/alpha_max).*sin(alpha_max*x/lx);
3  f2 = @(x,y,z)   y;
4  f3 = @(x,y,z)   (z+lx/alpha_max).*cos(alpha_max*x/lx)-lx/alpha_max;
```

The deformation into a hourglass: type 1 is described in Code - Matlab 11 and the deformation into a hourglass: type 2 in Code - Matlab 12.

Code - Matlab 11: A deformation into a hourglass: type 1.

```
1  lx = params.lx;
2  f1 = @(x,y,z)   x;
3  f2 = @(x,y,z)   y;
4  f3 = @(x,y,z)   z.*(-2*x/lx+1);
```

Code - Matlab 12: A deformation into a hourglass: type 2.

```
1  lx = params.lx;
2  f1 = @(x,y,z)   x;
3  f2 = @(x,y,z)   y.*(-2*x/lx+1);
4  f3 = @(x,y,z)   z.*(-2*x/lx+1);
```

B.2   Codes for different density models

Other changes are made in '**densityGradientVector.m**' to evaluate and illustrate the values of the different density models. The part in Code - Matlab 13 is replaced by the following codes depending on the density model.

Code - Matlab 13: Neo-Hookean density model.

```
1  % determinant term
2  J = F{1,1}.*F{2,2}.*F{3,3} + F{1,3}.*F{2,1}.*F{3,2} + ...
3      F{1,2}.*F{2,3}.*F{3,1} - F{1,3}.*F{2,2}.*F{3,1} - ...
4      F{1,2}.*F{2,1}.*F{3,3} - F{1,1}.*F{2,3}.*F{3,2};
5  % trace term
6  I = F{1,1}.^2 + F{1,2}.^2 + F{1,3}.^2 + ...
7      F{2,1}.^2 + F{2,2}.^2 + F{2,3}.^2 + ...
8      F{3,1}.^2 + F{3,2}.^2 + F{3,3}.^2;
9  % densities
10 densities = params.C1*(I -3 -2*log(J)) + params.D1*(J -1).^2;
```

The linear elasticity density model is shown in Code - Matlab 14.

Code - Matlab 14: Linear elasticity density.

```
1  eNormSq=(F{1,1}-1).^2+(F{2,2}-1).^2+(F{3,3}-1).^2+...
2   (1/2)*((F{1,2}+F{2,1}).^2+(F{1,3}+F{3,1}).^2+(F{2,3}+F{3,2}).^2);
3  eTraceSq=(F{1,1}+F{2,2}+F{3,3}-3).^2;
4  densities=(params.mu)*eNormSq+1/2*(params.lambda)*eTraceSq;
```

The code for the Saint Venant-Kirchhoff model is shown in Code - Matlab 15.

Code - Matlab 15: Saint Venant-Kirchhoff density.

```
ENormSq=(1/4)*((F{1,1}.^2+F{2,1}.^2+F{3,1}.^2-1).^2+...
               (F{1,2}.^2+F{2,2}.^2+F{3,2}.^2-1).^2+...
               (F{1,3}.^2+F{2,3}.^2+F{3,3}.^2-1).^2)+...
        (1/2)*((F{1,1}.*F{1,2}+F{2,1}.*F{2,2}+F{3,1}.*F{3,2}).^2+...
               (F{1,1}.*F{1,3}+F{2,1}.*F{2,3}+F{3,1}.*F{3,3}).^2+...
               (F{1,2}.*F{1,3}+F{2,2}.*F{2,3}+F{3,2}.*F{3,3}).^2);
ETraceSq =(1/4)*(F{1,1}.^2+F{1,2}.^2+F{1,3}.^2+...
                 F{2,1}.^2+F{2,2}.^2+F{2,3}.^2+...
                 F{3,1}.^2+F{3,2}.^2+F{3,3}.^2-3).^2;
densities=(params.mu)*ENormSq+1/2*(params.lambda)*ETraceSq;
```

Bibliography

[1] M. E. Gurtin: *An Introduction to Continuum Mechanics*, Academic Press, 1981.

[2] M. Kružík, T. Roubíček: *Mathematical Methods in Continuum Mechanics of Solids*, Springer, 2019.

[3] J. N. Reddy: *An Introduction to Continuum Mechanics*, Cambridge University Press, Second Edition, 2013.

[4] MATLAB. 9.10.0.1684407 (R2021a) Update 3. Natick, Massachusetts: The MathWorks Inc.

[5] Alexej Moskovka, Jan Valdman: *Fast MATLAB evaluation of nonlinear energies using FEM in 2D and 3D: nodal elements*, Applied Mathematics and Computation 424, 127048 (2022).

[6] Table of MODULI OF ELASTICITY AND POISSON'S RATIO, `https://www.essom.com/upload/eng_data/23.pdf`