

#### MASTER THESIS

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## Implicit constitutive relations in lower dimensional models in continuum mechanics

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Abstract: We study implicit constitutive equations and their possible applications in the description of the elastic and plastic response of isotropic solids. We develop a thermodynamic framework for the elastic and plastic response of isotropic solids and we perform simple numerical simulations of the elastic as well as plastic response of solids (beams) using implicit constitutive equations.

Keywords: implicit constitutive relations; beams; elasticity; thermodynamics; plasticity.

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#### Introduction

In this thesis, we investigate the possible use of so-called implicit constitutive relations in the description of response of continuous solid bodies. While the classical approach to constitutive relations is based on the assumption that the Cauchy stress tensor  $\mathbb{T}$  is a function of the deformation, that is

$$\mathbb{T} = \mathfrak{f}(\mathbb{B}),\tag{1}$$

where  $\mathbb{B}$  denotes the left Cauchy–Green tensor, we follow [1] and [2], and we consider implicit constitutive relations of the type

$$\mathfrak{g}\left(\mathbb{B},\mathbb{T}\right) = \mathbf{0},\tag{2}$$

and

$$\mathfrak{h}\left(\mathbb{B}, \stackrel{\square}{\mathbb{B}}, \mathbb{T}, \stackrel{\square}{\mathbb{T}}\right) = \mathbf{0},\tag{3}$$

where  $\mathfrak{f},\mathfrak{g}$  and  $\mathfrak{h}$  denote tensor-valued functions and  $\mathbb{A}$  denotes an objective rate of the given tensor.

In Chapter 1, we focus on elastic materials and we provide a counterpart to the classical representation formula

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B} \tag{4}$$

for isotropic hyperelastic solids, where  $\psi$  denotes the specific Helmholtz free energy. In the case of implicit constitutive relations, we derive, see Theorem 5, the representation formula

$$\mathbb{H} = \frac{1}{3} \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right) \mathbb{I} + \frac{\partial g}{\partial I_2} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} - \left[ \frac{\partial g}{\partial I_3} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2 \right]_{\delta}, \tag{5}$$

where  $\mathbb{H}$  denotes the Hencky strain tensor and g denotes the specific Gibbs free energy. Unlike in the previous studies on the subject matter, see [3], the representation formula (5) allows us to split the deformation to the volume-preserving and volume-changing part, analyze the corresponding stress response and identify certain natural restrictions regarding the choice of the formula for the specific Gibbs free energy.

In Chapter 2, we focus on the elastic-plastic response. In particular, we focus on the one-dimensional response described by an analogy of (3), that is on the response described by the formula

$$f\left(\epsilon, \dot{\epsilon}, \sigma, \dot{\sigma}\right) = 0,\tag{6}$$

where f is a scalar function,  $\epsilon$  denotes the relative deformation,  $\sigma$  denotes the stress and the symbol  $\dot{\alpha}$  denotes the time derivative of the corresponding quantity. Following [4] we investigate a one-dimensional constitutive relation

$$\dot{\sigma} - E\dot{\epsilon} = -EH_n(\sigma\dot{\epsilon})H_n(|\sigma| - \sigma_y)\dot{\epsilon},\tag{7}$$

where E denotes the Young modulus,  $\sigma_y$  denotes the yield stress and H denotes the Heaviside step function. We show that the constitutive relation (7) can be indeed used to describe the elastic-perfectly plastic response and we briefly discuss several variants of equation (7), as well as the motivation behind this evolution equation.

In Chapter 3, we propose a proof-of-concept numerical simulations of the deformation of an elastic-plastic beam. We follow [5], and we propose a numerical scheme for the solution of governing equations for the elastic-plastic beam. We solve governing equations in the quasistatic approximation, and we use the constitutive relation of the type (6), that now takes the form

$$g\left(\kappa, \dot{\kappa}, M, \dot{M}\right) = 0,\tag{8}$$

where g is a scalar function and  $\kappa$  and M denote the curvature and the bending moment. The numerical simulations are based on a straightforward implementation of the proposed numerical scheme in Mathematica programming language and they document the viability of the concept of implicit constitutive relations in the study of the elastic-plastic response. The scripts are attached as an electronic attachment to this thesis.

Finally, in Chapter 4 we return back to the one-dimensional constitutive relations of the type (6), and we generalize them to the fully three-dimensional setting. This problem has been already studied in [2], but unlike [2] we provide a complete thermodynamic basis for the corresponding model. In particular, we explicitly describe a procedure that allows one to design models for the inelastic response that have the structure (3), and that are guaranteed to satisfy the first and second law of thermodynamics. (This procedure otherwise shares all the benefits of the procedure used in the purely mechanical setting in [2] and [4]. Namely, there is no need to directly introduce the concept of plastic strain and so forth.) As a side effect we also obtain an evolution equation for the temperature; for example, the complete system of evolution equations for mechanical and thermal quantities for an elastic-perfectly plastic material reads

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \operatorname{div} \mathbf{v} = 0, \tag{9a}$$

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T},\tag{9b}$$

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e, \tag{9c}$$

$$\hat{\mathbb{B}}_{e} = [1 - H(\mathbb{T} : \mathbb{D}) H(|\mathbb{T}| - T_{y})] (\mathbb{DB}_{e} + \mathbb{B}_{e}\mathbb{D}), \qquad (9d)$$

$$\overset{\triangle}{\mathbb{B}}_{e} = [1 - H(\mathbb{T} : \mathbb{D}) H(|\mathbb{T}| - T_{y})] (\mathbb{DB}_{e} + \mathbb{B}_{e} \mathbb{D}), \qquad (9d)$$

$$\rho c_{V,R} \frac{d\theta}{dt} = H(\mathbb{T} : \mathbb{D}) H(|\mathbb{T}| - T_{y}) \mathbb{T} : \mathbb{D} + \kappa \triangle \theta, \qquad (9e)$$

where  $\rho$  is the density, **v** is the velocity gradient,  $\mathbb{B}_e$  is the elastic part of the left Cauchy-Green tensor,  $\mathbb{D}$  denotes the symmetric part of the velocity gradient,  $T_u$ is the yield stress,  $\theta$  denotes the thermodynamic temperature,  $c_{V,R}$  is the specific heat at the constant volume,  $\kappa$  is the thermal conductivity,  $\mathbb{T}:\mathbb{D}$  denotes the matrix scalar product of  $\mathbb{T}$  and  $\mathbb{D}, \frac{\mathrm{d}\rho}{\mathrm{d}t}$  and  $\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}$  denote material time derivatives of the corresponding quantities and  $\mathbb{B}_e$  denotes the corotational derivative of  $\mathbb{B}_e$ . In the end, we briefly comment on the flexibility of the proposed approach in the development of models for more complex material response.

# 1. Representation formula for isotropic solids described by implicit constitutive relations

The aim of this chapter is to provide a characterization for isotropic elastic solids described by implicit constitutive relations. In the beginning, we summarize several known results for homogeneous hyperelastic solids. In particular, we recall the standard representation formula

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B} \tag{1.1}$$

for isotropic hyperelastic solids.

Next, we derive a counterpart to (1.1) for isotropic elastic solids specified by a constitutive relation of the form

$$\mathbb{B} = \mathfrak{g}\left(\mathbb{T}\right). \tag{1.2}$$

At the end of this chapter, we show that the linearization of the resulting representation formula has a well-known counterpart in the theory of linearized elasticity. This chapter is based mainly on [6], but we provide detailed explanations and derivations.

#### 1.1 Summary of known results

First, let us consider an isotropic homogeneous elastic solid. Let us define the specific<sup>1</sup> Helmholtz free energy  $\psi$  as a function of the thermodynamic temperature  $\theta$  and the left Cauchy–Green tensor  $\mathbb B$  as

$$\psi =_{\text{def}} \psi (\theta, \mathbb{B}), \tag{1.3}$$

where  $\psi$  is an isotropic scalar-valued function. Isotropic functions are defined in (1.8). The specific Helmholtz free energy is related to the specific internal energy  $e =_{\text{def}} e(\eta, \mathbb{B})$  by the Legendre transformation

$$\psi(\theta, \mathbb{B}) = e(\eta, \mathbb{B}) \Big|_{\eta = \eta(\theta, \mathbb{B})} - \theta \eta(\theta, \mathbb{B}), \tag{1.4}$$

where  $\eta$  is the specific entropy. If we assume the following expression of the Cauchy stress tensor  $\mathbb{T}$  in terms of the left Cauchy–Green tensor as

$$\mathbb{T} = \mathfrak{f}(\mathbb{B}),\tag{1.5}$$

<sup>&</sup>lt;sup>1</sup>The adjective specific is important here as the Helmholtz free energy  $\psi$  must be measured as the energy per unit mass. If we were dealing with the specific Helmholtz free energy per unit volume, we would need to specify whether we are working in the reference or current configuration, since the same part of the material can occupy a different volume in a different configuration. Measurement as the energy per unit mass is also used for other thermodynamic potentials and for the entropy that appear in this thesis.

then the standard manipulation leads us to (1.1), which provides a relation between the stress and the derivatives of the specific Helmholtz free energy.

An essential part of the following calculations are the matrix<sup>2</sup> invariants  $I_1$ ,  $I_2$  and  $I_3$ , which are defined for a matrix  $\mathbb{A}$  as

$$I_1(\mathbb{A}) =_{\text{def}} \text{Tr } \mathbb{A},$$
 (1.6a)

$$I_2(\mathbb{A}) =_{\text{def}} \frac{1}{2} \left[ (\operatorname{Tr} \mathbb{A})^2 - \operatorname{Tr} \mathbb{A}^2 \right], \tag{1.6b}$$

$$I_3(\mathbb{A}) =_{\text{def}} \det \mathbb{A}. \tag{1.6c}$$

In the following calculations, formulae for the derivatives of the tensor invariants, which we recall without their derivations (see, for example, [7, pp. 362–363]), are also useful. The derivatives are

$$\frac{\partial I_1}{\partial \mathbb{A}} = \mathbb{I},\tag{1.7a}$$

$$\frac{\partial \mathbb{A}}{\partial \mathbb{A}} = \text{Tr}(\mathbb{A}) \mathbb{I} - \mathbb{A}^{\mathrm{T}}, \tag{1.7b}$$

$$\frac{\partial I_3}{\partial \mathbb{A}} = (\det \mathbb{A}) \, \mathbb{A}^{-T}. \tag{1.7c}$$

Furthermore, we formulate important well-known representation theorems for isotropic scalar-valued and tensor-valued functions. Let us start by defining the terms used in these theorems.

- A matrix  $\mathbb{Q}$  is a proper orthogonal matrix if and only if  $\mathbb{Q}\mathbb{Q}^T = \mathbb{Q}^T\mathbb{Q} = \mathbb{I}$  and  $\det \mathbb{Q} = 1$ , where  $\mathbb{I}$  denotes the unit matrix.
- A scalar-valued function  $\phi$  of a tensor is said to be isotropic if and only if

$$\phi\left(\mathbb{Q}\mathbb{A}\mathbb{Q}^{\mathrm{T}}\right) = \phi\left(\mathbb{A}\right) \tag{1.8a}$$

holds for any matrix  $\mathbb{A}$  and any proper orthogonal matrix  $\mathbb{Q}$ .

• A tensor-valued function f of a tensor is said to be isotropic if and only if

$$\mathfrak{f}\left(\mathbb{Q}\mathbb{A}\mathbb{Q}^{\mathrm{T}}\right) = \mathbb{Q}\mathfrak{f}\left(\mathbb{A}\right)\mathbb{Q}^{\mathrm{T}} \tag{1.8b}$$

holds for any matrix  $\mathbb{A}$  and any proper orthogonal matrix  $\mathbb{Q}$ .

Now we can formulate the mentioned representation theorems, which are a very useful tool for our future calculations.

<sup>&</sup>lt;sup>2</sup>As is common in continuum mechanics, we assume in this thesis that the terms matrix and tensor coincide, although this is not formally the case.

**Theorem 1** (Representation theorem for an isotropic scalar-valued function of a tensor). Let  $\mathbb{A}$  be a symmetric tensor. Then a scalar-valued function  $\epsilon(\mathbb{A})$  is isotropic if and only if it can be expressed as a function of the invariants of  $\mathbb{A}$ , i.e.

$$\epsilon(\mathbb{A}) = \epsilon(I_1, I_2, I_3). \tag{1.9}$$

*Proof.* See, for example, [8, p. 28].

**Theorem 2** (Representation theorem for an isotropic tensor-valued function of a tensor). Let  $\mathbb{A}$  and  $\mathbb{D}$  be symmetric tensors. Then a tensor-valued function  $\mathbb{D} = \mathfrak{g}(\mathbb{A})$  is isotropic if and only if it has a representation of the form

$$\mathbb{D} = \psi_0 \mathbb{I} + \psi_1 \mathbb{A} + \psi_2 \mathbb{A}^2, \tag{1.10}$$

where  $\psi_i = \psi_i(I_1, I_2, I_3)$  are functions of the invariants of A.

*Proof.* Also this theorem is presented here without its proof. It can be found, for instance, in [8, pp. 32-33].

Recall that the evolution equation for the specific internal energy e has the form

$$\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \mathbb{T} : \mathbb{D} - \mathrm{div}\,\mathbf{j}_e, \tag{1.11}$$

where  $\rho$  is the density,  $\mathbf{j}_e$  is the heat flux that can be expressed, for example, from Fourier's law and the other terms are defined in (1.19).

Evaluating the derivative of the specific internal energy leads to the evolution equation for the specific entropy

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{\theta} \left[ \left( \mathbb{T} - 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B} \right) : \mathbb{D} - \mathrm{div} \, \mathbf{j}_e \right]. \tag{1.12}$$

Therefore, the entropy production due to mechanical processes is given by the term

$$\left(\mathbb{T} - 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B}\right) : \mathbb{D},$$

and this term vanishes for all mechanical processes (i.e. the material is hyperelastic) if and only if

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B},\tag{1.13}$$

which is the well-known formula. The complete derivation of it can be found, for instance, in [9, p. 537]. Using Theorem 2, we see that

$$\mathbb{T} = \alpha_0 \mathbb{I} + \alpha_1 \mathbb{B} + \alpha_2 \mathbb{B}^2, \tag{1.14}$$

where  $\alpha_i = \psi_i(I_1, I_2, I_3)$  are functions of the invariants of  $\mathbb{B}$ . With (1.13) it is easy to determine these functions. The chain rule and using formulae for derivatives of matrix invariants (1.7) imply

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}} \mathbb{B} = 2\rho \left( \frac{\partial \psi}{\partial I_1} \frac{\partial I_1}{\partial \mathbb{B}} + \frac{\partial \psi}{\partial I_2} \frac{\partial I_2}{\partial \mathbb{B}} + \frac{\partial \psi}{\partial I_3} \frac{\partial I_3}{\partial \mathbb{B}} \right) \mathbb{B} = 
= 2\rho \left[ I_3 \frac{\partial \psi}{\partial I_3} \mathbb{I} + \left( \frac{\partial \psi}{\partial I_1} + I_1 \frac{\partial \psi}{\partial I_2} \right) \mathbb{B} - \frac{\partial \psi}{\partial I_2} \mathbb{B}^2 \right].$$
(1.15)

Comparing (1.14) with (1.15) we see that

$$\alpha_0 = 2\rho I_3 \frac{\partial \psi}{\partial I_2},\tag{1.16a}$$

$$\alpha_1 = 2\rho \left( \frac{\partial \psi}{\partial I_1} + I_1 \frac{\partial \psi}{\partial I_2} \right),$$
(1.16b)

$$\alpha_2 = -2\rho \frac{\partial \psi}{\partial I_2}.\tag{1.16c}$$

Having recalled the classical result (1.13), we are now in a position to investigate its counterpart to isotropic solids specified by the so-called implicit constitutive relation. As a counterpart to (1.5), assume the following constitutive relation

$$\mathbb{B} = \mathfrak{g}(\mathbb{T}). \tag{1.17}$$

We want to derive an analogy of equation (1.13), but using the implicit constitutive relation. We do not work directly with the left Cauchy–Green tensor, but we define the Hencky strain  $\mathbb{H}$  tensor as

$$\mathbb{H} =_{\text{def}} \frac{1}{2} \log \mathbb{B}. \tag{1.18}$$

The Hencky strain tensor has some nice properties, which we can formulate into Proposition 3. Before we do that, we introduce some notation.

• For matrices  $\mathbb{A}$  and  $\mathbb{B}$  is the matrix scalar product defined as

$$\mathbb{A} : \mathbb{B} =_{\operatorname{def}} \operatorname{Tr} \left( \mathbb{A} \mathbb{B}^{\mathrm{T}} \right). \tag{1.19a}$$

• The deviatoric (traceless) part of a matrix A is defined as

$$\mathbb{A}_{\delta} =_{\operatorname{def}} \mathbb{A} - \frac{1}{3} \left( \operatorname{Tr} \mathbb{A} \right) \mathbb{I}. \tag{1.19b}$$

- The symbol  $\dot{\alpha}$  denotes the time derivative of a scalar function  $\alpha(t)$ .
- The symbol  $\dot{\mathbf{r}}$  denotes the time derivative of a vector function  $\mathbf{r}(t)$ .
- The material time derivative of a scalar field  $\varphi(\mathbf{x},t)$  is defined as

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial\varphi}{\partial t} + \mathbf{v} \cdot \nabla\varphi, \tag{1.19c}$$

where  $\mathbf{v}$  is the velocity field.

• The material time derivative of a vector field  $\Phi(\mathbf{x},t)$  is defined as

$$\frac{\mathrm{d}\mathbf{\Phi}}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial\mathbf{\Phi}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{\Phi}. \tag{1.19d}$$

• The material time derivate of a tensor field  $\mathbb{A}(\mathbf{x},t)$  is defined as

$$\frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial \mathbb{A}}{\partial t} + \mathbf{v} \cdot \nabla \mathbb{A}. \tag{1.19e}$$

• The velocity gradient tensor L is defined as

$$\mathbb{L} =_{\mathrm{def}} (\nabla \mathbf{v})^{\mathrm{T}}. \tag{1.19f}$$

• The symmetric part of the velocity gradient  $\mathbb D$  is defined as

$$\mathbb{D} =_{\text{def}} \frac{1}{2} \left( \mathbb{L} + \mathbb{L}^{\text{T}} \right). \tag{1.19g}$$

• The deviatoric strain measure  $\overline{\mathbb{B}}$  is defined as

$$\overline{\mathbb{B}} =_{\text{def}} \frac{\mathbb{B}}{J_{3}^{2}},\tag{1.19h}$$

where J denotes the determinant of the deformation gradient defined as

$$J =_{\text{def}} \det \mathbb{F}. \tag{1.19i}$$

The purpose of defining the deviatoric strain measure is that  $\det \overline{\mathbb{B}} = 1$ , which means that volume does not change, hence  $\overline{\mathbb{B}}$  is called the volume-preserving strain measure.

• As in (1.18), we introduce the corresponding deviatoric Hencky strain tensor  $\overline{\mathbb{H}}$  as

$$\overline{\mathbb{H}} =_{\text{def}} \frac{1}{2} \log \overline{\mathbb{B}}. \tag{1.19j}$$

The introduction of these new deviatoric variables is motivated by the fact that for some models it is convenient to work with a deviatoric strain measure and the determinant of the deformation gradient. Some examples are in [10]. In these models it is possible to split the Cauchy stress tensor into its deviatoric and spherical part, as well as subsequently characterize the volume-changing in addition to the volume-preserving deformations and the corresponding parts of the Cauchy stress tensor. This motivates us to find such a decomposition into the volume-changing and volume-preserving parts also for our Hencky strain tensor  $\mathbb{H}$ .

Now that we have introduced all the necessary definitions, we can therefore formulate and prove the following proposition about the properties of the Hencky strain tensor.

<sup>&</sup>lt;sup>3</sup>Another undeniable advantage of Hencky strain tensor is the fact that in the onedimensional case it tends to infinity as F (one-dimensional deformation gradient) tends to zero, thus in a very natural way bounding the regime of applicability to the case F > 0 as it is claimed in [11, p. 42]. In our three-dimensional case, we extend it as J > 0, which provides us the correctness of definition (1.19h).

#### **Proposition 3.** The Hencky strain tensor $\mathbb{H}$ has the following properties:

(i) The Hencky strain tensor is stress-conjugate to the Cauchy stress tensor, which means that

 $\mathbb{T}: \mathbb{D} = \mathbb{T}: \frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t}.$  (1.20)

(ii) The deviatoric Hencky strain tensor is equal to the deviatoric part of the Hencky strain tensor, i.e.

 $\overline{\mathbb{H}} = \mathbb{H}_{\delta}. \tag{1.21}$ 

(iii) For an incompressible material the constrain  $\det \mathbb{F} = 1$  can be rewritten in terms of the Hencky strain tensor as  $\operatorname{Tr} \mathbb{H} = 0$ .

Proof.

- (i) The proof of equality (1.20) is more demanding and is not the subject of this thesis. The equality is proven, for example, in [12]. We note that equality (1.20) neither means nor implies that  $\mathbb{D} = \frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t}$ .
- (ii) First, due to the rule of the product of the determinants and the determinant of the transposed matrix we get

$$\det \mathbb{B} = (\det \mathbb{F}) (\det \mathbb{F}^{\mathrm{T}}) = (\det \mathbb{F})^2 = J^2. \tag{1.22}$$

Second, we use the following identity of the determinant of the matrix exponential

$$\det e^{\mathbb{A}} = e^{\operatorname{Tr} \mathbb{A}},\tag{1.23}$$

which is proven, for instance, in [13, p. 60]. Using (1.23), the definition of the Hencky strain tensor  $\mathbb{H}$  and (1.22) implies that

$$e^{2 \operatorname{Tr} \mathbb{H}} = \det e^{2 \mathbb{H}} = (\det \mathbb{F})^2 = J^2.$$
 (1.24)

This equation finally leads to the desired result

$$\overline{\mathbb{H}} = \frac{1}{2} \log \frac{\mathbb{B}}{J_3^2} = \frac{1}{2} \left[ \log \mathbb{B} - \frac{2}{3} (\log J) \mathbb{I} \right] = \mathbb{H} - \frac{1}{3} (\operatorname{Tr} \mathbb{H}) \mathbb{I} = \mathbb{H}_{\delta}. \quad (1.25)$$

(iii) The last part of this proposition is a direct consequence of identity (1.23) and the fact that  $\det \mathbb{F} = 1$  for incompressible materials. This directly implies that  $\operatorname{Tr} \mathbb{H} = 0$ .

In fact, equation (1.25) gives us a simple additive volumetric-isochoric split<sup>4</sup> of the Hencky strain tensor as

$$\mathbb{H} = \overline{\mathbb{H}} + \frac{1}{3} (\operatorname{Tr} \mathbb{H}) \mathbb{I}, \tag{1.26}$$

<sup>&</sup>lt;sup>4</sup>In fact, according to [14], [15] or [16], the Hencky strain is the only strain measure for which exists the additive volumetric-isochoric split.

as it is proven, for example, in [14, p. 28]. Next applying the logarithm to both sides of equation (1.24) implies

$$\operatorname{Tr} \mathbb{H} = \log J, \tag{1.27}$$

and substituting (1.27) into equation (1.26) yields

$$\mathbb{H} = \overline{\mathbb{H}} + \frac{1}{3} (\log J) \mathbb{I}. \tag{1.28}$$

The next approach is therefore as follows. We want to gradually determine the individual terms of the right-hand side of equation (1.28) and then substitute them back into (1.28). Let us start with the tensor  $\overline{\mathbb{H}}$ .

Let us think about a different scalar function e used in the definition of the specific internal energy, where the deviatoric Hencky strain  $\overline{\mathbb{H}}$  and the determinant of the deformation gradient J are used instead of  $\mathbb{B}$ . Assume that

$$e =_{\operatorname{def}} e\left(\eta, J, \overline{\mathbb{H}}\right). \tag{1.29}$$

Differentiation yields

$$\frac{\mathrm{d}e}{\mathrm{d}t} = \frac{\partial e}{\partial \eta} \frac{\mathrm{d}\eta}{\mathrm{d}t} + \frac{\partial e}{\partial J} \frac{\mathrm{d}J}{\mathrm{d}t} + \frac{\partial e}{\partial \overline{\mathbb{H}}} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t}.$$
 (1.30)

Now we use formula (1.21) from Proposition 3 and we show that

$$\frac{\partial e}{\partial \overline{\mathbb{H}}} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t} = \frac{\partial e}{\partial \overline{\mathbb{H}}} : \frac{\mathrm{d}\mathbb{H}_{\delta}}{\mathrm{d}t} = \frac{\partial e}{\partial \overline{\mathbb{H}}} : \left(\frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t}\right)_{\delta} = \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta} : \left(\frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t}\right)_{\delta} = \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t}.$$
(1.31)

Using this relation and the standard definition of the thermodynamic temperature (see, for example, [17, p. 6])

$$\theta =_{\text{def}} \frac{\partial e}{\partial \eta},\tag{1.32}$$

we can rewrite equation (1.30) to the form

$$\frac{\mathrm{d}e}{\mathrm{d}t} = \theta \frac{\mathrm{d}\eta}{\mathrm{d}t} + \frac{\partial e}{\partial J} \frac{\mathrm{d}J}{\mathrm{d}t} + \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta} : \frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t}.$$
 (1.33)

Furthermore, we can substitute this expression into the evolution equation for the specific internal energy (1.11) and we get the evolution equation for the specific entropy

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} + \mathrm{div}\left(\frac{\mathbf{j}_e}{\theta}\right) = \frac{1}{\theta} \left[ \mathbb{T} : \mathbb{D} - \rho \frac{\partial e}{\partial J} \frac{\mathrm{d}J}{\mathrm{d}t} - \rho \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\xi} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t} \right] - \frac{\mathbf{j}_e \cdot \nabla \theta}{\theta^2}. \tag{1.34}$$

Next, we manipulate with this equation to define the thermodynamic pressure and thermodynamic stress tensor, similarly as with the thermodynamic temperature. It is obvious that the expression  $\mathbb{T}:\mathbb{D}$  should be examined. We exploit formula (1.20) from Proposition 3 and use the fact, that  $\overline{\mathbb{H}}$  is traceless, that we also know from Proposition 3. This motivates us to decompose the Cauchy stress tensor to its deviatoric and spherical part as

$$\mathbb{T} = m\mathbb{I} + \mathbb{T}_{\delta},\tag{1.35}$$

where m is the mean normal stress defined by the formula

$$m =_{\text{def}} \frac{1}{3} \operatorname{Tr} \mathbb{T}. \tag{1.36}$$

Using this decomposition and again Proposition 3, we rewrite the matrix scalar product  $\mathbb{T} : \mathbb{D}$  as

$$\mathbb{T}: \mathbb{D} = \mathbb{T}: \frac{\mathrm{d}\mathbb{H}}{\mathrm{d}t} = (\mathbb{T}_{\delta} + m\mathbb{I}): \frac{\mathrm{d}}{\mathrm{d}t} \left( \overline{\mathbb{H}} + \frac{1}{3} \operatorname{Tr} \left( \mathbb{H} \right) \mathbb{I} \right) = \mathbb{T}_{\delta}: \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t} + m \frac{\mathrm{d}}{\mathrm{d}t} \operatorname{Tr} \mathbb{H}.$$
(1.37)

Furthermore, differentiating both sides of equation (1.27) gives us

$$\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{Tr} \mathbb{H} = \frac{1}{J} \frac{\mathrm{d}J}{\mathrm{d}t}.$$
(1.38)

Now we are ready to rewrite the evolution equation for the specific entropy (1.34) using relations (1.37) and (1.38) as

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} + \mathrm{div}\left(\frac{\mathbf{j}_e}{\theta}\right) = \frac{1}{\theta} \left( \left[ \frac{m}{J} - \rho \frac{\partial e}{\partial J} \right] \frac{\mathrm{d}J}{\mathrm{d}t} + \left[ \mathbb{T}_{\delta} - \rho \left( \frac{\partial e}{\partial \overline{\mathbb{H}}} \right)_{\delta} \right] : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t} \right) - \frac{\mathbf{j}_e \cdot \nabla \theta}{\theta^2}. \tag{1.39}$$

Based on this version of the evolution equation for the specific entropy, we define the thermodynamic pressure  $p_{th}$  as

$$p_{th} =_{\text{def}} -\rho J \frac{\partial e}{\partial J} \tag{1.40a}$$

and the thermodynamic (traceless) stress tensor  $(\mathbb{T}_{th})_{\delta}$  as

$$(\mathbb{T}_{th})_{\delta} =_{\text{def}} \rho \left( \frac{\partial e}{\partial \overline{\mathbb{H}}} \right)_{\delta}.$$
 (1.40b)

This definition of the thermodynamic pressure is absolutely consistent with the classical definition used, for example, for compressible gas. To show this, let us first recall the balance of the mass in the Lagrangian description, which is

$$\rho_R = \rho J, \tag{1.41}$$

where  $\rho_R$  is the density in the reference configuration. Now is also a good time to recall the balance of mass in the Eulerian description, which is also used in future calculations, as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \operatorname{div} \mathbf{v} = 0. \tag{1.42}$$

Derivations of (1.41) and (1.42) can be found, for instance, in [18, p. 19]. Using (1.41) and the chain rule, we get

$$p_{th} = -\rho J \frac{\partial e}{\partial J} = -\rho J \frac{\partial e}{\partial \rho} \frac{\partial \rho}{\partial J} = \rho J \frac{\partial e}{\partial \rho} \frac{\rho_R}{J^2} = \rho^2 \frac{\partial e}{\partial \rho},$$

which is the desired formula. Going back to our definition of the thermodynamic pressure and the thermodynamic traceless tensor (1.40), we rewrite the evolution equation for the specific entropy (1.39) to its final form

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} + \mathrm{div}\left(\frac{\mathbf{j}_e}{\theta}\right) = \frac{1}{\theta} \left(\frac{1}{J} \left[m + p_{\mathrm{th}}\right] \frac{\mathrm{d}J}{\mathrm{d}t} + \left[\mathbb{T}_\delta - (\mathbb{T}_{\mathrm{th}})_\delta\right] : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t}\right) - \frac{\mathbf{j}_e \cdot \nabla \theta}{\theta^2}. \quad (1.43)$$

Again, the elastic material is defined as a material, which does not produce the entropy during mechanical processes. In words of formula (1.43), this condition is satisfied if and only if

$$\frac{1}{J}\left[m+p_{\rm th}\right]\frac{\mathrm{d}J}{\mathrm{d}t}+\left[\mathbb{T}_{\delta}-\left(\mathbb{T}_{\rm th}\right)_{\delta}\right]:\frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t}=0,$$

and it occurs if

$$m = -p_{th}, (1.44a)$$

$$\mathbb{T}_{\delta} = (\mathbb{T}_{th})_{\delta}. \tag{1.44b}$$

Note that we could work also with the specific Helmholtz free energy  $\psi$  defined as

$$\psi =_{\operatorname{def}} \psi \left( \theta, J, \overline{\mathbb{H}} \right),$$

and repeating the same approach, but evaluating derivatives of  $\psi$  with respect to  $\overline{\mathbb{H}}$  and J gives us the following counterparts to (1.13)

$$m = \rho J \frac{\partial \psi}{\partial J},\tag{1.45a}$$

$$\mathbb{T}_{\delta} = \left(2\rho\overline{\mathbb{B}}\frac{\partial\psi}{\partial\overline{\mathbb{B}}}\right)_{\delta}.\tag{1.45b}$$

#### 1.2 Specific Gibbs free energy

Having defined the thermodynamic pressure  $p_{th}$  and the thermodynamic tensor  $(\mathbb{T}_{th})_{\delta}$ , we can introduce a new thermodynamic potential. Firstly, to simplify our future calculations, we slightly modify the definition of the thermodynamic (traceless) tensor, where we get rid of the density. Starting now,  $(\mathbb{T}_{th})_{\delta}$  takes over the role of the thermodynamic (traceless) tensor and it is defined as

$$(\mathbb{T}_{th,\rho})_{\delta} =_{\text{def}} \frac{(\mathbb{T}_{th})_{\delta}}{\rho} = \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta}.$$
 (1.46)

The new potential is the specific Gibbs free energy g and it is defined as the Legendre transformation of the specific internal energy with respect to  $\eta$ , J and  $\overline{\mathbb{H}}$ , which are the corresponding variables from definition (1.29). The defining formula is

$$g\left(\theta, p_{\rm th}, (\mathbb{T}_{\rm th,\rho})_{\delta}\right) =_{\rm def} \left[e - \frac{\partial e}{\partial \eta} \eta - \frac{\partial e}{\partial J} J - \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta} : \overline{\mathbb{H}}\right] \Big|_{\substack{\eta = \eta(\theta, p_{\rm th}, (\mathbb{T}_{\rm th,\rho})_{\delta}) \\ J = J(\theta, p_{\rm th}, (\mathbb{T}_{\rm th,\rho})_{\delta}) \\ \overline{\mathbb{H}} = \overline{\mathbb{H}}(\theta, p_{\rm th}, (\mathbb{T}_{\rm th,\rho})_{\delta})}}, \quad (1.47)$$

where  $e = e(\eta, J, \overline{\mathbb{H}})$ . The next step is to differentiate g with respect to its variables. Using definitions of the temperature (1.32), the thermodynamic pressure (1.40a) and the thermodynamic tensor (1.46), formula (1.47) can be rewritten

to the form

$$g\left(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}\right) = e\left(\eta, J, \overline{\mathbb{H}}\right) \begin{vmatrix} \eta = \eta(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}) \\ J = J(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}) \end{vmatrix} - \theta \eta \begin{vmatrix} + \eta(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}) \\ \eta = \eta(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}) \end{vmatrix} + \frac{p_{th}}{\rho} \begin{vmatrix} - (\mathbb{T}_{th,\rho})_{\delta} & \overline{\mathbb{H}} \\ \rho = \rho(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta}) \end{vmatrix} = \overline{\mathbb{H}}(\theta, p_{\mathrm{th}}, (\mathbb{T}_{\mathrm{th},\rho})_{\delta})$$

$$(1.48)$$

Differentiating (1.48) with respect to time we get

$$\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{\partial e}{\partial \eta} \frac{\mathrm{d}\eta}{\mathrm{d}t} + \frac{\partial e}{\partial J} \frac{\mathrm{d}J}{\mathrm{d}t} + \left(\frac{\partial e}{\partial \overline{\mathbb{H}}}\right)_{\delta} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t} - \frac{\mathrm{d}\theta}{\mathrm{d}t} \eta - \theta \frac{\mathrm{d}\eta}{\mathrm{d}t} + \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{\rho}\right) p_{th} + \\
+ \frac{1}{\rho} \frac{\mathrm{d}p_{th}}{\mathrm{d}t} - \frac{\mathrm{d}\left(\mathbb{T}_{\mathrm{th},\rho}\right)_{\delta}}{\mathrm{d}t} : \overline{\mathbb{H}} - (\mathbb{T}_{\mathrm{th},\rho})_{\delta} : \frac{\mathrm{d}\overline{\mathbb{H}}}{\mathrm{d}t}.$$
(1.49)

Let us look again at the balance of mass (1.41). It implies that

$$\frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{1}{\rho} \right) = \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{J}{\rho_R} \right) = \frac{1}{\rho_R} \frac{\mathrm{d}J}{\mathrm{d}t} = \frac{1}{\rho J} \frac{\mathrm{d}J}{\mathrm{d}t}. \tag{1.50}$$

In the next step, we use this relation and the same definitions triplet of the temperature (1.32), the thermodynamic pressure (1.40a) and the thermodynamic tensor (1.46), and reduce the previous equation (1.49) to

$$\frac{\mathrm{d}g}{\mathrm{d}t} = -\eta \frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{1}{\rho} \frac{\mathrm{d}p_{th}}{\mathrm{d}t} - \overline{\mathbb{H}} : \frac{\mathrm{d}\left(\mathbb{T}_{\mathrm{th},\rho}\right)_{\delta}}{\mathrm{d}t}.$$
(1.51)

On the other hand, if we differentiate the specific Gibbs free energy g directly (i.e. as a composed function) with respect to time, we have

$$\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{\partial g}{\partial \theta} \frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{\partial g}{\partial p_{th}} \frac{\mathrm{d}p_{th}}{\mathrm{d}t} + \frac{\partial g}{\mathrm{d}(\mathbb{T}_{\mathrm{th},\rho})_{\delta}} : \frac{\mathrm{d}(\mathbb{T}_{\mathrm{th},\rho})_{\delta}}{\mathrm{d}t}, \tag{1.52}$$

which can be further rewritten as:

$$\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{\partial g}{\partial \theta} \frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{\partial g}{\partial p_{th}} \frac{\mathrm{d}p_{th}}{\mathrm{d}t} + \left(\frac{\partial g}{\partial (\mathbb{T}_{\mathrm{th},\rho})_{\delta}}\right)_{\delta} : \frac{\mathrm{d}(\mathbb{T}_{\mathrm{th},\rho})_{\delta}}{\mathrm{d}t}, \tag{1.53}$$

Comparing (1.51) with (1.53) we can finally identify formulae for the derivatives of g as

$$\frac{\partial g}{\partial \theta} = -\eta,\tag{1.54a}$$

$$\frac{\partial g}{\partial p_{th}} = \frac{J}{\rho_R},\tag{1.54b}$$

$$\left(\frac{\partial g}{\partial \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}}\right)_{\delta} = -\overline{\mathbb{H}}.$$
(1.54c)

## 1.3 Representation theorem for isotropic elastic solids with given specific Gibbs free energy

Further we assume that  $\overline{\mathbb{H}} = \mathfrak{g} \Big( (\mathbb{T}_{th,\rho})_{\delta} \Big)$ , which is in the form of the implicit constitutive relation (1.17). We also assume that we are dealing with isotropic material. One of the aims of this chapter is to derive a representation theorem for isotropic elastic solids. The procedure for its derivation is as follows. First, we derive the representation theorem only for the deviatoric part of the Hencky strain tensor, then we use the definition of deviatoric part and get the desired theorem from it.

Let us start with Theorem 2, which implies

$$\overline{\mathbb{H}} = \alpha_0 \mathbb{I} + \alpha_1 \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} + \alpha_2 \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2, \tag{1.55}$$

where  $\alpha_i = \alpha_i(I_1, I_2, I_3)$ , i = 0, 1, 2, are functions of the tensor invariants of the tensor  $(\mathbb{T}_{\text{th},\rho})_{\delta}$ . Thanks to the fact, that  $(\mathbb{T}_{\text{th},\rho})_{\delta}$  is a traceless tensor, we can find some relations between these functions. We see that

$$I_1 = 0,$$
 (1.56a)

$$I_{2} = \frac{1}{2} \left[ \left( \operatorname{Tr} \left( (\mathbb{T}_{\operatorname{th},\rho})_{\delta} \right) \right)^{2} - \operatorname{Tr} \left( (\mathbb{T}_{\operatorname{th},\rho})_{\delta} \right)^{2} \right] = -\frac{1}{2} \left[ \operatorname{Tr} \left( (\mathbb{T}_{\operatorname{th},\rho})_{\delta} \right)^{2} \right], \quad (1.56b)$$

$$I_3 = \det\left( (\mathbb{T}_{\text{th},\rho})_{\delta} \right). \tag{1.56c}$$

The next step is applying a trace operator to both sides of equation (1.55). Using again the facts that  $\overline{\mathbb{H}}$  and  $(\mathbb{T}_{th,\rho})_{\delta}$  are traceless tensors, we get

$$0 = 3\alpha_0 + \alpha_2 \operatorname{Tr} \left[ \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2 \right], \tag{1.57}$$

from which we can identify  $\alpha_0$  using (1.56b) as

$$\alpha_0 = -\frac{1}{3}\alpha_2 \operatorname{Tr}\left[ (\mathbb{T}_{\text{th},\rho})_{\delta}^2 \right] = \frac{2}{3}\alpha_2 I_2. \tag{1.58}$$

Substituting (1.58) into representation formula (1.55) yields

$$\overline{\mathbb{H}} = \frac{2}{3} \alpha_2 I_2 \mathbb{I} + \alpha_1 \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} + \alpha_2 \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2. \tag{1.59}$$

Using Theorem 1 for our isotropic scalar valued function, which is the specific Gibbs free energy g, we can see that it must take the form

$$g = g(\theta, p_{th}, I_2, I_3). (1.60)$$

Moreover, if we use the chain rule and formula (1.54c), we identify the deviatoric Hencky strain  $\overline{\mathbb{H}}$  as

$$\overline{\mathbb{H}} = -\left(\frac{\partial g}{\partial \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}}\right)_{\delta} = -\left(\frac{\partial g}{\partial I_{2}}\frac{\partial I_{2}}{\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}} + \frac{\partial g}{\partial I_{3}}\frac{\partial I_{3}}{\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}}\right)_{\delta}.$$
 (1.61)

Here we can use formulae for derivatives of matrix invariants, which we have introduced in (1.7). With the property that  $(\mathbb{T}_{th,\rho})_{\delta}$  is a symmetric traceless

tensor, the derivatives of invariants  $I_2$  and  $I_3$  are

$$\frac{\partial I_2}{\partial \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}} = \text{Tr}\left(\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}\right) \mathbb{I} - \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^{\text{T}} = -\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}, \tag{1.62a}$$

$$\frac{\partial I_3}{\partial \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}} = \det\left(\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}\right) \left(\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}\right)^{-T} = I_3 \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^{-1}. \tag{1.62b}$$

We substitute these formulae into equation (1.61) and we get

$$\overline{\mathbb{H}} = \left(\frac{\partial g}{\partial I_2} \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta} - \frac{\partial g}{\partial I_3} I_3 \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^{-1}\right)_{\delta}.$$
 (1.63)

Only partial derivatives of g with respect to  $I_2$  and  $I_3$  remain to be determined. We use the following well-known theorem to determine them.

**Theorem 4** (Cayley–Hamilton). A tensor  $\mathbb{A}$  satisfies its own characteristic equation, i.e.

$$\mathbb{A}^3 - I_1 \mathbb{A}^2 + I_2 \mathbb{A} - I_3 \mathbb{I} = \mathbf{0}. \tag{1.64}$$

*Proof.* See, for example, [19, p. 28].

In our situation, using (1.56a) with Cayley–Hamilton theorem implies

$$\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^{3} + I_{2}\left(\mathbb{T}_{\text{th},\rho}\right)_{\delta} - I_{3}\mathbb{I} = \mathbf{0}. \tag{1.65}$$

From this equation, we can express  $(\mathbb{T}_{\text{th},\rho})_{\delta}^{-1}$  as

$$(\mathbb{T}_{\text{th},\rho})_{\delta}^{-1} = \frac{1}{I_3} \left( I_2 \mathbb{I} + (\mathbb{T}_{\text{th},\rho})_{\delta}^2 \right).$$
 (1.66)

Substituting this relation into formula (1.63) yields

$$\overline{\mathbb{H}} = \left(\frac{\partial g}{\partial I_2} \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta} - I_2 \frac{\partial g}{\partial I_3} \mathbb{I} - \frac{\partial g}{\partial I_3} \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^2\right)_{\delta} = 
= -\frac{2}{3} I_2 \frac{\partial g}{\partial I_3} \mathbb{I} + \frac{\partial g}{\partial I_2} \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta} - \frac{\partial g}{\partial I_3} \left(\mathbb{T}_{\text{th},\rho}\right)_{\delta}^2.$$
(1.67)

Comparing (1.67) with representation formula (1.59), we identify  $\alpha_1$  and  $\alpha_2$  as

$$\alpha_1 = \frac{\partial g}{\partial I_2},\tag{1.68a}$$

$$\alpha_2 = -\frac{\partial g}{\partial I_3},\tag{1.68b}$$

and the final form of the relation for  $\mathbb{H}$  is

$$\overline{\mathbb{H}} = -\frac{2}{3} I_2 \frac{\partial g}{\partial I_3} \mathbb{I} + \frac{\partial g}{\partial I_2} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} - \frac{\partial g}{\partial I_3} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2. \tag{1.69}$$

From the volumetric-isochoric split of the Hencky strain (1.28) the second term, which is  $\log J$ , remains to be expressed. Fortunately, it is a lot easier than the

first term. The formula for the derivative of g with respect to  $p_{th}$  (1.54b) implies

$$\log J = \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right). \tag{1.70}$$

The final step is to obtain the representation theorem for the complete Hencky strain tensor  $\mathbb{H}$ . In order to do that, we substitute (1.69) and (1.70) into the volumetric-isochoric split (1.28). Since  $\overline{\mathbb{H}} = \mathbb{H}_{\delta}$  is traceless, we see that  $\overline{\mathbb{H}} = \overline{\mathbb{H}}_{\delta}$ , and it leads to the formula

$$\mathbb{H} = \overline{\mathbb{H}} + \frac{1}{3} \log J = \overline{\mathbb{H}}_{\delta} + \frac{1}{3} \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right) \mathbb{I} = 
= \frac{1}{3} \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right) \mathbb{I} + \frac{\partial g}{\partial I_2} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} - \left[ \frac{\partial g}{\partial I_3} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2 \right]_{\delta}.$$
(1.71)

Summing up this approach, we can formulate the following version of the representation theorem for isotropic elastic solids.

**Theorem 5** (Representation theorem for isotropic elastic solids with a given specific Gibs free energy). Let us consider an isotropic elastic solid with a given specific Gibbs energy of the form

$$g = g(\theta, p_{th}, I_2, I_3), \tag{1.72}$$

where  $I_2 = I_2\left((\mathbb{T}_{th,\rho})_{\delta}\right)$  and  $I_3 = I_3\left((\mathbb{T}_{th,\rho})_{\delta}\right)$  are the second invariant and the third invariant of the tensor  $(\mathbb{T}_{th,\rho})_{\delta}$ . Then the constitutive relation between the Hencky strain tensor  $\mathbb{H}$  and the Cauchy stress tensor  $\mathbb{T}$  is

$$\mathbb{H} = \frac{1}{3} \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right) \mathbb{I} + \frac{\partial g}{\partial I_2} \left( \mathbb{T}_{th,\rho} \right)_{\delta} - \left[ \frac{\partial g}{\partial I_3} \left( \mathbb{T}_{th,\rho} \right)_{\delta}^2 \right]_{\delta}. \tag{1.73}$$

#### 1.4 Full system of governing equations

In this section, we formulate a full system of governing equations for isotropic elastic solids in the Eulerian description with given specific Gibbs free energy g, which is in the form

$$g = g\left(\theta, p_{th}, (\mathbb{T}_{th,\rho})_{\delta}\right). \tag{1.74}$$

This system of governing equations consists of four equations. The first one is the well-known balance of the linear momentum in which we do not take into account the body force **b**. Thus, the balance of the linear momentum is

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T},\tag{1.75}$$

where the Cauchy stress tensor  $\mathbb{T}$  is given by the formula

$$\mathbb{T} = -p_{th}\mathbb{I} + \rho \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}, \tag{1.76}$$

see (1.35), (1.44) and (1.46).

The second equation is representation formula (1.73) from Theorem 5. To derive the third equation, we start with a definition of the upper convected derivative of a matrix  $\mathbb{A}$  as

$$\overset{\nabla}{\mathbb{A}} =_{\text{def}} \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} - \mathbb{L}\mathbb{A} - \mathbb{A}\mathbb{L}^{\mathrm{T}}.$$
(1.77)

Recall that

$$\frac{\mathrm{d}\mathbb{F}}{\mathrm{d}t} = \mathbb{L}\mathbb{F}.\tag{1.78}$$

Using (1.78) we calculate the upper convected derivative of the left Cauchy–Green tensor  $\mathbb B$  as

$$\overset{\triangledown}{\mathbb{B}} = \frac{\mathrm{d}\mathbb{F}}{\mathrm{d}t}\mathbb{F}^{\mathrm{T}} + \mathbb{F}\frac{\mathrm{d}\mathbb{F}^{\mathrm{T}}}{\mathrm{d}t} - \mathbb{L}\mathbb{B} - \mathbb{B}\mathbb{L}^{\mathrm{T}} = \mathbf{0}.$$
 (1.79)

Moreover, the definition of the Hencky strain tensor  $\mathbb{H}$  (1.18) implies

$$\overline{e^{2\mathbb{H}}} = \overset{\triangledown}{\mathbb{B}}.\tag{1.80}$$

And from (1.79) and (1.80), we get our third equation as the evolution equation for  $\mathbb{H}$  as

$$\overline{e^{2\mathbb{H}}} = \mathbf{0}. \tag{1.81}$$

In the last equation, we want to include the evolution equation for the temperature  $\theta$ . Dealing with the elastic solid, the dissipative term in the evolution equation for the specific entropy (1.43) has to be zero, so we get

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} + \mathrm{div}\left(\frac{\mathbf{j}_e}{\theta}\right) = -\frac{\mathbf{j}_e \cdot \nabla \theta}{\theta^2}.$$
 (1.82)

Furthermore, the relation (1.54a) for the derivative of g implies

$$-\rho \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{\partial g}{\partial \theta} \right) + \mathrm{div} \left( \frac{\mathbf{j}_e}{\theta} \right) = -\frac{\mathbf{j}_e \cdot \nabla \theta}{\theta^2}. \tag{1.83}$$

It remains to deal with the heat flux  $\mathbf{j}_e$ . For it we use Fourier's law

$$\mathbf{j}_e = -\kappa \nabla \theta, \tag{1.84}$$

where  $\kappa > 0$  is the thermal conductivity and it is a constant. Overall, equation (1.83) can be rewritten as

$$-\rho \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{\partial g}{\partial \theta} \right) - \kappa \operatorname{div} \left( \frac{\nabla \theta}{\theta} \right) = \kappa \frac{\nabla \theta \cdot \nabla \theta}{\theta^2}$$
 (1.85)

or after using the identity div  $\left(\frac{\nabla \theta}{\theta}\right) = \frac{\triangle \theta}{\theta} + \nabla \theta \cdot \nabla \left(\frac{1}{\theta}\right)$  as

$$-\rho \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{\partial g}{\partial \theta} \right) - \kappa \frac{\triangle \theta}{\theta} - \kappa \nabla \theta \cdot \nabla \left( \frac{1}{\theta} \right) - \kappa \frac{\nabla \theta \cdot \nabla \theta}{\theta^2} = 0. \tag{1.86}$$

And finally after evaluating that  $\nabla \left(\frac{1}{\theta}\right) = -\frac{\nabla \theta}{\theta^2}$  we get

$$-\rho\theta \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{\partial g}{\partial \theta} \right) = \kappa \triangle \theta. \tag{1.87}$$

The density  $\rho$ , which appears in (1.75) and (1.87), is expressed from the relation

$$\rho e^{\text{Tr}\,\mathbb{H}} = \rho_R,\tag{1.88}$$

which comes from the balance of mass (1.41) and relation (1.24). Now we are finally able to formulate the full system of governing equations

$$\frac{\rho_R}{e^{\text{Tr}\,\mathbb{H}}}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T},\tag{1.89a}$$

$$\mathbb{H} = \frac{1}{3} \log \left( \rho_R \frac{\partial g}{\partial p_{th}} \right) \mathbb{I} + \frac{\partial g}{\partial I_2} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta} - \left[ \frac{\partial g}{\partial I_3} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}^2 \right]_{\delta}, \quad (1.89b)$$

$$\overline{e^{2\mathbb{H}}} = \mathbf{0},\tag{1.89c}$$

$$-\theta \frac{\rho_R}{e^{\text{Tr} \mathbb{H}}} \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{\partial g}{\partial \theta} \right) = \kappa \triangle \theta, \tag{1.89d}$$

which should be solved for unknowns  $\mathbb{H}$ ,  $\mathbf{v}$  and  $\theta$ .

### 1.5 Restrictions on specific Gibbs free energy and relation to standard linearized elasticity

We have almost completed the theoretical part of this chapter and at the end we look at a specific example. The main result, Theorem 5, works with the assumption that we have the specific Gibbs free energy. However, the specific Gibbs free energy cannot be just any function of the respective variables. In addition, it must have a certain structure. But what are the requirements that a given function must meet to be the specific Gibbs free energy? The best way to investigate this question is to study the behavior of the density.

We can see that in formula (1.54b) for the partial derivative of the specific Gibbs free energy g with respect to the thermodynamic pressure  $p_{th}$ , the referential density  $\rho_R$  appears. Nevertheless, we are interested in the density  $\rho$  in the current configuration. Using the balance of mass (1.41) in formula (1.54b) leads to the desired relation with  $\rho$  as

$$\frac{\partial g}{\partial p_{th}} = \frac{1}{\rho}. (1.90)$$

Since the density at point P, which is the interior point of the body located in a small element of volume  $\Delta V$  whose mass is  $\Delta m$ , is defined as the limit

$$\rho =_{\text{def }} \lim_{\Delta V \to 0} \frac{\Delta V}{\Delta m},\tag{1.91}$$

and because  $\Delta V$  and  $\Delta m$  are positive, the density  $\rho$  has to be positive as well, and using (1.90) we get the first condition as

$$\frac{\partial g}{\partial p_{th}} > 0. {(1.92)}$$

The second condition stems from the physical assumption that the material stretches in the direction of the highest tensile force. It means that if there

is an increasing tension in the elastic material, the density is decreasing. This can be expressed as

$$\frac{\partial \rho}{\partial p_{th}} > 0.$$

We use this inequality again in formula (1.54b), which leads to the restriction

$$\frac{\partial^2 g}{\partial p_{th}^2} = \frac{\partial}{\partial p_{th}} \left( \frac{1}{\rho} \right) = -\frac{1}{\rho^2} \frac{\partial \rho}{\partial p_{th}} < 0. \tag{1.93}$$

Now we are ready to formulate the following proposition, about the necessary conditions for the specific Gibbs free energy g.

**Proposition 6** (Necessary conditions for the specific Gibbs free energy). Let us consider an isotropic elastic solid with a given specific Gibbs free energy of the form

$$g = g(\theta, p_{th}, I_2, I_3). \tag{1.94}$$

Then the specific Gibbs free energy g must satisfy

$$\frac{\partial g}{\partial p_{th}} > 0, \tag{1.95a}$$

$$\frac{\partial^2 g}{\partial p_{th}^2} < 0. \tag{1.95b}$$

Next we want to show the practical application of this proposition. Let us define functions  $g_1$  and  $g_2$  as

$$g_1(\theta, p_{th}, I_2, I_3) =_{\text{def}} -c_{V,R}\theta \left[ \log \left( \frac{\theta}{\theta_R} \right) - 1 \right] - \frac{K_R}{\rho_R} e^{-\frac{p_{th}}{K_R}} + \frac{\rho_R}{2\mu_R} I_2, \quad (1.96a)$$

$$g_2(\theta, p_{th}, I_2, I_3) =_{\text{def}} -c_{V,R}\theta \left[ \log \left( \frac{\theta}{\theta_R} \right) - 1 \right] - \frac{K_R}{\rho_R} e^{-\frac{p_{th}^2}{K_R}} + \frac{\rho_R}{2\mu_R} I_2, \quad (1.96b)$$

where  $c_{V,R}$  is the specific heat at the constant volume,  $\theta_R$  is the reference temperature and  $K_R$  and  $\mu_R$  are the positive parameters, which denote the bulk and shear moduli. Later, we show their relation to the usual definitions of the bulk K and shear  $\mu$  moduli, which are defined in the standard linearized elasticity.

First, we check for both functions the first necessary condition from Proposition 6.

$$\frac{\partial g_1}{\partial p_{th}} = \frac{e^{-\frac{p_{th}}{K_R}}}{\rho_R},\tag{1.97}$$

which is always positive. On the other hand, the same check for the function  $g_2$  leads to

$$\frac{\partial g_2}{\partial p_{th}} = \frac{2p_{th}}{\rho_R} e^{-\frac{p_{th}}{K_R}},\tag{1.98}$$

which might be negative. Therefore, the function  $g_2$  cannot be the specific Gibbs free energy. So, continue only with the function  $g_1$  and verify the second condition for it. We have

$$\frac{\partial^2 g_1}{\partial p_{th}^2} = \frac{\partial}{\partial p_{th}} \left( \frac{e^{-\frac{p_{th}}{K_R}}}{\rho_R} \right) = -\frac{e^{-\frac{p_{th}}{K_R}}}{K_R \rho_R}, \tag{1.99}$$

which is negative as required. So we can say that  $g_1$  is an example of the specific Gibbs free energy.<sup>5</sup>

The next step is to express the Hencky strain tensor  $\mathbb{H}$  based on the function  $g_1$  using Theorem 5. Since the function  $g_1$  does not depend on the third tensor invariant  $I_3$ , formula (1.73) is reduced as

$$\mathbb{H} = \frac{1}{3} \log \left( \rho_R \frac{\partial g_1}{\partial p_{th}} \right) \mathbb{I} + \frac{\partial g_1}{\partial I_2} \left( \mathbb{T}_{\text{th},\rho} \right)_{\delta}. \tag{1.100}$$

All that remains is to calculate  $\frac{\partial g_1}{\partial I_2}$ , which is

$$\frac{\partial g_1}{\partial I_2} = \frac{\rho_R}{2\mu_R}. (1.101)$$

Since (1.90) and (1.97) imply that

$$\frac{1}{\rho} = \frac{e^{-\frac{p_{th}}{K_R}}}{\rho_R},\tag{1.102}$$

formula (1.101) can be rewritten as

$$\frac{\partial g_1}{\partial I_2} = \frac{\rho}{2\mu_R} e^{-\frac{p_{th}}{K_R}}. (1.103)$$

Substituting (1.97) and (1.103) into (1.100) and using definition (1.44b) leads to the desired result

$$\mathbb{H} = -\frac{p_{th}}{3K_R} \mathbb{I} + \frac{1}{2\mu_R} e^{-\frac{p_{th}}{K_R}} \left( \mathbb{T}_{th} \right)_{\delta}. \tag{1.104}$$

As mentioned, now we want investigate the linearized version of this result.

First, we briefly recall the theory of linearization. Let us assume that the deformation  $\chi$  can be decomposed as  $\chi = \mathbf{X} + \mathbf{U}$ , where  $\mathbf{X}$  is the position in the reference configuration and  $\mathbf{U}$  is the displacement. We also assume that  $|\nabla \mathbf{U}| \ll 1$ . In the words of the displacement gradient, the linearized strain  $\epsilon$  is defined as

$$\boldsymbol{\epsilon} =_{\text{def}} \frac{1}{2} \left( \nabla \mathbf{U} + (\nabla \mathbf{U})^{\mathrm{T}} \right), \tag{1.105}$$

 $\rho c_{V,R} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \kappa \triangle \theta.$ 

<sup>&</sup>lt;sup>5</sup>Let us justify the choice of the thermal part of the specific Gibbs energy  $g_1$  defined in (1.96a). Substituting  $g_1$  into (1.89d) leads to the linear partial differential equation for the temperature  $\theta$  known as the heat equation

and the deformation gradient  $\mathbb{F}$  can be expressed as

$$\mathbb{F} = \nabla \chi = \mathbb{I} + \nabla \mathbf{U}. \tag{1.106}$$

Substituting this relation into the definition of the Hencky strain tensor (1.18) yields

$$\mathbb{H} = \frac{1}{2} \log \mathbb{B} = \frac{1}{2} \log \left( (\mathbb{I} + \nabla \mathbf{U}) (\mathbb{I} + \nabla \mathbf{U})^{\mathrm{T}} \right) \approx \frac{1}{2} \log \left( \mathbb{I} + (\nabla \mathbf{U} + (\nabla \mathbf{U})^{\mathrm{T}}) \right),$$
(1.107)

where we neglected terms  $(\nabla \mathbf{U})^{\mathrm{T}}(\nabla \mathbf{U})$  and  $(\nabla \mathbf{U})(\nabla \mathbf{U})^{\mathrm{T}}$  as we assume that they are small. Note, that in (1.107) we have also derived the formula for the linearized left Cauchy–Green tensor as

$$\mathbb{B} \approx \mathbb{I} + 2\epsilon. \tag{1.108}$$

The next step is to take into account the standard approximation  $\log (1+x) \approx x$  for |x| < 1 that gives us

$$\mathbb{H} \approx \frac{1}{2} \left( \nabla \mathbf{U} + (\nabla \mathbf{U})^{\mathrm{T}} \right) = \boldsymbol{\epsilon}. \tag{1.109}$$

Note that this also justifies why the coefficient  $\frac{1}{2}$  appears in the definition of the Hencky strain tensor (1.18).

The next step is to deal with a linearization of the right-hand side of (1.104) with respect to the stress. We see that the spherical part is already linear. On the other hand, we have to appropriately approximate the deviatoric part as the exponential function represents non-linearity there. The most straightforward and in this case fully sufficient is to use the Taylor series for the exponential function  $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$ , specifically only the first term. All together gives us the complete linearization of equation (1.104) as

$$\boldsymbol{\epsilon} = -\frac{p_{th}}{3K_R} \mathbb{I} + \frac{1}{2\mu_R} \left( \mathbb{T}_{th} \right)_{\delta}. \tag{1.110}$$

From the decomposition of the Cauchy stress tensor  $\mathbb{T}$  to the deviatoric and spherical part (1.35) and from (1.44) we calculate that

$$\mathbb{T}_{\delta} = (\mathbb{T}_{\text{th}})_{\delta}, \qquad (1.111a)$$

$$\operatorname{Tr} \mathbb{T} = -3p_{th}. \tag{1.111b}$$

Substituting these relations into formula (1.110) gives us

$$\epsilon = \frac{1}{9K_R} \left( \text{Tr } \mathbb{T} \right) \mathbb{I} + \frac{1}{2\mu_R} \mathbb{T}_{\delta}. \tag{1.112}$$

Recall now the standard constitutive relation for the linearized elasticity (which can be found, for instance, in [20, p. 140])

$$\tau = \lambda \left( \operatorname{Tr} \boldsymbol{\epsilon} \right) \mathbb{I} + 2\mu \boldsymbol{\epsilon}, \tag{1.113}$$

where  $\tau$  is the stress tensor in the linearized theory, while  $\lambda$  and  $\mu$  are material constants called Lamé coefficients. The first Lamé coefficient  $\mu$  we have already

defined specifically as the shear modulus. Now we want to invert this equation. Applying the trace operator to the both sides of (1.113) implies

$$\operatorname{Tr} \boldsymbol{\tau} = (3\lambda + 2\mu) \operatorname{Tr} \boldsymbol{\epsilon}, \tag{1.114}$$

which can be substituted back into (1.113) and we can get inverted relation (1.113) as

$$\boldsymbol{\epsilon} = -\frac{\lambda}{2\mu} \left( \operatorname{Tr} \boldsymbol{\epsilon} \right) \mathbb{I} + \frac{1}{2\mu} \boldsymbol{\tau} = \left( \frac{1}{3} \cdot \frac{1}{2\mu} - \frac{\lambda}{2\mu} \cdot \frac{1}{3\lambda + 2\mu} \right) \left( \operatorname{Tr} \boldsymbol{\tau} \right) \mathbb{I} + \frac{1}{2\mu} \boldsymbol{\tau}_{\delta} =$$

$$= \frac{1}{9\lambda + 6\mu} \left( \operatorname{Tr} \boldsymbol{\tau} \right) \mathbb{I} + \frac{1}{2\mu} \boldsymbol{\tau}_{\delta}. \tag{1.115}$$

Defining the bulk modulus K as  $K =_{\text{def}} \lambda + \frac{2}{3}\mu$  leads to the relation

$$\boldsymbol{\epsilon} = \frac{1}{9K} \left( \operatorname{Tr} \boldsymbol{\tau} \right) \mathbb{I} + \frac{1}{2\mu} \boldsymbol{\tau}_{\delta}. \tag{1.116}$$

This shows an evident similarity in equation (1.112). It also explains the chosen form of the specific Gibbs free energy  $g_1$  in definition (1.96a).

# 2. Elasto-plastic response of one-dimensional models described implicitly

The aim of this chapter is to introduce one-dimensional models for the inelastic response of the material. These models are based on the concept of implicit constitutive relations. In standard plasticity, we consider strain decomposition into its elastic and plastic part, see, for example, [21]. On the other hand, for some specific materials (such as Aluminium), which shows only negligible elastic response, this decomposition is not appropriate. Also in soil and rock mechanics, the plastic strain is viewed with some difficulty and many papers have been written describing the elimination process (see, for instance, [22]). As we shall see this theory, based on the implicit constitutive relation, does not need this decomposition. This theory of describing the inelastic response of the material is based on [4].

In the first part of this chapter, we introduce the relation between the stress, the strain, the temperature and their time derivatives to describe the inelastic response of the material. Then we include discontinuity in this description. This leads to some complications in our numerical implementations that we have to deal with, but it also gives us a tool to consider hysteretic materials, wherein the current state depends on the complete history of the material. Furthermore, we show some examples describing the elastic-perfectly plastic response (the response that contains sharp yield points), where we also show just the mentioned hysteresis of the material. However, since in fact most materials do not have these points, we eliminate them and observe the elasto-plastic response of the material, also with some examples. The implementation of all figures in this chapter is done in Mathematica programming language using the standard library function NDSolve.

## 2.1 General form of constitutive equations for elastic-perfectly plastic response

In the previous chapter, we assumed in (1.5) a relation between the Cauchy stress tensor  $\mathbb{T}$  and the left Cauchy–Green tensor  $\mathbb{B}$ . That is commonly used assumption for the standard version of the implicit equation (see, for instance, [23])

$$f(\mathbb{B}, \mathbb{T}, \theta) = \mathbf{0} \tag{2.1}$$

for the thermoelastic material. Implicit thermoelasticity is also our starting point for our analysis. At first, however, for one-dimensional models, we work with the stress  $\sigma$ , the small strain  $\epsilon$  and the temperature  $\theta$ . As a counterpart to equation (2.1) in three dimensions, we assume the following implicit constitutive equation for a thermoelastic material in one dimension

$$h\left(\epsilon, \sigma, \theta\right) = 0. \tag{2.2}$$

Differentiating this equation with respect to time we get

$$\frac{\partial h}{\partial \epsilon} \dot{\epsilon} + \frac{\partial h}{\partial \sigma} \dot{\sigma} + \frac{\partial h}{\partial \theta} \dot{\theta} = 0. \tag{2.3}$$

Unlike the previous chapter, we now want to describe the plastic material (inelastic). The idea is that for certain ranges of the strain, the stress and the temperature, the material response is elastic, as described in the previous equation. On the other hand, if we are outside this range, the material could exhibit an inelastic response (perfectly plastic response). Therefore, we modify equation (2.3) by changing its right-hand side as

$$\frac{\partial h}{\partial \epsilon} \dot{\epsilon} + \frac{\partial h}{\partial \sigma} \dot{\sigma} + \frac{\partial h}{\partial \theta} \dot{\theta} = w(\mathbf{r}) \frac{\mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}} + |\mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}}|}{2}, \tag{2.4}$$

where  $\mathbf{r} =_{\text{def}} [\epsilon, \sigma, \theta]^{\text{T}}$  and w and  $\mathbf{p}$  are scalar and vector functions of  $\mathbf{r}$ . To explain why we are considering this form of equation, we rewrite it as

$$\nabla h \cdot \dot{\mathbf{r}} = w(\mathbf{r}) H(\mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}}) \mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}}, \tag{2.5}$$

where the notation H stands for the Heaviside step function defined as

$$H(x) =_{\text{def}} \begin{cases} 0, & x < 0, \\ 1, & x \ge 0. \end{cases}$$
 (2.6)

Thus, we can rewrite equation (2.4) into the form

$$\nabla h \cdot \dot{\mathbf{r}} =_{\text{def}} \begin{cases} w(\mathbf{r}) \mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}}, & \mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}} > 0, \\ 0, & \text{otherwise.} \end{cases}$$
 (2.7)

Now when we have this form of equation, we can see that the term  $H(\mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}})$  represents the whole group for loading and unloading criteria based on the stress, the strain or the temperature for elasto-plastic materials. We can also see this term as a counterpart to the loading and unloading criteria for three dimensional elasto-plastic materials (see, for example, [24]). Furthermore, depending on a sign of the term  $\mathbf{p}(\mathbf{r}) \cdot \dot{\mathbf{r}}$  we can observe the hysteretic behavior of the material. On the other hand, this term with the Heaviside function cannot handle a yield criterion. This is the purpose of the scalar function  $\omega(\mathbf{r})$  that contains the yield criterion in itself.

#### 2.2 Classical plasticity examples

Now when we have formulated the general form of the constitutive equation for elasto-plastic response (2.7), let us look further at some specific cases. Let us begin with the formulation of well-known Hooke's law. First, verbally as Robert Hooke did it in 1678 in his essay *Ut tensio sic vis*, followed by the well-known formula derived, for example, in [25, pp. 70–71].

**Theorem 7** (Hooke's law). The power of a springy body is in the same proportion as the extension. Thus, the stress  $\sigma$  and the small strain  $\epsilon$  are related by the Young modulus of elasticity E as

$$\sigma = E\epsilon. \tag{2.8}$$

It is Hooke's law (more precisely its derivative - differentiating both sides of equation (2.8) with respect to time) that forms an elastic response in our model, whose constitutive equation is

$$\dot{\sigma} - E\dot{\epsilon} = -EH(\sigma\dot{\epsilon})H(|\sigma| - \sigma_u)\dot{\epsilon}, \tag{2.9}$$

where  $\sigma_y$  is the yield stress.

Now we see how this equation relates to the formulated general constitutive equation (2.7). First, we notice that we do not include the temperature in this model, so our assumption is, that the function h depends only on  $\sigma$  and  $\epsilon$ . Furthermore, the scalar function  $\omega$  is defined as  $\omega(\mathbf{r}) =_{\text{def}} -\frac{E}{\sigma}H(|\sigma| - \sigma_y)$ , which includes the yield condition, the vector function  $\mathbf{p}$  is defined as  $\mathbf{p}(\mathbf{r}) =_{\text{def}} [\sigma, 0]^{\text{T}}$  and finally, we assume that the function h has such a form that its derivatives are  $\frac{\partial h}{\partial \epsilon} = -E$  and  $\frac{\partial h}{\partial \sigma} = 1$ . Let us now analyze the situations that may occur. We expect that we have the given small strain and we are interested in how it affects the stress.

- (i) If  $\sigma \dot{\epsilon} > 0$  and  $|\sigma| = \sigma_y$ , then  $\dot{\sigma} = 0$ . Thus, the stress is constant. It can be also explained that in the first condition  $\sigma \dot{\epsilon} > 0$  we consider tensile loading and the second condition  $|\sigma| = \sigma_y$  describes what happens if  $\sigma$  reaches a certain limit set by  $\sigma_y$ . This tells us that in this case  $\sigma = \sigma_y$  and we observe the perfectly plastic response.
- (ii) In other cases where the conditions of the previous point are not met, we observe the elastic response given by equation  $\dot{\sigma} = E\dot{\epsilon}$ .

Moreover, the model described by equation (2.9) is a rate-independent process, which means that if we rescale the time variable  $t \to \alpha \tilde{t}$  for some  $\alpha > 0$ , then the response of the material does not change. Indeed substituting  $t = \alpha \tilde{t}$  into equation (2.9) yields

$$\frac{1}{\alpha}\dot{\sigma} - \frac{E}{\alpha}\dot{\epsilon} = -\frac{E}{\alpha}H\left(\sigma\dot{\epsilon}\right)H\left(|\sigma| - \sigma_y\right)\dot{\epsilon},\tag{2.10}$$

which after multiplying the whole equation by  $\alpha$  gives us again equation (2.9).

Now we want to verify the elastic-perfectly plastic response of the material defined by equation (2.9) numerically. As mentioned, we have to deal with discontinuity given by the Heaviside function. Therefore, for every  $n \in \mathbb{N}$  we define the function  $H_n$  as

$$H_n(x) =_{\text{def}} \frac{1}{2} + \frac{1}{\pi} \arctan(xn). \tag{2.11}$$

As  $n \to \infty$ , these functions  $H_n$ , according to [26, p. 734], converge pointwise to the Heaviside step function H(x) = 1, if x > 0, and H(x) = 0, if x < 0, which, together with the continuity of  $H_n$ , is exactly what we need. In Figure 2.1 we can see that convergence is fast enough, just for n = 1000 we get a very good approximation.

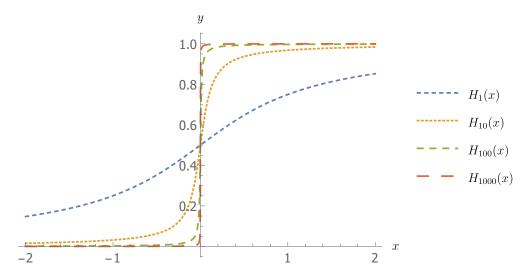


Figure 2.1: Convergence rate of the approximation of the Heaviside function  $H_n$ .

Now that we have solved the problem of implementation of the Heaviside function, let us look at equation (2.9) itself. First, we rewrite it using the approximation as

$$\dot{\sigma} - E\dot{\epsilon} = -EH_n(\sigma\dot{\epsilon})H_n(|\sigma| - \sigma_y)\dot{\epsilon}. \tag{2.12}$$

We further illustrate how the stress  $\sigma$  depends on the small strain  $\epsilon$ . For this illustration we need to specify values for the Young modulus E, which measures the stiffness of the material, the yield stress  $\sigma_y$  and also for the small strain  $\epsilon$ . We further consider that our small strain is given by the formula  $\epsilon(t) = \sin(t)$ . The value of n in definition (2.12) is set to  $10^{11}$ . First, let us analyze the situation, when E = 1 and  $\sigma_y = 0.5$ , as shown in Figure 2.2 and Figure 2.3.

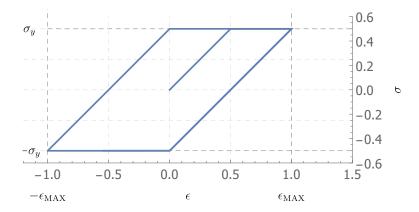


Figure 2.2: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=1 and the yield stress  $\sigma_y=0.5$ . The value of  $\epsilon_{\text{MAX}}$  is given by the definition of  $\epsilon$  as  $\epsilon_{\text{MAX}}=\sin(t)|_{t=\frac{\pi}{2}}=1$ .

<sup>&</sup>lt;sup>1</sup>We assume that each physical quantity is scaled by characteristic quantities such as a characteristic time, a characteristic length and a characteristic mass, while consequently we effectively work with dimensionless quantities.

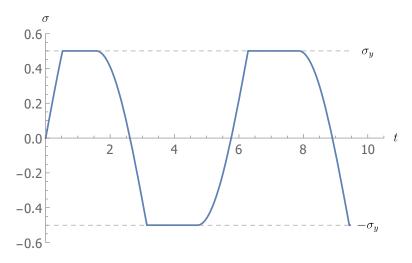


Figure 2.3: Dependence of the stress  $\sigma$  on time t with the Young modulus E=1 and the yield stress  $\sigma_y=0.5$ .

In Figure 2.2 we see that from the beginning the stress  $\sigma$  has increased to its limit value, which is the yield stress  $\sigma_y$  (on this interval we can see the elastic response of the material - elastic loading). When  $\sigma$  reaches the limit value, the stress does not change - the material response is perfectly plastic until the small strain  $\epsilon$  reaches its maximum value. Then the material performs the elastic unloading until the stress  $\sigma$  reaches its extreme value again, but now its minimum  $-\sigma_y$ . This is followed by the perfectly plastic response and this cyclic process repeats itself again and again. In Figure 2.2 we can also observe the hysteresis of the material. The moment when  $\epsilon$  reaches its maximum value  $\epsilon_{\rm MAX}$ , we then observe the elastic unloading, as we mentioned before. However, because of the plastic deformation, for  $\epsilon=0$  we get a different value of  $\sigma$  than we had at the beginning of the cycle. Since this part of Figure 2.2 for unloading has the same shape as for loading, it is only shifted (i.e. the material memory is manifested). Therefore, we call the material response hysteretic.

It is also interesting to look at the dependence of the stress on time shown in Figure 2.3. The information provided in this figure is similar. When the stress  $\sigma$  reaches the yield stress  $\sigma_y$ , we can see the perfectly plastic response of the material and that the stress is constant for a specific time interval. Then again unloading and so on as in the previous figure. We notice that due to the definition of the small strain  $\epsilon$ , the stress  $\sigma$  has a periodic waveform whose graph is similar to the sine function.

In Figure 2.4 and Figure 2.5 can see that if the stress does not reach the yield value, no plastic response is observed. This is achieved by setting  $\sigma_y = 1.1$ .

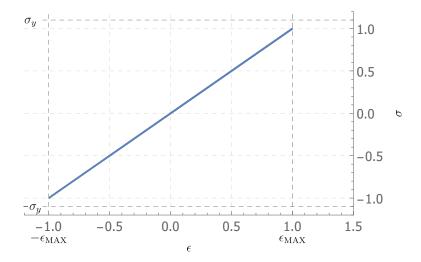


Figure 2.4: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=1 and the yield stress  $\sigma_y=1.1$  - completely elastic response as the stress  $\sigma$  never reaches the yield stress  $\sigma_y$ .

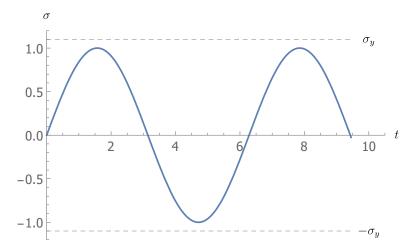


Figure 2.5: Dependence of the stress  $\sigma$  on time t with the Young modulus E=1 and the yield stress  $\sigma_y=1.1$ . The material response is completely elastic as the stress  $\sigma$  for any time t does not reach the yield stress  $\sigma_y$ .

We have just shown and verified, that the model based on the constitutive relation (2.9) or more precisely on its approximated version (2.12), actually works as expected.

Let us now look at the problem that occurs in this model. The problem is at the moment of transition from the elastic response of the material to the perfectly plastic. These sharp yield points are marked in Figure 2.6 and Figure 2.7.

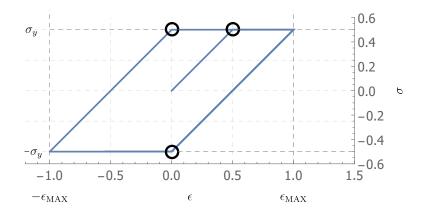


Figure 2.6: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=1 and the yield stress  $\sigma_y=0.5$  with marked sharp yield points.

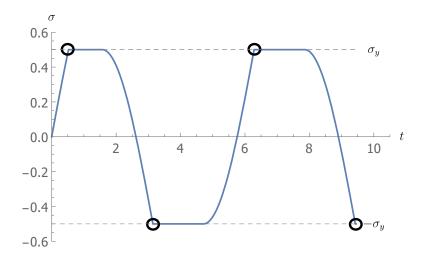


Figure 2.7: Dependence of the stress  $\sigma$  on time t with the Young modulus E=1 and the yield stress  $\sigma_y=0.5$  with marked sharp yield points.

Sharp yield points are consequences of the fact the approximated constitutive equation (2.12) has a very steep transition to plasticity at the moment when stress  $\sigma$  reaches  $\sigma_y$  due to the presence of the term  $H_n(|\sigma| - \sigma_y)$ . In fact, most materials do not show such a sharp yield condition, so we smooth this term including the Heaviside function.

Next, we modify the problematic term  $H_n(|\sigma| - \sigma_y)$  with respect to the remaining terms in equation (2.12). Consider a modified version of equation (2.12) in the form

$$\dot{\sigma} - E\dot{\epsilon} = -EH_n(\sigma\dot{\epsilon})\left[1 + \tanh\left(\alpha\left(|\sigma| - \sigma_y\right)\right)\right]\dot{\epsilon}.$$
 (2.13)

Let us justify this choice now. First, we remind in Figure 2.8 how the hyperbolic tangent function looks like. Second, in Figure 2.9 we can see the difference between  $H_n(x)$  with  $n = 10^{11}$  and  $1 + \tanh(\alpha x)$  as it appears in equation (2.13) with the parameter  $\alpha$  set to 30. The version of response relation with the hyperbolic tangent (2.13) obviously has a smoother transition between two value levels.

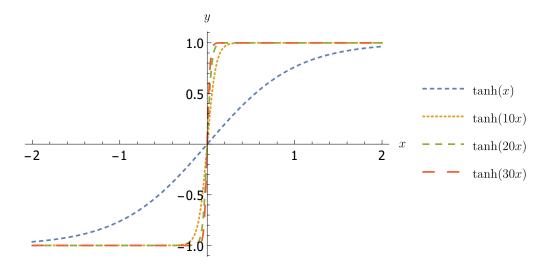


Figure 2.8: Functions  $\tanh(\alpha x)$  for different values of  $\alpha$ .

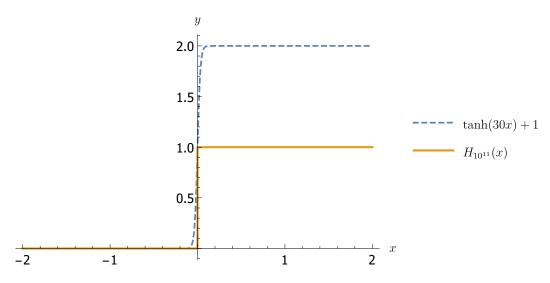


Figure 2.9: The difference between functions  $1 + \tanh(30x)$  and  $H_{10^{11}}(x)$ . The hyperbolic tangent gives a worse approximation. On the other hand, it is much smoother than the approximation of the Heaviside function.

So, we can see that this approximation can be smooth enough. However, another question arises from Figure 2.9. Is it not a problem that the positive values of the function  $1+\tanh{(\alpha x)}$ , independent of the choice of the parameter  $\alpha$ , are greater than one, which is contrary to what we expect from the role of the Heaviside function? Next, we show that this is not the problem.

From definition (2.13) we see that it happens if and only if

$$|\sigma| > \sigma_v. \tag{2.14}$$

But can this even happen? Suppose yes and that this situation arises at the point  $\sigma_1$ , which we fix for this moment. First, we assume that  $\sigma_1 > \sigma_y$  (for negative  $\sigma_1$  the approach is similar). Moreover, we assume that the stress  $\sigma$  is increasing on the interval  $[\sigma_y, \sigma_1]$ , so  $\dot{\sigma} > 0$  on the interval  $[\sigma_y, \sigma_1]$ . Then

$$1 + \tanh\left(\alpha\left(|\sigma_1| - \sigma_y\right)\right) = \delta, \tag{2.15}$$

for some  $\delta > 1$ . In the same way we use the expression

$$H_n\left(\sigma_1\dot{\epsilon}\right) = 1 - \lambda,\tag{2.16}$$

for some non-negative  $\lambda$ , for which  $\frac{\delta-1}{\delta} > \lambda$ . This can be achieved by taking larger n in the definition of  $H_n$ . Otherwise, if we cannot express  $H_n$  as we did, it does not make sense to discuss this situation because the right-hand side of (2.13) is zero. Then (2.13) can be rewritten as

$$\dot{\sigma}_1 = E\left(1 - (1 - \lambda)\delta\right)\dot{\epsilon} = E\left(1 - \delta + \lambda\delta\right)\dot{\epsilon} < E\left(1 - \delta + \delta - 1\right)\dot{\epsilon} = 0, \quad (2.17)$$

which is a contradiction with the fact that  $\dot{\sigma} > 0$  on the interval  $[\sigma_y, \sigma_1]$ . Using the similar approach for  $\sigma_1 < \sigma_y$  also leads to the contradiction. Thus, it implies that  $\sigma_1 = \sigma_y$ . So, we proved that our response relation (2.13) is right and doing what we expect it to do.

Successful elimination of sharp yield points given by (2.13) is shown in Figure 2.10 and Figure 2.11.

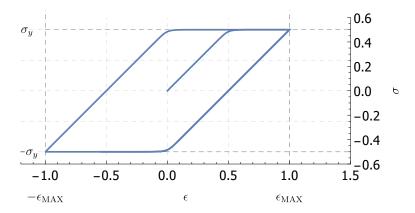


Figure 2.10: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=1 and the yield stress  $\sigma_y=0.5$  with eliminated sharp yield points by replacing the Heaviside function with a smooth transition as shown in equation (2.13) with the parameter  $\alpha=30$ .

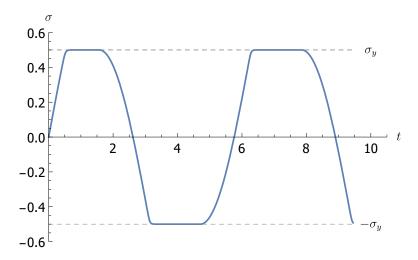


Figure 2.11: Dependence of the stress  $\sigma$  on time t with the Young modulus E=1 and the yield stress  $\sigma_y = 0.5$  with eliminated sharp yield points by replacing the Heaviside function with a smooth transition as shown in equation (2.13) with the parameter  $\alpha = 30$ .

We can see that Figure 2.10 and Figure 2.11 that describe the elasto-plastic response of the material preserv all properties (e.g. hysteresis of the material) that we observed in Figure 2.2 and Figure 2.3 for the elastic-perfectly plastic response of the material.

It is worth mentioning how different values of  $\alpha$  deal with sharp yield points. In Figure 2.12 we can see that smaller  $\alpha$  generates a smoother transition from the elastic to plastic deformation.

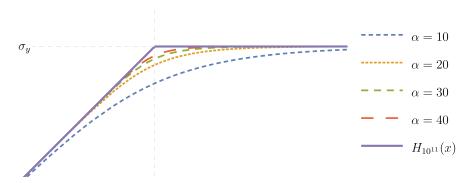


Figure 2.12: Detail on a transition from the elastic to the plastic deformation in dependence on the value of  $\alpha$  and comparison with the original (approximated) relation (2.12) with  $n = 10^{11}$ .

In Figure 2.4 and Figure 2.5 we investigated how the change of the yield stress  $\sigma_y$  affects the response of the material. Let us look at the end of this chapter how the change of the Young modulus E affects the response of the material.

Let us analyze the role of the Young modulus in the original constitutive relation (2.9) and consider that we have previously defined the small strain  $\epsilon$  as the sine function. Starting from t = 0 and continuing to some specific time  $t_1$ , the stress  $\sigma$  is definitely less than  $\sigma_y$ . On the interval  $[0, t_1]$  equation (2.9) yields

$$\dot{\sigma}(t) = E\dot{\epsilon}(t), \qquad (2.18)$$

which is a differential equation for the stress  $\sigma$  with the initial condition  $\sigma(0) = 0$ , whose solution on the interval  $[0, t_1]$  is

$$\sigma(t) = E\sin(t). \tag{2.19}$$

From this solution on the interval  $[0, t_1]$  we can distinguish two cases:

(i)  $E < \sigma_y$ 

In this case, the stress  $\sigma$  never reaches the yield value  $\sigma_y$ . So, the right-hand side of the constitutive equation (2.9) is always zero, thus  $\sigma(t) = E \sin(t)$  on the whole time interval. In this case we observe the purely elastic response of the material. In Figure 2.13 and Figure 2.14 we can see that the same is valid also for the discussed approximated relation (2.13). We used  $\alpha = 30$  for both figures.

(ii)  $E \geq \sigma_y$ 

In this case, there are situations, in which  $\sigma(t) = \sigma_y$ , so the "plastic" part of the response relation (2.9) is activated at periodically repeating intervals, and in the case  $E = \sigma_y$  at points. The larger the Young modulus E is, the faster the stress  $\sigma$  increases and decreases. In other words, in these situations the larger E extends the duration of the plastic response of the material. Again in Figure 2.15 and Figure 2.16 we can see that the same is true also for the approximated relation (2.13). We used  $\alpha = 30$  for both figures.

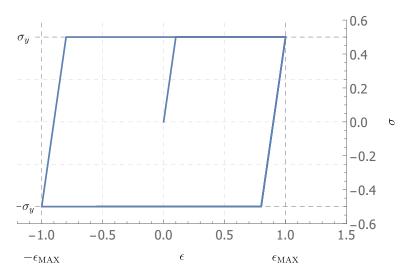


Figure 2.13: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=0.4 and the yield stress  $\sigma_y=0.5$ . We can see that the stress  $\sigma$  never reaches the yield value  $\sigma_y$  as its maximum is equal to the Young modulus E, therefore the response of the material is purely elastic.

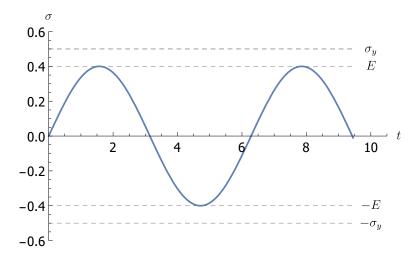


Figure 2.14: Dependence of the stress  $\sigma$  on time t with the Young modulus E = 0.4 and the yield stress  $\sigma_y = 0.5$ . We can see that the stress  $\sigma$  never reaches the yield value  $\sigma_y$  as its maximum is equal to the Young modulus E, therefore the response of the material is purely elastic.

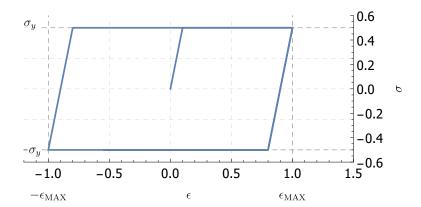


Figure 2.15: Dependence of the stress  $\sigma$  on the small strain  $\epsilon$  with the Young modulus E=5.0 and the yield stress  $\sigma_y=0.5$ . We can see that the stress  $\sigma$  reaches the yield value  $\sigma_y$  very fast and the response of the material is mostly plastic.

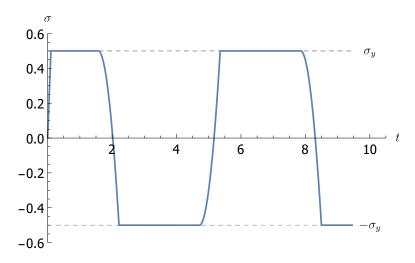


Figure 2.16: Dependence of the stress  $\sigma$  on time t with the Young modulus E=5.0 and the yield stress  $\sigma_y=0.5$ . We can see that the stress  $\sigma$  reaches the yield value  $\sigma_y$  very fast and the response of the material is mostly plastic.

# 3. Simulation of elasto-plastic response of inextensible beams

The aim of this chapter is to simulate the elasto-plastic response of an inextensible beam undergoing bending by using the implicit constitutive relation of the form (2.13), which we developed in the previous chapter. The constitutive relation of the inextensible elasto-plastic beam is very similar to (2.13), except that the variables are replaced by other suitable variables associated with beam theory. The simulation of the elasto-plastic behavior of the beam is performed again in Mathematica programming language using the standard library function NDSolve. We restrict ourselves to a two-dimensional setting - the beam moves in a plane. The simulation is done by discretizing the beam into N rigid elements of equal length. In addition to constitutive relations, we formulate other discretized equations based on kinematics, equilibrium of forces and the balance of angular momentum for the beam and our approach is quasistatic approximation. Finally, when we are done with discretization, we show that the model works as expected and we present simulations of the elastic and elasto-plastic material responses. The approach used in this chapter is motivated by [5].

## 3.1 Discrete elasto-plastic beam

We consider an inextensible elasto-plastic beam of length L. The beam is discretized into N rigid elements of equal length  $l = \frac{L}{N}$ .

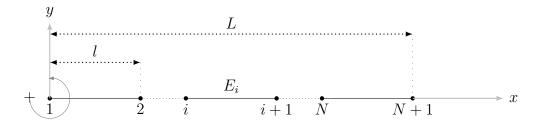


Figure 3.1: The elasto-plastic beam of length L is discretized into N rigid elements of equal length  $l = \frac{L}{N}$ . Each element  $E_i$  is described by positions of its nodes. The default state for discretizing the beam is the position of the first node 1 at the origin [0,0], the second node 2 at [l,0], ..., the Nth node at [(N-1)l,0] and the (N+1)th node at [Nl,0].

Forces acting on each beam element are shown in Figure 3.2.

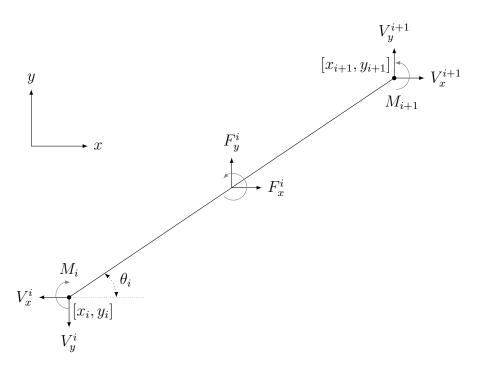


Figure 3.2: Forces acting on the discrete beam element  $E_i$ . Deformations occur only at the beam joints. The position of each discrete beam element is described by the position of its nodes (beam joints), here  $[x_i, y_i]$  and  $[x_{i+1}, y_{i+1}]$ ,  $\theta_i$  is the angle between the element  $E_i$  and the x-axis,  $\mathbf{F}^i = [F_x^i, F_y^i]$  is the external force vector (such as gravity) applied to the center of the element  $E_i$  respectively,  $\mathbf{V}^i = [V_x^i, V_y^i]$  is the net force vector on the cross section and  $M_i$  is the bending moment at the beam joint.

The bending moments  $M_i$  are rotational forces within beam elements  $E_i$  that cause bending. Similar to standard beam bending calculations (see, for example, [27]), we describe the shape of the beam by the curvature  $\kappa$ , which is defined as

$$\kappa =_{\text{def}} \frac{\mathrm{d}\theta}{\mathrm{d}s},\tag{3.1}$$

where s is the length of the arc. In the standard theory of beam bending the moment-curvature relationship (derived, for instance, in [28]) in the continuous setting reads

$$M = EI\kappa, \tag{3.2}$$

where E is the Young modulus of elasticity and I is the second moment of area of a shape of a beam. The product EI is referred to as the bending stiffness of a beam. Note that (3.2) can be viewed as a kind of a counterpart to Hooke's law (2.8). In fact the bending stiffness EI is obviously the same for all elements  $E_i$  so relation (3.2) can be rewritten for each discrete element  $E_i$  as

$$M_i = EI\kappa_i. (3.3)$$

In the previous chapter, we considered a class of constitutive relations of the form

$$f\left(\epsilon, \dot{\epsilon}, \sigma, \dot{\sigma}\right) = 0,\tag{3.4}$$

that is capable of describing the elasto-plastic response. So it motivates us (together with (3.2)) to consider the same constitutive relation for each discrete element  $E_i$ , just instead of  $\sigma$  we use  $M_i$  and instead of  $\epsilon$  we use  $\kappa_i$ , i.e.

$$f\left(\kappa_i, \dot{\kappa}_i, M_i, \dot{M}_i\right) = 0. \tag{3.5}$$

Since we want to present a model that does not have a sharp yield point and instead smoothly transits between the elastic and inelastic response (which is required for each discrete beam element  $E_i$ ), the appropriate constitutive relation is (2.13), which in terms of the bending moment  $M_i$  and the curvature  $\kappa_i$  for each element  $E_i$  reads

$$\dot{M}_i - EI \ \dot{\kappa}_i = -EI \ H_n \left( M_i \dot{\kappa}_i \right) \left[ 1 + \tanh \left( \alpha \left( |M_i| - M_y \right) \right) \right] \dot{\kappa}_i, \tag{3.6}$$

where three adjustable parameters, namely the yield bending moment  $M_y$ , which is a counterpart to  $\sigma_y$ , the bending stiffness EI, and the parameter  $\alpha$ , are the same for each discrete element  $E_i$  and thanks to them we can simulate the hysteretic response of the beam. Since the curvature can be in the discrete setting approximated as

$$\dot{\kappa}_i \approx \frac{\dot{\theta}_i - \dot{\theta}_{i-1}}{l},\tag{3.7}$$

response equation (3.6) can be written (also using the Heaviside function properties) in the following discretized form

$$\dot{M}_{i} = \{1 - H_{n} \left( M_{i} \left( \dot{\theta}_{i} - \dot{\theta}_{i-1} \right) \right) [1 + \tanh \left( \alpha \left( |M_{i}| - M_{y} \right) \right)] \} EI \frac{\dot{\theta}_{i} - \dot{\theta}_{i-1}}{I}, \quad (3.8)$$

where i = 2, ..., N, i.e. we observe the response relation only in the inner joints of the beam. The values of the bending moments  $M_1$  and  $M_{N+1}$  in the edge nodes are determined by the boundary conditions, which are discussed later.

Let us look back at Figure 3.2. It is straightforward to deduce the following kinematic relations for the positions of the beam joints for each discrete element  $E_i$ 

$$x_{i+1} - x_i = l\cos\theta_i,\tag{3.9a}$$

$$y_{i+1} - y_i = l\sin\theta_i,\tag{3.9b}$$

where i = 1, ..., N. (These kinematic equations hold at each beam joint.) Next, equilibrium of forces described in Figure 3.2 in discrete beam element  $E_i$  implies

$$V_x^i - V_x^{i+1} - F_x^i = 0, (3.10a)$$

$$V_x^i - V_x^{i+1} - F_x^i = 0,$$

$$V_y^i - V_y^{i+1} - F_y^i = 0,$$
(3.10a)
(3.10b)

where i = 1, ..., N. Finally, we use also the balance of angular momentum in each beam element

$$M_i - M_{i+1} - M_F^i = 0, (3.11)$$

where  $M_F^i$  denotes a sum of the moments of the force acting on the element  $E_i$ . For the force **F** acting at a point **A**, the angular momentum **M** of this force with respect to a reference point **O** is defined as

$$\mathbf{M} = \mathbf{r} \times \mathbf{F},\tag{3.12}$$

where  $\mathbf{r}$  is a vector joining the reference point  $\mathbf{O}$  to the point of application of the force. The sum  $M_F^i$  consist of three parts, namely the momentum of the force  $\mathbf{V^i}$ , the momentum of the force  $\mathbf{F^i}$  and the momentum of the force  $\mathbf{V^{i+1}}$  and because of the sign convention introduced in Figure 3.1

$$M_F^i = M_{V_i}^i - M_{F_i}^i - M_{V_{i+1}}^i. (3.13)$$

Since our reference point is at the node  $[x_{i+1}, y_{i+1}]$ , where the force  $V_{i+1}$  is acting, then  $M_{V_{i+1}}^i = 0$ . Equation (3.12) gives us formulae for  $M_{V_i}^i$  and  $M_{F_i}^i$  as

$$\mathbf{M}_{F_i} = -\frac{l}{2} \begin{bmatrix} \cos \theta_i \\ \sin \theta_i \\ 0 \end{bmatrix} \times \begin{bmatrix} F_x^i \\ F_y^i \\ 0 \end{bmatrix} = -\frac{l}{2} \begin{bmatrix} 0 \\ 0 \\ F_y^i \cos \theta_i - F_x^i \sin \theta_i \end{bmatrix}, \quad (3.14)$$

from which we can immediately see that  $M_{F_i}^i = -\frac{l}{2} \left( F_y^i \cos \theta_i - F_x^i \sin \theta_i \right)$ . Similarly

$$\mathbf{M}_{V_i} = -l \begin{bmatrix} \cos \theta_i \\ \sin \theta_i \\ 0 \end{bmatrix} \times \begin{bmatrix} V_x^i \\ V_y^i \\ 0 \end{bmatrix} = -l \begin{bmatrix} 0 \\ 0 \\ V_y^i \cos \theta_i - V_x^i \sin \theta_i \end{bmatrix}, \tag{3.15}$$

which gives us that  $M_{V_i}^i = -l(V_y^i \cos \theta_i - V_x^i \sin \theta_i)$ . Substituting these formulae into (3.13) and then into (3.11) gives us the final form of the balance of angular momentum for each discrete beam element  $E_i$  as

$$M_i - M_{i+1} + \left(V_x^i - \frac{1}{2}F_x^i\right)l\sin\theta_i - \left(V_y^i - \frac{1}{2}F_y^i\right)l\cos\theta_i = 0,$$
 (3.16)

where  $i = 1, \ldots, N$ .

Finally, we can formulate a system of discretized equations, consisting discrete response equation (3.8), kinematic equations (3.9), equilibrium of forces (3.10) and the balance of angular momentum (3.16), which describes the elasto-plastic behavior of the whole beam.

$$\dot{M}_{i} = \{1 - H_{n} \left( M_{i} \left( \dot{\theta}_{i} - \dot{\theta}_{i-1} \right) \right) [1 + \tanh \left( \alpha \left( |M_{i}| - M_{y} \right) \right)] \} E I^{\frac{\dot{\theta}_{i} - \dot{\theta}_{i-1}}{l}}$$
(3.17a)

$$x_{i+1} - x_i - l\cos\theta_i = 0, (3.17b)$$

$$y_{i+1} - y_i - l\sin\theta_i = 0, (3.17c)$$

$$V_x^i - V_x^{i+1} - F_x^i = 0, (3.17d)$$

$$V_y^i - V_y^{i+1} - F_y^i = 0, (3.17e)$$

$$M_i - M_{i+1} + \left(V_x^i - \frac{1}{2}F_x^i\right)l\sin\theta_i - \left(V_y^i - \frac{1}{2}F_y^i\right)l\cos\theta_i = 0,$$
 (3.17f)

where i = 2, ..., N for (3.17a) and i = 1, ..., N for (3.17b) - (3.17f).

#### Numerical simulation of bending of inexten-3.2 sible elasto-plastic beam

Now we want to solve equations (3.17) numerically and simulate the elasto-plastic behaviour of an inextensible beam. We consider the setting, where the beam is clamped at its left end and there is a force acting at its right end as shown in Figure 3.3.

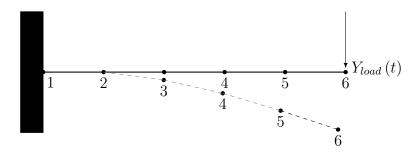


Figure 3.3: Simulation of the beam bending, where the beam is divided into five rigid elements. The beam is clamped at its left end (beam joint 1) and the force  $Y_{load}(t)$  is acting at its right end (beam joint 6).

In the simulation, we assume that there are no external forces acting on the beam. Further we have to specify the boundary conditions for the system of equations (3.17). Assuming that the origin of the coordinate system is at the beam joint 1, the following three conditions hold

$$\theta_1(t) = 0, \tag{3.18a}$$

$$x_1(t) = 0,$$
 (3.18b)

$$y_1(t) = 0.$$
 (3.18c)

The remaining three boundary conditions arise from the fact that the right end of the beam, which is at the beam joint N+1, is subject to displacement under the action of the force  $\mathbf{V}^{N+1} = \left[0, Y_{load}\left(t\right)\right]^{\mathrm{T}}$  and there are no external forces as described in Figure 3.3. These conditions are

$$M_{N+1}(t) = 0, (3.19a)$$

$$V_x^{N+1}(t) = 0, (3.19b)$$

$$V_x^{N+1}(t) = 0,$$
 (3.19b)  
 $V_y^{N+1}(t) = Y_{load}(t).$  (3.19c)

Now that we are done with the boundary conditions for the whole beam, we must further specify the initial conditions for calculation in each discrete element  $E_i$ for time t=0 (start of the simulation). Again, because we have placed our first beam joint 1 at the origin of the coordinate system and because there are no forces or moments acting on the beam at time t=0, the initial conditions are

$$x_i(0) = (i-1)l,$$
 (3.20a)

$$y_i\left(0\right) = 0,\tag{3.20b}$$

$$\theta_i(0) = 0, \tag{3.20c}$$

$$M^{i}(0) = 0,$$
 (3.20d)

$$V_x^i(0) = 0,$$
 (3.20e)

$$V_u^i(0) = 0, (3.20f)$$

for i = 1, ..., N + 1.

The last problem we have to solve is the description of the force  $Y_{load}(t)$  acting on the right end of the beam. The approach that is physically consistent is that the function  $Y_{load}(t)$  is linear up to the given time limit of  $t_{limit}$ , where the function takes the extreme value  $Y_{load}(t_{limit})$  and then from the limit time  $t_{limit}$  the force stops acting and we observe the reaction of the beam. This can be described by the equation

$$Y_{load}(t) = \begin{cases} At, & 0 < t \le t_{limit}, \\ 0, & t > t_{limit}, \end{cases}$$

$$(3.21)$$

where  $A \in \mathbb{R}^-$  is a constant (the chosen parameter) that determines the slope of the function  $Y_{load}(t)$ , i.e. the rate of loading. Negativity of the parameter A is determined by the direction of the force  $Y_{load}(t)$  in Figure 3.3.

This definition is ideal from a physical point of view, but unfortunately it is not smooth on the interval [0,T], where  $T > t_{limit}$  (the problem is at time  $t_{limit}$ ). The problem arises when the numerical software solves equation (3.17f) on the interval [0,T] and expresses the time derivative of the bending moment M so that it can be substituted into equation (3.17a). To overcome this problem, we have to redefine the function  $Y_{load}(t)$  in two steps.

In the first step, we make the function  $Y_{load}(t)$  continuous. This is achieved simply by adding a very steep transition between the extreme value of  $Y_{load}(t)$  at time  $t_{limit}$  and the constant zero value at times t after  $t_{limit}$  as

$$Y_{load}(t) = \begin{cases} At, & 0 < t \le t_{limit}, \\ Bt + (A - B) t_{limit}, & t_{limit} < t \le \frac{B - A}{B} t_{limit}, \\ 0, & t > \frac{B - A}{B} t_{limit}, \end{cases}$$
(3.22)

where  $B \in \mathbb{R}^+$  is a constant (the chosen parameter) that determines the slope of the transition between the extreme value of  $Y_{load}(t)$  at time  $t_{limit}$  and the constant zero value at times t after  $t_{limit}$ . Positivity of the parameter B is implied by negativity of A. Note that we want to take the parameter B large enough to get the steepest and fastest possible transition.

The second step is to smooth the piecewise function  $Y_{load}(t)$  defined by formula (3.22). Using the procedure described in [29], we get the smooth function on the interval [0, T] for any positive T as

$$Y_{load}(t) = K_A + \sum_{i=1}^{2} K_{B_i} \log[1 + e^{-\beta(t - \gamma_i)}], \qquad (3.23)$$

where

- $\beta$  is the chosen control parameter,
- $\gamma_1 =_{\text{def}} t_{limit}$ ,

• 
$$\gamma_2 =_{\text{def}} \frac{B - A}{B} t_{limit}$$
,

• 
$$K_A =_{\text{def}} - (B - A) \gamma_1 + B \gamma_2$$
,

• 
$$K_{B_1} =_{\operatorname{def}} \frac{B-A}{\beta}$$
,

• 
$$K_{B_2} =_{\operatorname{def}} \frac{-B}{\beta}$$
.

Figure 3.4 shows an example of the function defined by (3.23) with different values of  $\beta$ .

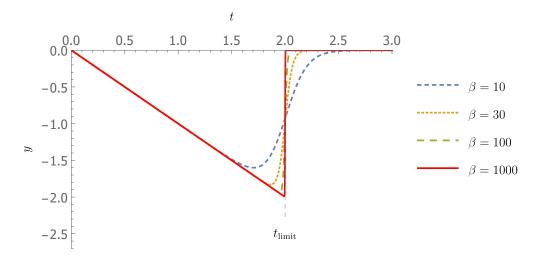


Figure 3.4: An example of functions given by (3.23) for several different values of  $\beta$  for A = -1,  $B = 10^5$  and  $t_{limit} = 2$ . We can see that the larger  $\beta$  values, the more similar the function is to the definition of the piecewise function (3.22).

Now we have completed the full description of the model given in Figure 3.3 and together with the corresponding system of equations (3.17), the boundary conditions (3.18) - (3.19), the initial conditions (3.20) and the loading function (3.23) and after specifying all needed parameters, we can simulate the behavior of the beam.

Two possibilities may now arise depending on the yield moment  $M_y$ . The first is that in all discrete elements  $E_i$ , the bending moment  $M_i$  is less than  $M_y$  so equation (3.17a) results in the time-differentiated moment-curvature relation-ship (3.3). This is something similar to what we have already examined in the previous chapter and we got the elastic response of the material as discussed and shown in Figure 2.4 and Figure 2.5. This situation is described in the first subsection. On the other hand, in the second subsection we discuss the second possibility, that is that the parameter  $M_y$  is chosen so that some bending moments  $M_i$  reach the yield value  $M_y$  and we follow an analogy of the plastic deformation, which we observed in the previous chapter in Figure 2.10 and Figure 2.11.

### 3.2.1 Elastic response

First, we want to show that for a suitably chosen parameter  $M_y$ , which is together with the other parameters defined in Table 3.1, we get the purely elastic response of the beam in our numerical simulation. The value of N is the highest on which the simulation went through using **Mathematica** version 10.3.

Parameter	Value
N	14
$\parallel$ L	14
$\parallel t_{limit}$	2
$\parallel$ $n$	$10^{11}$
$\parallel$ $\alpha$	30
$\parallel M_y$	10
$\parallel$ $EI$	5
$\beta$	$10^{3}$
$\ $ A	-1
B	$10^{5}$

Table 3.1: Parameter values for the first simulation. (Parameter values are given in a dimensionless form.)

We are interested in how the shape of the beam changes (i.e. how the position of the coordinates  $x_i$ ,  $y_i$  for each discrete beam element  $E_i$  changes) on a certain time interval [0, T]. Numerical calculations were done on the interval [0, 100], but interesting things happen on a substantially shorter time interval. Hence the following figures are plotted for T = 10.

Let us look first at the time evolution of the position of the end beam joint in Figure 3.5 and Figure 3.6. These figures should give us an idea whether we have chosen the appropriate parameter  $M_y$  (i.e. big enough) and if our response is indeed elastic. However, we check this explicitly in Figure 3.7, where we show that on our time interval [0, 10], none of the bending moments  $M_i$ , which corresponds to the inner beam joints, is larger than the yield bending moment  $M_y$ , i.e. there is no plastic deformation. In the last Figure 3.8, we look at the shape of the beam at several different time instants.

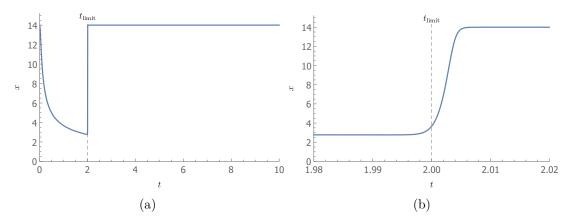


Figure 3.5: Figure (a) shows the x-position of the end beam joint (in our case it is  $x_{15}$ ) as a function of time. Figure (b) shows the x-position of the node  $x_{15}$  as a function of time on a short time interval including  $t_{limit}$ .

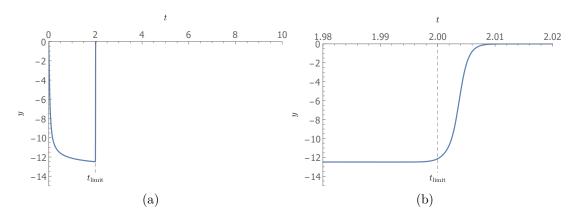


Figure 3.6: Figure (a) shows the y-position of the end beam joint (in our case it is  $y_{15}$ ) as a function of time. Figure (b) shows the y-position of the node  $y_{15}$  as a function of time on a short time interval including  $t_{limit}$ .

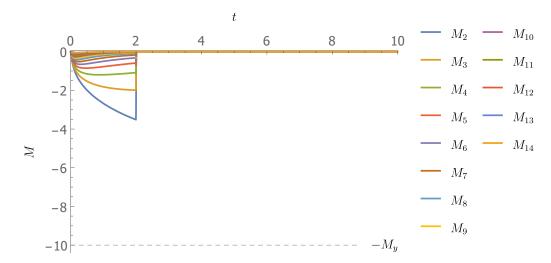


Figure 3.7: Values of the bending moments  $M_i$  of the inner beam joints (i.e. i = 2, 3, ..., 14 in our case) as a function of time. We can see that none of the moments in the absolute value reaches the value of  $M_y$ . Parameter  $t_{limit}$  is chosen as  $t_{limit} = 2$ .

In Figure 3.5, Figure 3.6 and Figure 3.7 we can see that we are actually observing the elastic response of the material - especially in Figure 3.7 we see that there is no inner beam joint i in the beam, for which the corresponding bending moment  $M_i$  reaches the value of the yield bending moment  $M_y$ . This leads to the fact that the right-hand side of discretized response equation (3.17a) does not contain "plastic" terms, that is, only the terms characterizing elasticity left. We also see that when the force stops acting (i.e. at time  $t > t_{limit} = 2$ ), we observe that the values of bending moments  $M_i$  in all internal nodes of the beam very quickly reach zero. In Figure 3.5 and Figure 3.6 we notice, that when the force stops acting, the beam returns to its original position very quickly. These observations are also documented in Figure 3.8 that shows the shape of the beam at various time instants.

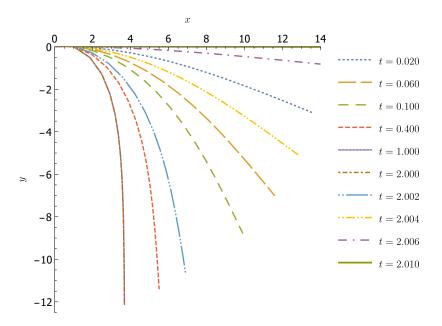


Figure 3.8: The shape of the beam as a function of time. We observe the elastic behavior of the material - the beam quickly returns to its original position after unloading. Value of  $t_{limit}$  is chosen as  $t_{limit} = 2$ .

Figure 3.8 can be seen as one of the two main results of this chapter and the thesis itself. It is a numerical verification of a physical model of beam bending described in Figure 3.3 and mathematically formulated in a discretized version by equations (3.17) with the relevant boundary conditions (3.18) and (3.19) and initial conditions (3.20). As we have shown in Figure 3.7, there is no bending moment  $M_i$  of the inner beam joints in our simulation, that reaches in the absolute value the critical value given by the parameter  $M_y$ . This gives us an a priori estimate that we observe the purely elastic behavior of the beam, which is verified in Figure 3.8.

As can be seen in Figure 3.8, even though the force is applied up to time  $t_{limit}$ , the beam at time t = 1 already reaches its critical position in which it remains until time  $t_{limit}$ . As soon as the force stops acting, we observe a rapid reaction of the beam as the material returns to its original position very quickly.

## 3.2.2 Elasto-plastic response

Our second simulation is based on the parameter values shown in Table 3.2. The parameters in this table (especially  $M_y$ ) are chosen in that way that we can observe the elasto-plastic behavior of the beam as shown in the following figures. The value of N is the highest on which the simulation went through using Mathematica version 10.3.

Parameter	Value
N	14
$\parallel$ L	14
$\parallel t_{limit}$	2
$\parallel$ $n$	$10^{11}$
$\parallel$ $\alpha$	30
$M_y$	1
$\parallel$ $EI$	5
$\beta$	$10^{3}$
$\ $ A	-1
B	$10^{5}$

Table 3.2: Parameter table for the second simulation. (Parameter values are given in a dimensionless form.)

We are therefore interested in how the shape of the beam changes on a certain time interval [0, T]. Let us look first at the time evolution of the position of the end beam joint in Figure 3.9 and Figure 3.10. As in the previous simulation, these figures should give us information whether we have chosen the appropriate parameter  $M_y$ . This is further verified in Figure 3.11. In the last Figure 3.12 the shape of the beam is shown at several different time instants. Again we chose T = 10.

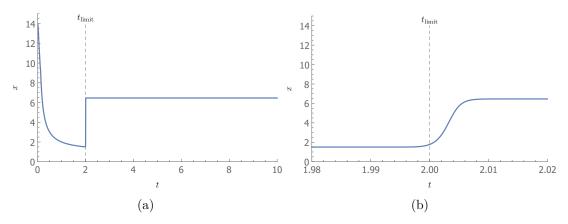


Figure 3.9: Figure (a) shows the x-position of the end beam joint (in our case it is  $x_{15}$ ) as a function of time. Figure (b) shows the x-position of the node  $x_{15}$  as a function of time on a short time interval including  $t_{limit}$ .

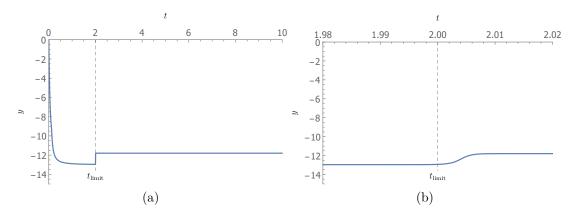


Figure 3.10: Figure (a) shows the y-position of the end beam joint (in our case it is  $y_{15}$ ) as a function of time. Figure (b) shows the y-position of the node  $y_{15}$  as a function of time on a short time interval including  $t_{limit}$ .

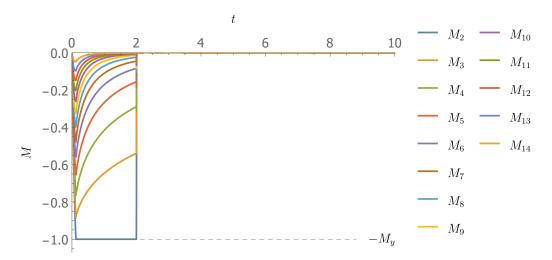


Figure 3.11: Values of the bending moments  $M_i$  of the inner beam joints (i.e. i = 2, 3, ..., 14 in our case) as a function of time. We can see that the moment  $M_2$  reaches the value of  $-M_y$ , but none of the moments exceeds it.

In Figure 3.9, Figure 3.10 and Figure 3.11 we see that, unlike the previous simulation, we now observe the plastic response of the material. Especially in Figure 3.11 we see that in the beam joint 2, the corresponding bending moment  $M_2$  reaches the value of the yield bending moment  $M_y$  (more precisely, the absolute value of  $M_2$  is equal to  $M_y$ ). This implies that the right-hand side of discretized response equation (3.17a) contains "plastic" terms. In Figure 3.9 and Figure 3.10 we notice that when the force stops acting, the beam quickly reaches a static position, but different from the original position - we observe the plastic deformation. These statements are further documented in Figure 3.12 that shows the shape of the beam at various time instants.

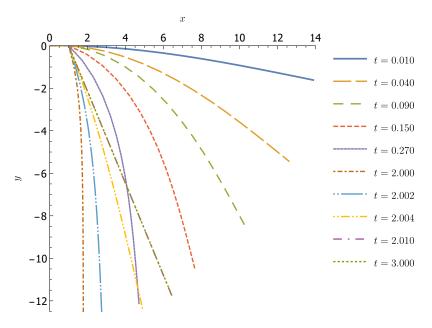


Figure 3.12: The shape of the beam as a function of time. We observe the plastic response of the material - the beam quickly reaches the deformed position where it remains after unloading. The shape of the beam at t = 2.010 is almost identical to the shape of the beam at t = 3.000.

Figure 3.12 shows the second main results of this chapter. The only difference in this simulation compared to the previous one is that we took the lower value of the parameter  $M_y$ . However, as is shown in Figure 3.11, the bending moment of the first inner beam joint  $M_2$  reaches the yield bending moment, specifically  $-M_y$ . Based on the theory that we have built, this gives us an a priori estimate that we observe the elasto-plastic behavior of the material, which is verified in Figure 3.12.

During the time interval when the force is acting at the right end of the beam (i.e.  $t \leq t_{limit} = 2.000$ ), the beam is bent to its critical position. Subsequently, when the force stops acting, we can observe the effort of the beam to return to its original position, but unlike the previous simulation, this does not happen. Already at time t = 2.010, the beam remains in a deformed bent position, in which it remains permanently (as shown at time t = 3.000, there is no further displacement of the beam position). Thus, we observe the elasto-plastic response of the beam.

# 4. Three-dimensional analogy of elastic-perfectly plastic response

In Chapter 2, we have developed a constitutive relation (2.9), which describes the elastic-perfectly plastic response of the material in the one-dimensional setting. The aim of this final chapter is to derive a similar constitutive relation for three-dimensional isotropic solids and to provide a thermodynamic basis for such a constitutive relation. We achieve this by a similar procedure based on thermodynamics as we did in Chapter 1, where we worked with the hyperelastic material. An important part of our approach is, as in Chapter 2, that we want to avoid calculations involving plastic strain.

## 4.1 Thermodynamic framework for plasticity

#### 4.1.1 Preliminaries

Let us introduce the corotational derivative, which is for a matrix  $\mathbb{A}$  defined as

$$\stackrel{\triangle}{\mathbb{A}} =_{\text{def}} \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} - \mathbb{W}\mathbb{A} + \mathbb{A}\mathbb{W}, \tag{4.1}$$

where W is the skew-symmetric part of the velocity gradient L, that is

$$W =_{\operatorname{def}} \frac{1}{2} \left( \mathbb{L} - \mathbb{L}^{\mathrm{T}} \right). \tag{4.2}$$

The corotational derivative given by definition (4.1) means that the rate is calculated with respect to a frame that is rotated. Furthermore, the equality  $\mathbb{B} = \mathbf{0}$ , proven in (1.79), together with the fact that  $\mathbb{W}$  is the skew-symmetric tensor and  $\mathbb{D}$  is the symmetric tensor yields

$$\overset{\triangle}{\mathbb{B}} = \frac{d\mathbb{B}}{dt} - \mathbb{W}\mathbb{B} + \mathbb{B}\mathbb{W} = \frac{d\mathbb{B}}{dt} - (\mathbb{L} - \mathbb{D}) \,\mathbb{B} - \mathbb{B} \,(\mathbb{L} - \mathbb{D})^{\mathrm{T}} = 
= \overset{\nabla}{\mathbb{B}} + \mathbb{D}\mathbb{B} + \mathbb{B}\mathbb{D} = \mathbb{D}\mathbb{B} + \mathbb{B}\mathbb{D}.$$
(4.3)

The classical elastoplasticity (see, for example, [30, p. 165]) is based on a decomposition of the deformation gradient  $\mathbb{F}$  into the elastic and plastic part. The decomposition takes the form of the multiplicative decomposition of  $\mathbb{F}$  as

$$\mathbb{F} = \mathbb{F}_e \mathbb{F}_p, \tag{4.4}$$

where  $\mathbb{F}_e$  is the elastic part of the deformation gradient and  $\mathbb{F}_p$  is the plastic part of the deformation gradient. Based on this decomposition, we can define the elastic part of the left Cauchy–Green tensor  $\mathbb{B}_e$  as

$$\mathbb{B}_e =_{\operatorname{def}} \mathbb{F}_e \mathbb{F}_e^{\operatorname{T}}. \tag{4.5}$$

Motivated by relation (1.78) we denote the term  $\frac{d\mathbb{F}_p}{dt}\mathbb{F}_p^{-1}$  as  $\mathbb{L}_p$ . Note that here we do not use the term definition for this relation, but only denotation as  $\mathbb{L}_p$  does

not have any direct physical meaning unlike the velocity gradient  $\mathbb{L}$ . Having  $\mathbb{L}_p$ , we define the plastic strain rate  $\mathbb{D}_p$  as

$$\mathbb{D}_p =_{\operatorname{def}} \frac{1}{2} \left( \mathbb{L}_p + \mathbb{L}_p^{\mathrm{T}} \right). \tag{4.6}$$

Next, we find a similar evolution equation for  $\mathbb{B}_e$  as we did it already for  $\mathbb{B}$  in (4.3). For that we also need a formula for the time derivative of the matrix inverse, which for an invertible matrix  $\mathbb{A}$  is

$$\frac{\mathrm{d}\mathbb{A}^{-1}}{\mathrm{d}t} = -\mathbb{A}^{-1} \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} \mathbb{A}^{-1}.$$
 (4.7)

Now using formulae (4.4), (4.5), (4.6) and (4.7) we can express  $\frac{d\mathbb{B}_e}{dt}$  as

$$\frac{d\mathbb{B}_{e}}{dt} = \frac{d}{dt} \left( \mathbb{F}_{e} \mathbb{F}_{e}^{T} \right) = \frac{d\mathbb{F}_{e}}{dt} \mathbb{F}_{e}^{T} + \mathbb{F}_{e} \frac{d\mathbb{F}_{e}^{T}}{dt} = \frac{d}{dt} \left( \mathbb{F} \mathbb{F}_{p}^{-1} \right) \mathbb{F}_{e}^{T} + \mathbb{F}_{e} \frac{d}{dt} \left( \mathbb{F}_{p}^{-T} \mathbb{F}^{T} \right) =$$

$$= \mathbb{L} \mathbb{B}_{e} + \mathbb{B}_{e} \mathbb{L}^{T} - \mathbb{F}_{e} \frac{d\mathbb{F}_{p}}{dt} \mathbb{F}_{p}^{-1} \mathbb{F}_{e}^{T} - \mathbb{F}_{e} \left( \frac{d\mathbb{F}_{p}}{dt} \mathbb{F}_{p}^{-1} \right)^{T} \mathbb{F}_{e}^{T} =$$

$$= \mathbb{L} \mathbb{B}_{e} + \mathbb{B}_{e} \mathbb{L}^{T} - 2\mathbb{F}_{e} \mathbb{D}_{p} \mathbb{F}_{e}^{T}. \tag{4.8}$$

Substituting this result into the definition of  $\widehat{\mathbb{B}}_e$  and performing the same manipulation as in (4.3) implies the evolution equation for  $\mathbb{B}_e$  as

$$\stackrel{\triangle}{\mathbb{B}}_e = \mathbb{D}\mathbb{B}_e + \mathbb{B}_e\mathbb{D} - 2\mathbb{F}_e\mathbb{D}_p\mathbb{F}_e^{\mathrm{T}}.$$
(4.9)

Furthermore, we write for better clarity the evolution equation for  $\mathbb{B}$  (4.3) and the evolution equation for  $\mathbb{B}_e$  (4.9) below each other

$$\hat{\mathbb{B}} = \mathbb{DB} + \mathbb{BD}, \tag{4.10a}$$

$$\overset{\triangle}{\mathbb{B}}_e = \mathbb{D}\mathbb{B}_e + \mathbb{B}_e\mathbb{D} - 2\mathbb{F}_e\mathbb{D}_p\mathbb{F}_e^{\mathrm{T}}.$$
(4.10b)

Note that equation (4.10b) implies, that the tensor  $\stackrel{\triangle}{\mathbb{B}}_e$  is symmetric.

In our approach, we want to avoid direct calculations involving plastic quantities such as  $\mathbb{D}_p$  in (4.10b). Comparing equation (4.10a) with equation (4.10b) gives us an idea of rewriting them as one common equation, which is consistent with both evolution equations for  $\mathbb{B}$  and  $\mathbb{B}_e$ . The natural candidate is an equation in the form

$$\stackrel{\triangle}{\mathbb{B}}_e = \mathbb{D}\mathbb{B}_e + \mathbb{B}_e\mathbb{D} + \mathbb{X},\tag{4.11}$$

where  $\mathbb{X}$  denotes a tensor, which we want to determine now. To preserve the symmetry of the tensor  $\mathbb{B}_e$ , our first requirement for the tensor  $\mathbb{X}$  is to be symmetrical as well. The reason for defining the evolution equation this way stems from the fact that if  $\mathbb{X} = \mathbf{0}$ , then the evolution equation of  $\mathbb{B}_e$  of the form (4.11) coincides with the evolution equation of  $\mathbb{B}$  given by (4.10a).

### 4.1.2 Specific Helmholtz free energy

We assume that the specific Helmholtz free energy is given by the formula

$$\psi =_{\operatorname{def}} \psi \left( \theta, \mathbb{B}_e \right). \tag{4.12}$$

Recall the relation between the specific Helmholtz free energy  $\psi$ , the specific internal energy e and the specific entropy  $\eta$  in terms of  $\mathbb{B}_e$  as a counterpart to (1.4) as

$$\psi(\theta, \mathbb{B}_e) = e(\eta, \mathbb{B}_e) \Big|_{\eta = \eta(\theta, \mathbb{B}_e)} - \theta \eta(\theta, \mathbb{B}_e), \tag{4.13}$$

which in fact is the Legendre transformation of the specific internal energy.

Substituting (4.13) into the evolution equation for the specific internal energy of the form (1.11) only with a slight change that  $e =_{\text{def}} e(\eta, \mathbb{B}_e)$  yields

$$\rho \left( \frac{\partial \psi}{\partial \theta} \frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{\partial \psi}{\partial \mathbb{B}_e} : \frac{\mathrm{d}\mathbb{B}_e}{\mathrm{d}t} + \frac{\mathrm{d}\theta}{\mathrm{d}t} \eta + \theta \frac{\mathrm{d}\eta}{\mathrm{d}t} \right) = \mathbb{T} : \mathbb{D} - \mathrm{div} \, \mathbf{j}_e. \tag{4.14}$$

Further using the formula  $\frac{\partial \psi}{\partial \theta} = -\eta$ , we obtain the standard evolution equation for the specific entropy in the form

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{\theta} \left( \mathbb{T} : \mathbb{D} - \rho \frac{\partial \psi}{\partial \mathbb{B}_e} : \frac{\mathrm{d}\mathbb{B}_e}{\mathrm{d}t} - \mathrm{div}\,\mathbf{j}_e \right),\tag{4.15}$$

as a counterpart of the evolution equation (1.12). Now we want to modify this equation in such a way that it includes  $\mathbb{D}$  and the corotational derivative of  $\mathbb{B}_e$ . In the first step, we want to substitute the corotational derivate of  $\mathbb{B}_e$  into this equation. The obvious way how to do it is by modifying the term  $\frac{\partial \psi}{\partial \mathbb{B}_e}$ :  $\frac{d\mathbb{B}_e}{dt}$  because the definition (4.1) of  $\mathbb{B}_e$  implies

$$\frac{\partial \psi}{\partial \mathbb{B}_e} : \frac{\mathrm{d}\mathbb{B}_e}{\mathrm{d}t} = \frac{\partial \psi}{\partial \mathbb{B}_e} : \left( \stackrel{\triangle}{\mathbb{B}}_e + \mathbb{W}\mathbb{B}_e - \mathbb{B}_e \mathbb{W} \right). \tag{4.16}$$

Next, we want to evaluate the matrix scalar product on the right-hand side of (4.16). Theorem 1 implies that

$$\frac{\partial \psi}{\partial \mathbb{B}_e} = \sum_{n=1}^3 \frac{\partial \psi}{\partial I_i} \frac{\partial I_i}{\partial \mathbb{B}_e},\tag{4.17}$$

where  $I_i$ , i = 1, 2, 3, are the matrix invariants of  $\mathbb{B}_e$ . Using formulae (1.7) for the derivatives of matrix invariants together with the fact that  $\mathbb{B}_e$  is the symmetric tensor yields

$$\frac{\partial \psi}{\partial \mathbb{B}_e} = \frac{\partial \psi}{\partial I_1} \mathbb{I} + I_1 \frac{\partial \psi}{\partial I_2} \mathbb{I} - \frac{\partial \psi}{\partial I_2} \mathbb{B}_e + I_3 \frac{\partial \psi}{\partial I_3} \mathbb{B}_e^{-1}. \tag{4.18}$$

Substituting (4.18) into (4.16) together with the cyclic property of the trace (i.e. for matrices  $\mathbb{A}$  and  $\mathbb{B}$  the equality  $\operatorname{Tr}(\mathbb{AB}) = \operatorname{Tr}(\mathbb{BA})$  holds) implies

$$\frac{\partial \psi}{\partial \mathbb{B}_e} : \frac{\mathrm{d}\mathbb{B}_e}{\mathrm{d}t} = \frac{\partial \psi}{\partial \mathbb{B}_e} : \overset{\triangle}{\mathbb{B}}_e. \tag{4.19}$$

Moreover, having expression (4.18) we notice, that  $\frac{\partial \psi}{\partial \mathbb{B}_e}$  commutes with  $\mathbb{B}_e$ .

In the second step, we want to deal with the symmetric part of the velocity gradient  $\mathbb{D}$ . We want to express  $\mathbb{D}$  from equation (4.11), so that we can substitute it into equation (4.15). For this we need the following theorem (see, for example, [31, pp. 7–8]).

**Theorem 8** (Solution of the algebraic Lyapunov equation). Let  $\mathbb{A}$  and  $\mathbb{Q}$  be given matrices and suppose that all the eigenvalues of the matrix  $\mathbb{A}$  have negative real parts. Then equation

$$\mathbb{A}^{\mathrm{T}}\mathbb{P} + \mathbb{P}\mathbb{A} = -\mathbb{Q} \tag{4.20}$$

has a unique solution

$$\mathbb{P} = \int_{\tau=0}^{\infty} e^{\tau \mathbb{A}^{\mathrm{T}}} \mathbb{Q} \ e^{\tau \mathbb{A}} \ \mathrm{d}\tau. \tag{4.21}$$

Since  $\mathbb{B}_e$  is the symmetric positive definite matrix, then all eigenvalues of the matrix  $-\mathbb{B}_e$  are negative (and real). We see that if we rewrite (4.11) as

$$(-\mathbb{B}_e)^{\mathrm{T}} \mathbb{D} + \mathbb{D} (-\mathbb{B}_e) = -\left(\stackrel{\triangle}{\mathbb{B}}_e - \mathbb{X}\right), \tag{4.22}$$

we obtain the  $algebraic\ Lyapunov\ equation$  as in (4.20). Then Theorem 8 implies that

$$\mathbb{D} = \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \left( \stackrel{\triangle}{\mathbb{B}}_e - \mathbb{X} \right) e^{-\tau \mathbb{B}_e} d\tau.$$
 (4.23)

Now substituting (4.19) and (4.23) into (4.15) yields

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{\theta} \left\{ \underbrace{\mathbb{T} : \left[ \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \left( \stackrel{\triangle}{\mathbb{B}}_e - \mathbb{X} \right) e^{-\tau \mathbb{B}_e} \, \mathrm{d}\tau \right]}_{\mathbf{I}} - \underbrace{\rho \frac{\partial \psi}{\partial \mathbb{B}_e} : \stackrel{\triangle}{\mathbb{B}}_e}_{\mathbf{II}} - \underbrace{\mathrm{div} \, \mathbf{j}_e}_{\mathbf{III}} \right\}. \tag{4.24}$$

The right-hand side of equation (4.24) is divided into three terms I, II and III. First, we want to manipulate term I and term II. At this moment, we leave term III unchanged.

Let us start with term I. The definition of the matrix scalar product (1.19a), the fact that for two (real) matrices  $\mathbb A$  and  $\mathbb B$  the equality  $\mathbb A:\mathbb B=\mathbb B:\mathbb A$  holds and the symmetry of the Cauchy stress tensor  $\mathbb T$  implies that term I can be rewritten as

$$\operatorname{Tr}\left[\left(\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_{e}} \left(\stackrel{\triangle}{\mathbb{B}}_{e} - \mathbb{X}\right) e^{-\tau \mathbb{B}_{e}} \, d\tau\right) \mathbb{T}\right]. \tag{4.25}$$

Since the trace of the matrix product is by definition a finite sum, we can exchange the integral and the trace, which together with the cyclic property of the trace yields

$$\int_{\tau=0}^{\infty} \operatorname{Tr} \left[ \mathbb{T} e^{-\tau \mathbb{B}_e} \left( \stackrel{\triangle}{\mathbb{B}}_e - \mathbb{X} \right) e^{-\tau \mathbb{B}_e} \right] d\tau. \tag{4.26}$$

Next, we recall the fact that the cyclic property of the trace can be extended to the product of four matrices  $\mathbb{A}$ ,  $\mathbb{B}$ ,  $\mathbb{C}$  and  $\mathbb{D}$  as  $\operatorname{Tr}(\mathbb{ABCD}) = \operatorname{Tr}(\mathbb{DABC})$  which we use as

$$\int_{\tau=0}^{\infty} \operatorname{Tr} \left[ e^{-\tau \mathbb{B}_e} \, \mathbb{T} e^{-\tau \mathbb{B}_e} \left( \stackrel{\triangle}{\mathbb{B}}_e - \mathbb{X} \right) \right] d\tau. \tag{4.27}$$

The last expression can be further rewritten as

$$\operatorname{Tr}\left[\left(\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_{e}} \, \mathbb{T}e^{-\tau \mathbb{B}_{e}} \, d\tau\right) \stackrel{\triangle}{\mathbb{B}}_{e}\right] - \operatorname{Tr}\left[\left(\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_{e}} \, \mathbb{T}e^{-\tau \mathbb{B}_{e}} \, d\tau\right) \mathbb{X}\right]. \tag{4.28}$$

Using the same approach as before (but in the reverse direction), we can rewrite the previous expression as

$$\operatorname{Tr}\left[\left(\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_{e}} \, \mathbb{T}e^{-\tau \mathbb{B}_{e}} \, d\tau\right) \overset{\triangle}{\mathbb{B}}_{e}\right] - \operatorname{Tr}\left[\left(\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_{e}} \, \mathbb{X}e^{-\tau \mathbb{B}_{e}} \, d\tau\right) \mathbb{T}\right], \qquad (4.29)$$

which by the definition of the matrix scalar product (1.19a) and by the fact that  $\hat{\mathbb{B}}_{e}$  is symmetric implies that

$$I = \left( \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \, \mathbb{T} e^{-\tau \mathbb{B}_e} \, d\tau \right) : \overset{\triangle}{\mathbb{B}}_e - \mathbb{T} : \left( \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \, \mathbb{X} e^{-\tau \mathbb{B}_e} \, d\tau \right). \tag{4.30}$$

We start dealing with term II. First, we mention the following formula for calculating the definite integral

$$\int_{\tau=0}^{\infty} e^{-2\tau \mathbb{B}_e} d\tau = \left[ -\frac{1}{2} (\mathbb{B}_e)^{-1} e^{-2\tau \mathbb{B}_e} \right]_{\tau=0}^{\infty} = \frac{1}{2} (\mathbb{B}_e)^{-1}.$$
 (4.31)

Next, term II from (4.24) can be rewritten as

$$\operatorname{Tr}\left(\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \stackrel{\triangle}{\mathbb{B}}_e\right). \tag{4.32}$$

Furthermore, using equality (4.31) implies

$$\operatorname{Tr}\left(2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e \int_{\tau=0}^{\infty} e^{-2\tau \mathbb{B}_e} \, d\tau \, \stackrel{\triangle}{\mathbb{B}}_e\right), \tag{4.33}$$

which is equal to

$$\operatorname{Tr}\left(\int_{\tau=0}^{\infty} 2\rho \frac{\partial \psi}{\partial \mathbb{B}_{e}} \,\mathbb{B}_{e} \,e^{-2\tau \mathbb{B}_{e}} \,\mathrm{d}\tau \,\stackrel{\triangle}{\mathbb{B}}_{e}\right). \tag{4.34}$$

Next, we need observations that  $\mathbb{B}_e$  commutes with  $e^{-\tau \mathbb{B}_e}$ , and that  $\frac{\partial \psi}{\partial \mathbb{B}_e}$  commutes with  $e^{-\tau \mathbb{B}_e}$ . The commutative property of  $e^{-\tau \mathbb{B}_e}$  and  $\mathbb{B}_e$  can be seen from the definition of the matrix exponential

$$e^{-\tau \mathbb{B}_e} =_{\operatorname{def}} \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\tau \mathbb{B}_e \right)^n. \tag{4.35}$$

Then

$$e^{-\tau \mathbb{B}_e} \ \mathbb{B}_e = \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} (\mathbb{B}_e)^{n+1} = \mathbb{B}_e \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} (\mathbb{B}_e)^n = \mathbb{B}_e \ e^{-\tau \mathbb{B}_e}.$$
 (4.36)

The commutative property of  $\frac{\partial \psi}{\partial \mathbb{B}_e}$  and  $e^{-\tau \mathbb{B}}$  can be shown similarly, only we need to use formula (4.18) for the partial derivative of  $\psi$ . Then (4.34) is equal to

$$\operatorname{Tr}\left[\int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \left(2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e\right) e^{-\tau \mathbb{B}_e} \, \mathrm{d}\tau \, \stackrel{\triangle}{\mathbb{B}}_e\right],\tag{4.37}$$

which after using the definition of the matrix scalar product and the symmetry of  $\hat{\mathbb{B}}_e$  leads to the equality

$$II = \left( \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \left( 2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e \right) e^{-\tau \mathbb{B}_e} \, d\tau \right) : \stackrel{\triangle}{\mathbb{B}}_e$$
 (4.38)

Finally, substituting (4.30) and (4.38) into (4.24) leads to the following form of the evolution equation for the specific entropy

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{\theta} \left\{ \left[ \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \left( \mathbb{T} - 2\rho \mathbb{B}_e \frac{\partial \psi}{\partial \mathbb{B}_e} \right) e^{-\tau \mathbb{B}_e} \, \mathrm{d}\tau \right] : \mathring{\mathbb{B}}_e + \right. \\ \left. - \mathbb{T} : \left[ \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \mathbb{X} \, e^{-\tau \mathbb{B}_e} \, \mathrm{d}\tau \right] - \mathrm{div} \, \mathbf{j}_e \right\}. \quad (4.39)$$

Now we see that if  $\mathbb{X} = \mathbf{0}$ , which happens if  $\mathbb{B}_e = \mathbb{B}$ , and using the requirement that the material should not produce entropy due to mechanical processes, we get a counterpart to the constitutive relation (1.13) as

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e. \tag{4.40}$$

Now we need to specify the constitutive relation for  $\mathbb{X}$ , in such a way that the response of the material is elastic-perfectly plastic, similar to Chapter 2. We assume the Cauchy stress tensor in the form (4.40). Thus, only the following term (except the heat flux) remains on the right-hand side of the evolution equation for the specific entropy (4.39)

$$-\mathbb{T}: \left[ \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \mathbb{X} e^{-\tau \mathbb{B}_e} d\tau \right]. \tag{4.41}$$

As we want to have non-negative entropy production, we need this term to be non-negative as well. If we denote the integral part as

$$\mathbb{Y} =_{\operatorname{def}} \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \mathbb{X} \ e^{-\tau \mathbb{B}_e} \ \mathrm{d}\tau, \tag{4.42}$$

and using again Theorem 8, then X solves the algebraic Lyapunov equation

$$YB_e + B_eY = X. (4.43)$$

Next, we want to include in the constitutive equation for  $\mathbb{X}$  both elastic ( $\mathbb{X} = \mathbf{0}$ ) and perfectly-plastic ( $\mathbb{X} \neq \mathbf{0}$ ) responses. We choose our constitutive relation as a counterpart to (2.9) as

$$\mathbb{Y} =_{\text{def}} -H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_y\right) \mathbb{D},\tag{4.44}$$

where  $T_y$  is the yield stress, which is a counterpart to  $\sigma_y$  from the constitutive relation (2.9).

Substituting  $\mathbb{Y}$  of the form (4.44) into (4.41) yields

$$-\mathbb{T}: \left[ \int_{\tau=0}^{\infty} e^{-\tau \mathbb{B}_e} \mathbb{X} \ e^{-\tau \mathbb{B}_e} \ d\tau \right] = -\mathbb{T}: \mathbb{Y} = H \left( \mathbb{T} : \mathbb{D} \right) H \left( |\mathbb{T}| - T_y \right) \mathbb{T}: \mathbb{D} \ge 0,$$

$$(4.45)$$

where the non-negativity is assured thanks to the definition of the Heaviside function (2.6) and the presence of the product  $H(\mathbb{T}:\mathbb{D})\mathbb{T}:\mathbb{D}$ . However, our goal is to find the evolution equation for  $\mathbb{B}_e$ . Substituting (4.44) into (4.43) gives us

$$\mathbb{X} = -H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_y\right) \left(\mathbb{DB}_e + \mathbb{B}_e \mathbb{D}\right), \tag{4.46}$$

which after substitution into (4.11) implies that the evolution equation for  $\mathbb{B}_e$  is

$$\overset{\triangle}{\mathbb{B}}_{e} = \left[1 - H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_{y}\right)\right] \left(\mathbb{DB}_{e} + \mathbb{B}_{e}\mathbb{D}\right). \tag{4.47}$$

The updated version of the evolution equation for the specific entropy (4.39) is also useful for deriving governing equations, which is done in the following section. Substituting (4.40) and (4.45) into (4.39) yields

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{\theta} \left[ H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_y\right) \mathbb{T} : \mathbb{D} - \operatorname{div} \mathbf{j}_e \right]. \tag{4.48}$$

Let us now analyze the evolution equation (4.47), that is implied by the constitutive relation (4.44). First, we have already shown that this definition always implies non-negative entropy production. Moreover, the following two situations may occur:

(i) If  $\mathbb{T} : \mathbb{D} < 0$ , which means that the material is being unloaded or if the yield value for the stress has not been reached, i.e.  $|\mathbb{T}| < T_y$ , then (4.47) reads

$$\overset{\triangle}{\mathbb{B}}_e = (\mathbb{D}\mathbb{B}_e + \mathbb{B}_e \mathbb{D}), \tag{4.49}$$

thus  $\mathbb{B}_e$  satisfies the same evolution equation as  $\mathbb{B}$ , hence the response is elastic.

(ii) If  $\mathbb{T}: \mathbb{D} \geq 0$ , which means that the material is not being unloaded and if the yield value for the stress has been reached, i.e.  $|\mathbb{T}| = T_y$ , then (4.47) reads

$$\stackrel{\triangle}{\mathbb{B}}_e = \mathbf{0},\tag{4.50}$$

which indicates the plastic response.

Now let us take a look at the well-known von Mises yield criterion that is in a general form (see [9, p. 473]) and [32, p. 4]) defined as

$$\left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right] = 2\sigma_0^2, \tag{4.51}$$

where  $\sigma_0$  is the flow stress, which is defined as the instantaneous value of stress required to continue plastically deforming the material - to keep the material "flowing" (for example, for wires it can be determined with a tensile testing) and  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  are called principal stresses because they act on faces that have no shear stress acting upon them. The relation (4.51) can be further expressed by the definition of the stress deviator (1.19b) as

$$\sqrt{\frac{3}{2}} \left| \mathbb{T}_{\delta} \right| = \sigma_0, \tag{4.52}$$

and if we define the yield stress as  $T_y =_{\text{def}} \sqrt{\frac{2}{3}} \sigma_0$  it gives us

$$|\mathbb{T}_{\delta}| - T_y = 0, \tag{4.53}$$

which is exactly in the form of (4.44).

The von Mises yield criterion provides good predictions for most polycrystalline metals, which are metals that are composed of many crystallites of varying size and orientation and is used for modelling of rock and soil materials. This yield condition might be used, for example, for malleable iron.

# 4.2 Full system of governing equations

Now that we have found the relation for the evolution equation for  $\mathbb{B}_e$ , we further derive a full system of governing equations in the Eulerian description as an

analogy of the system of governing equations (1.89) in the implicit elastic theory. Compared to the implicit elasticity, where we had the relation (1.88) between the Hencky strain tensor  $\mathbb{H}$  and the density  $\rho$ , thanks to which we did not need the evolution equation for the density  $\rho$ , now we are in a situation where we do not have a counterpart to (1.88), and therefore the evolution equation for the density  $\rho$  must necessarily be part of governing equations. As a natural candidate for the description of the evolution of the density, the balance of mass (1.42) offers itself. We also need to deal with the specific Helmholtz free energy  $\psi$  instead of the specific Gibbs free energy g and with it we start now.

We assume the additive decomposition of the specific Helmholtz free energy into the thermal and mechanical part as

$$\psi = \psi_e \left( \mathbb{B}_e \right) + \psi_\theta \left( \theta \right), \tag{4.54}$$

where the thermal part  $\psi_{th}$  is given by the standard formula

$$\psi_{\theta}(\theta) = -c_{V,R}\theta \left[ \log \left( \frac{\theta}{\theta_R} \right) - 1 \right],$$
(4.55)

where  $c_{V,R}$  is the specific heat at the constant volume,  $\theta_R$  is the reference temperature.

Next, we substitute formula (4.55) into the evolution equation for the specific entropy (4.48) to get the evolution equation for the temperature. The standard formula

$$\eta = -\frac{\partial \psi}{\partial \theta},\tag{4.56}$$

implies that the entropy is in our case (4.54) and (4.55) given by the formula

$$\eta = c_{V,R} \log \left( \frac{\theta}{\theta_R} \right).$$
(4.57)

This implies that the evolution equation for the specific entropy (4.48) can be rewritten as the evolution equation for the temperature

$$\rho c_{V,R} \frac{\mathrm{d}\theta}{\mathrm{d}t} = H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_y\right) \mathbb{T} : \mathbb{D} - \operatorname{div} \mathbf{j}_e, \tag{4.58}$$

which can be thanks to Fourier's law (1.84) further rewritten as

$$\rho c_{V,R} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \kappa \triangle \theta + H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_y\right) \mathbb{T} : \mathbb{D}. \tag{4.59}$$

Finally, we are now in a position to summarize the obtained results. The balance of mass (1.42), the balance of linear momentum without the body force (1.75), the representation formula for the Cauchy stress tensor (4.40), the evolution equation for  $\mathbb{B}_e$  (4.47) and the evolution equation for the temperature (4.59) form the full system of governing equations in the Eulerian description for un-

knowns  $\mathbb{B}_e$ ,  $\mathbf{v}$ ,  $\theta$  and  $\rho$ .

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \,\mathrm{div}\,\mathbf{v} = 0,\tag{4.60a}$$

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T},\tag{4.60b}$$

$$\mathbb{T} = 2\rho \frac{\partial \psi}{\partial \mathbb{B}_e} \mathbb{B}_e, \tag{4.60c}$$

$$\hat{\mathbb{B}}_{e} = \left[1 - H\left(\mathbb{T} : \mathbb{D}\right) H\left(|\mathbb{T}| - T_{y}\right)\right] \left(\mathbb{DB}_{e} + \mathbb{B}_{e}\mathbb{D}\right), \tag{4.60d}$$

$$\rho c_{V,R} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \kappa \triangle \theta + H(\mathbb{T} : \mathbb{D}) H(|\mathbb{T}| - T_y) \mathbb{T} : \mathbb{D}. \tag{4.60e}$$

# 4.3 Linearization of governing equations

We show that the linearization of the evolution equation (4.60d) leads directly to the one-dimensional constitutive relation (2.9) for the elastic-perfectly plastic response which has been introduced in [4].

We use the same approach as at the end of Chapter 1. This linearization is very rough and takes into account several assumptions and simplifications. In addition to the linearized strain  $\epsilon$  we work now with the elastic part of the linearized strain tensor  $\epsilon_e$ . Moreover, we further assume that  $|\nabla U_e| \ll 1$ .

In the same way as in (1.108), where we derived that  $\mathbb{B} \approx \mathbb{I} + 2\epsilon$ , we can derive the formula for the linearized elastic part of the left Cauchy–Green tensor as

$$\mathbb{B}_e \approx \mathbb{I} + 2\epsilon_e. \tag{4.61}$$

From (1.108) we can further get that

$$\frac{\mathrm{d}\mathbb{B}}{\mathrm{d}t} \approx 2\frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t},\tag{4.62}$$

and its counterpart is

$$\frac{\mathrm{d}\mathbb{B}_e}{\mathrm{d}t} \approx 2\frac{\mathrm{d}\boldsymbol{\epsilon}_e}{\mathrm{d}t}.\tag{4.63}$$

Furthermore, we assume that

$$\frac{\mathrm{d}\mathbb{B}}{\mathrm{d}t} \approx 2\mathbb{D}.\tag{4.64}$$

Relations (4.62) and (4.64) imply that

$$\mathbb{D} \approx \frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t}.\tag{4.65}$$

Now we have completed linearization of the right-hand side of equation (4.60d) and we want to further linearize its left-hand side, where only the corotational derivative  $\hat{\mathbb{B}}_e$  occurs. From the definition of the corotational derivative (4.1) we get

$$\overset{\triangle}{\mathbb{B}}_{e} = \frac{\mathrm{d}\mathbb{B}_{e}}{\mathrm{d}t} - \mathbb{W}\mathbb{B} + \mathbb{B}\mathbb{W} \approx 2\frac{\mathrm{d}\boldsymbol{\epsilon}_{e}}{\mathrm{d}t} - \mathbb{W} + \mathbb{W} = 2\frac{\mathrm{d}\boldsymbol{\epsilon}_{e}}{\mathrm{d}t},\tag{4.66}$$

where we used only the linear term from the approximation of  $\hat{\mathbb{B}}_e$  given by (4.61) and the approximation (4.63). Thus, equation (4.60d) can be linearized as

$$\frac{\mathrm{d}\boldsymbol{\epsilon}_{e}}{\mathrm{d}t} = \left[1 - H\left(\boldsymbol{\tau} : \frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t}\right) H\left(|\boldsymbol{\tau}| - T_{y}\right)\right] \frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t}.$$
(4.67)

We are now in a situation where on the left-hand side of equation (4.67) the elastic part of the linearized strain tensor  $\epsilon_e$  appears, but on the right-hand side there is the standard linearized strain  $\epsilon$ . Therefore, now we find the relation between  $\epsilon_e$  and  $\epsilon$ , that we can rewrite equation (4.67) into a form in which only the strain  $\epsilon$  is present. Thanks to formula (4.60c), we can get an analogy of (1.113) as

$$\boldsymbol{\tau} = \lambda \left( \operatorname{Tr} \boldsymbol{\epsilon}_e \right) \mathbb{I} + 2\mu \boldsymbol{\epsilon}_e. \tag{4.68}$$

This relation leads to an analogy of (1.114) as

$$\operatorname{Tr} \boldsymbol{\tau} = (3\lambda + 2\mu) \operatorname{Tr} \boldsymbol{\epsilon}_e. \tag{4.69}$$

Substituting Tr  $\epsilon_e$  expressed from (4.69) into (4.68) gives us the inverted relation

$$\boldsymbol{\epsilon}_{e} = -\frac{\lambda}{2\mu (3\lambda + 2\mu)} (\operatorname{Tr} \boldsymbol{\tau}) \mathbb{I} + \frac{1}{2\mu} \boldsymbol{\tau}. \tag{4.70}$$

Defining the Young modulus of elasticity E and the Poisson ratio  $\nu$  in a standard way (see, for example, [33, p. 203])

$$E =_{\text{def}} \frac{\mu (3\lambda + 2\mu)}{\lambda + \mu},\tag{4.71a}$$

$$\nu =_{\text{def}} \frac{\lambda}{2(\lambda + \mu)},\tag{4.71b}$$

implies that equation (4.70) can be rewritten as

$$\boldsymbol{\epsilon}_{e} = -\frac{\nu}{E} \left( \operatorname{Tr} \boldsymbol{\tau} \right) \mathbb{I} + \frac{1+\nu}{E} \boldsymbol{\tau}. \tag{4.72}$$

Substituting (4.72) back into (4.67) gives us the desired result

$$\frac{1}{E} \left[ (1+\nu) \frac{\mathrm{d}\boldsymbol{\tau}}{\mathrm{d}t} - \nu \left( \mathrm{Tr} \left( \frac{\mathrm{d}\boldsymbol{\tau}}{\mathrm{d}t} \right) \right) \mathbb{I} \right] = \left[ 1 - H \left( \boldsymbol{\tau} : \frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t} \right) H \left( |\boldsymbol{\tau}| - T_y \right) \right] \frac{\mathrm{d}\boldsymbol{\epsilon}}{\mathrm{d}t}.$$
(4.73)

Furthermore, if the stress tensor  $\tau$  has a form

$$\boldsymbol{\tau} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma \end{bmatrix}, \tag{4.74}$$

then the  $\hat{z}\hat{z}$  component of (4.73) reads

$$\dot{\sigma} - E\dot{\epsilon} = -EH(\sigma\dot{\epsilon})H(|\sigma| - T_u)\dot{\epsilon},\tag{4.75}$$

where  $\epsilon$  denotes the  $\hat{z}\hat{z}$  component of the linearized strain tensor  $\epsilon$ . Equation (4.75) is the one-dimensional equation (2.9) that has been introduced in [4].

# Conclusion

In this thesis, we have presented and deeply investigated several implicit constitutive relations. We can say that each chapter describes in its own way certain implicit constitutive relation or the whole class of these constitutive relations.

In Chapter 1, we have explained and deduced in detail, based on the implicit constitutive relation and the standard thermodynamic framework, three-dimensional representation formula, see Theorem 5. Then we linearized this formula and we have shown an important result that linearization based on this theory of implicit constitutive relations (1.112) gives the same result as linearization based on standard elasticity (1.116).

In Chapter 2, we have thoroughly discussed a relatively new approach for the inelastic response of solids in one dimension. We have shown the implicit constitutive relation (2.9), which led to the elastic-perfectly plastic response of the material (when the yield criterion was met). This response is then thoroughly discussed in Figure 2.2 and Figure 2.3. However, this kind of material response contains sharp yield points, that are almost absent from most materials. For this reason we have formulated the (approximated) implicit constitutive relation (2.13), and we discussed it in Figure 2.10 and Figure 2.11.

In Chapter 3, which is my most significant individual contribution, we have numerically analyzed the behavior of the inextensible beam. From considerations based on kinematics, equilibrium of forces, the balance of angular momentum, the implicit response relation and discretization of the whole beam, we formulated the system of equations (3.17).

We considered a specific example. The beam was clamped at its left end and the force was acting at its right end, as described in Figure 3.3. For this process, we have formulated boundary conditions (3.18) and (3.19) and initial conditions (3.20). Depending on the value of the yield bending moment  $M_y$ , we expected two possible material responses that also occurred.

In the first case we simulated the elastic response of the beam, i.e. in any element of the beam the absolute value of the bending moment did not reach the critical value determined by the parameter  $M_y$ . How the applied force affects the beam and especially that when the force stopped acting, while the material quickly returns to its original shape without any plastic deformation, is shown in Figure 3.8.

In the second case we have chosen the parameter  $M_y$  small enough, that in some beam element (specifically the second as seen in Figure 3.11) the absolute value of the bending moment reached value of  $M_y$ . This led to the elasto-plastic response, that we observed in Figure 3.12.

The numeric code was implemented in **Mathematica** programming language. Unfortunately, it did not allow us to discretize the beam to more than only 14 elements (N=14). However, as shown in Figure 3.8 and Figure 3.12, it is sufficient to claim that we have numerically verified the bending theory, which in our case is described by the system of equations (3.17), including, inter alia, constitutive equation (3.17a).

The next steps could possibly be, for example, taking into account the different situation than described in Figure 3.3, e.g. considering external forces such

as gravity. Another possible development could be to add a curvature history parameter to equation (3.17a), which provides better simulations of materials that hardens with bending (see [5]).

Finally, in Chapter 4 we derived the implicit constitutive relation (4.60d) based on the thermodynamic framework for plasticity. In deriving this equation, as in Chapter 2, it was crucial to avoid plastic strain tensor. We have also shown that the traditional von Mises yield criterion is in line with this derived implicit constitutive relation. At the end of this chapter and also of the whole thesis, by linearizing equation (4.60d), we inferred equation (2.9), which we discussed in detail in Chapter 2.

This relatively new approach, introduced in [4], which describes the elastoplastic behavior of the material without having to identify the plastic strain, apparently has not yet delivered all its results that we can achieve, and there are other steps that can be further developed. For example, we can adjust the yield stress  $T_y$  to be temperature-dependent.

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