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Firstname Lastname

Prüfer:	Prof. Dr.-Ing. habil. P. Steinmann
Betreuer:	Dr.-Ing. S. Pfaller
Ausgabe:	DD.MM.YYYY
Abgabe:	DD.MM.YYYY

Universität Erlangen-Nürnberg
Lehrstuhl für Technische Mechanik
Prof. Dr.-Ing. habil. P. Steinmann

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Acronyms

EER evaluated strain reactions.

ER evaluated reaction.

ESR evaluated stress reactions.

FEM finite element method.

MD molecular dynamics.

MSE mean squared error.

OLR optimized load reactions.

OMP optimized material parameters.

PBC periodic boundary conditions.

RLR reference load reactions.

RMSE root mean squared error.

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1 Introduction

research questions

2 Basics

This chapter lays the foundations to understand this thesis. First molecular dynamics (MD) is simulation method is introduced. Afterwards the constitutive model is presented. In the last section the used scripting tool with its plug-in for periodic boundary conditions is explained.

2.1 Molecular dynamics

Adhesive joints are important because of XXX FÜR POLYMERE. The extension of usage in further applications depends on a profound understanding of their material behaviour. For investigations on atomistic level molecular dynamics (MD) is a widely used approach [1]. From the interactions with neighbouring atoms Newtons equation is solved for every atom. These interactions are modeled via potentials. Non-bonded interactions like van der Waals potentials are considered within a cutoff radius. The total potential energy of the system helps to identify the acting forces and accelerations of each particle. To follow the movements of the particles time integration is necessary. Usual are small time step sizes in femtoseconds what makes only small time scales possible with suitable computational costs [1]. Similar restriction holds for the system size, due to the increasing number of interactions with increasing element dimensions. However, small dimensions lead to large surface-to-volume ratios which result in significant free surface effects. To avoid them periodic boundary conditions (PBC) are used. They constrain the simulated element as if it is integrated in an infinitely large volume. To achieve this the boundaries of the system close themselves, which results in a simulation of an infinitively long concatenation of the same element in each direction [2]. Regarding the particle tracking, a particle which leaves the system at one surface enters the system then at the opposite surface. For the deformation of the whole system is restricted in a way that parallel surfaces remain parallel during loading procedures. With these adaptions the results from MD simulations can be transferred to a larger system. Thus, MD simulations allow building samples with prescribed properties followed by deformation tests to study the material behaviour [3]. During a deformation test stress and strain values are measured for every simulation time step. This leads to discrete points describing the stress and strain evolutions over the loading process. To deduce general stress-strain curves from this discrete points, a mathematical expression is required. This is done by constitutive models, which describe the general qualitative relation between stresses and strains [4]. Through material parameters the material specific properties are considered. Depending on the deformation regime for that the constitutive model holds, different material parameters are useful. Polymers are usually modeled with elastoplastic models. In the elastic regime the material parameters Young's modulus E and Poisson's ratio ν are used to specify the material. They show elastic behaviour until a yield strength is reached. Then the plastification begins which can be described by various hardening models depending on the material characteristics [4].

This work focusses on the investigations by Ries et al. [5] who studied the curing and deformation properties of epoxy through MD simulation. They developed models with

numerous mixing ratios of resin and hardener[1]. Their performed deformation tests build the motivation for the here developed optimization process. Ries et al. [5] ran uniaxial tensile tests loading a sample with a linear strain up to a maximum value of 20 %. The test sample is constrained by PBC which allow lateral contractions. To record the stress-strain response without viscous amounts they developed a procedure to approximate the quasi-static material response. Then only elastic and plastic reactions are considered. Their choice of constitutive models is based on the assumption of isotropic material behaviour. To describe the elastic material behaviour they used the Neo-Hookean hyperelasticity model. The plastic reactions are modeled via the VOCE-model which defines the stresses during the hardening process through (Zitat voce)

$$\sigma = \sigma_0 + \alpha(1 - \exp(-\beta\varepsilon_{pl})) + \gamma\varepsilon_{pl} \tag{2.1}$$

$$\sigma_0 : \text{ Yield stress}$$
$$\varepsilon_{pl} : \text{ Plastic strain}$$
$$\alpha, \beta, \gamma : \text{ Hardening parameters}$$

Together with the elastic material parameters Young's modulus E and Poison's ratio ν, six constitutive parameters are available to fit the stress-strain pairs measured through MD simulation. Their values are calculated with a minimization algorithm. The detailed procedure is described in [5]. The procedure of Ries et al. [5] is important since their data are used for the model assessment of the optimization procedure developed in this work. A detailed description of the optimization setup is given in chapter 3. In the verification studies the optimization procedure is tested with mixing ratios 4:3, 6:3 and 8:3. To evaluate its performance the optimized material parameters (OMP) are compared to the material parameter governed by Ries et al. [5]. Though a valid comparison is only possible if first the stress strain data are collected under similar loading conditions. And second the same constitutive model is used to govern the material parameter values. Thus, a detailed understanding of the methods used by Ries et al. [5] is necessary, since they are adopted to the simulation process used in this work.

- jz mit FEM weil XXXX

2.2 Finite Element Method

The finite element method (FEM) is a widely used approach for XXX. The purpose of FEM is to find solutions for field problems in complex regimes [6]. Though an analytical solution is only possible for simple problem formulations. Therefore, the FEM discretizes the regime into a finite number of elements. The element behaviour is characterized by approximation functions with a finite number of parameters. Assembling the approximation functions of all elements leads to an equation system to approximate the solution for the whole regime [7]. The FEM is mostly used in structural mechanics to provide information about forces and deformations. The general procedure of the FEM is presented in the following:

[1] The mixing rato is specified in the notation resin:hardener

1. Discretization
2. Construction of stiffness matrix
3. Coordinate transformation
4. Assembling
5. Application of boundary conditions
6. Solving equation system

In the first step we discretize the continuum in finite elements. The shape and size of the elements depend on the geometry of the regime and the required level of precision. To achieve more accurate solutions smaller elements are necessary. Then we create for every element a local stiffness matrix $\boldsymbol{K}$, which connects the acting forces $\boldsymbol{S}$ with the element deformations $\boldsymbol{u}$ via

$$\boldsymbol{S} = \boldsymbol{K} \cdot \boldsymbol{u}. \tag{2.2}$$

Although the equation holds for an element, the calculated forces and deformations are defined at the element nodes. The entries in the stiffness matrix depend on the used element type. They contain material specific information through material parameters. The stiffness matrices were constructed in local coordinate systems. To connect them, a transformation into one global system is necessary. In the fourth step the equation systems of all elements are combined into one global system. In the assembly neighbouring elements share their nodes, which needs to be considered during the construction of the global equation system. Through prescribed loadings at the boundary of the continuum certain forces or deformations are known. They are inserted in the equation system as boundary conditions. In the last step the equation system is solved. The result are the deformations for every node [6], [7].

- various geometries possible - fast simulation time - easy to use in programs - high felxibility –> various constitutitve models voreingestellt - choose const model –> define material parameters - or define material behaviour through exp data (if mat par not known, exact const model not impemented) - mesh part: denepends on geometry –> el type and sizes - apply bc - possible to read out all stress and strain values - differente element types - fieldOutput: different vaiables which describe reactions (Energy, Stress,s train, deformation, etc) - FO in all directions available - per loadstep - decided for FEM because: - fast - direct results for material response - material parameter relation - easy to construct (for case of cube) -

load step erklären

2.3 ABAQUS PDE

2.3.1 EasyPBC Plug-In

2.4 Numerical optimization

To find the values of material parameters fitting best the material behaviour measured in the MD-simulation a mathematical formulation is necessary. This leads to an optimization problem, where a calculated error (see section 3.3), defined as an objective

function of the material parameter values, should be minimized. To solve this optimization problem various mathematical algorithms are available. We decided to use the Nelder-Mead algorithm, which is a widely used gradient-free optimization algorithm [8]. In a gradient-free algorithm the derivates of the function are not included in the process. Our objective function is based on results from a finite-element-analysis, which makes it impossible to determine its derivatives directly. Therefore, only gradient-free algorithms come into account. In addition, ignoring the derivatives saves significant computational costs, which leads to fast convergence times [9]. Due to its simple structure the algorithm is a standard feature in many numerical libraries [10]. In PYTHON it is available in the SciPy.optimize minimize -function. In **??** the function call is described in detail. Here we focus on the procedure of the algorithm. The algorithm is capable to find a local minimum of a scalar function depending on n optimization variables. In this work the optimization variables are the material parameters. The definition of the objective function can be found in section 3.1. Assuming the objective function is known, the first step is to create $n+1$ points $\mathbf{P}$ in an n-dimensional space. In the initial step of the algorithm the position of the points has to be determined. This is done by an initial guess $\hat{x}$ for every optimization variable value. To process six optimization variables the initial guess would look like

$$\hat{\mathbf{x}} = [\hat{x}^0, \hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{x}^4, \hat{x}^5]$$
$$\text{with } \hat{x}^i \equiv \text{initial guess of the } i\text{-th optimization variable}$$

Based on this the initial points $\hat{\mathbf{P}}_\mathbf{i}$ are constructed. The first one is defined as $\hat{\mathbf{P}}_\mathbf{1} = \hat{\mathbf{x}}$. For the other points the value of one variable in the initial guess is changed each. The points result in an n dimensional simplex. In the next step the function values corresponding to the points $\mathbf{P}_\mathbf{i}$ are evaluated and sorted by size. The highest function value y_h thus maps the worst value combination $\mathbf{P}_\mathbf{h}$ of the optimization parameters. Afterwards a centroid of all points of the simplex except $\mathbf{P}_\mathbf{h}$ is determined. Now there are four possible operations to improve the position of $\mathbf{P}_\mathbf{h}$. Reflection and expansion of $\mathbf{P}_\mathbf{h}$ at the centroid are the first two. Before the new point $\mathbf{P}^*$ is positioned the corresponding function value needs to be evaluated. Only if y^* is smaller than y_l, $\mathbf{P}^*$ is set as new point $\mathbf{P}_\mathbf{i}$ in the simplex. If y^* is larger than y_l, the new point is even worse than $\mathbf{P}_\mathbf{h}$. Therefore, the operations contraction or shrinking have to be performed. They should find a position $\mathbf{P}^{**}$ between $\mathbf{P}_\mathbf{h}$ and its reflection $\mathbf{P}^*$ which leads to a better function value y^{**}. This needs multiple iterations because for every guess $\mathbf{P}^{**}$ the function has to be evaluated. Only when a better position $\mathbf{P}_\mathbf{h}$ is replaced by $\mathbf{P}^*$ or $\mathbf{P}^{**}$ and the algorithm starts again with the new simplex [11]. Therefore multiple function evaluations are necessary during one iteration of the optimization. If the variations of the functions values y_i fall under a certain limit, the minimum with its corresponding parameter values is found. To ensure a successful search the initial simplex should be scaled regularly [12] which is possible through a regular distribution of the points $\hat{\mathbf{P}}_\mathbf{i}$ in space. This can be difficult if the values of the optimization variables differ much in size. Therefore, it is necessary to normalize the variable values within the range of 0 to 1.

XXX muss vmtl eig in BAsics To evaluate the quality of the material parameters we need a possibility to investigate the material response caused by the definition of the material parameters. Then we can compare this results with the load parameters and evaluate the quality of the current material parameters. Thus we have to use a simulation program to analyse the material behaviour for every iteration of material parameter values during the optimisation process. We decided to use ABAQUS as simulation software, because of the intern scripting tool. With the ABAQUS scripting tool one can run python scripts directly in ABAQUS (see chapter XX). With special ABAQUS commands one can use ABAQUS with the same opportunities as with the GUI. XXXX

Therefore we choose simple load cases, which are easy to recalculate. AS explained in the chpater XX about the mathematical problem formulation, we have to define a parameter which defines the quality of the mechanical responses calculated by ABAQUS compared to the ones from the MD-simulation. Therefore we first have to define adequate mechanical measurements which represent best the mechanical behaviour and contain information about the material parameters. Hence the stress and strain measurements in all normal and shear directions are possible quantities. Depending on the load case the measurements with the most useful information may vary.

3 Models and Methods

The remarks in chapter 2 demonstrate the necessity of an easy and fast procedure to determine material parameters for materials modeled with MD simulations. Deformation tests in MD simulations provide information about the mechanical behaviour of the materials. The aim of the developed optimisation process is to find material parameters which best represent this behaviour. In the following chapter we describe workflow of the optimisation algorithm. First we have a closer look at the structure of the process. Then we introduce the required input data. At the end the implementation is explained.

3.1 Theory

In deformation tests performed with MD simulations the material behaviour during the loading process is recorded (see section 2.1). Therefore stress and strain values in all directions at discrete simulation time steps are available. In the following stress and strain data, measured during a loading process, are referenced as load reactions. In subsection 3.2.2 we present their structure in detail. To extract material parameters from these load reactions, a constitutive model is required, which describes the stress-strain relation of a material through a functional relation. The constitutive model, with its corresponding material parameters, used in this work is presented in section 2.1. Therefore an evaluation of the material parameters found by the optimisation algorithm is possible. This is done with a FEM simulation as described in section 2.2. It returns the stress strain reactions from a material corresponding its prescribed material parameters, constitutive model and the loading process. Consequently, load reactions measured in MD simulations can be compared with the ones computed in FEM. To represent the mechanical behaviour measured in MD simulations best, a small difference between the load reactions is favourable. Since the material parameters define the load reactions from FEM, their quality is implicitly measured. In other words, we have to minimize the difference between the load reactions to find the best material parameters. We use the Nelder-Mead algorithm, introduced in section 2.4, to perform this optimisation. This numerical algorithm is capable to minimize the value of a scalar function by optimizing multiple parameters. Optimising all material parameters from our constitutive model is easily possible, while the scalar minimization function poses a challenge. Its function value defines the quality of the OMP. As explained before, we use the difference between the load reactions to define the OMP quality. Since we want to fit the whole loading process, the difference at all time steps should be taken into account. To achieve this, we design a procedure, explained in section 3.3, to summarize all these differences into one error value. However, some terms need to be introduced first.

3.2 Input data

HIER VLT NOCH EIN EINLEITENDER SATZ

3.2.1 Load cases and evaluated reactions

A load case defines the direction in which a load acts. Since we want reproducible and easy cases, we only allow loading in normal and principal shear directions. We use the Abaqus plug-in EasyPBC to apply these loadings. For a consistent naming, we adopt the naming from EasyPBC for the load cases, defined in Table 3.1. To model a more complex loading situation, it is possible to apply different load cases one after another. For example, we can apply a normal strain in xx-direction followed by a shear strain in xz-direction. Nevertheless, in one load case only one direction is loaded to avoid mutual influence. The optimisation algorithm requires the load reactions without any constrains for every load case. Only PBC are applies which are described in section 2.1. After the application of a load case, we have to decide which material responses we use to compare with our load parameters. We have the possibility to read out the stresses and strains in all normal and shear directions (see Table 3.2). The quantities we choose for the comparison are called evaluated reaction. For a high result quality of our material parameters, we try to choose evaluated reaction where we can extract the most information about our material behaviour. These measurements vary depending on the applied load case. In Figure 3.1 an exemplary load case E11 (green) with possible corresponding evaluated reactions (yellow) is depicted.

Table 3.1: Mapping of load directions to load cases.

Load direction	**Load case**
xx	E11
yy	E22
zz	E33
xy	G12
yz	G23
xz	G13

Table 3.2: list of possible evaluated reactions.

Evaluated stress reactions (ESR)	**Evaluated strain reactions (EER)**
σ_{xx}	ε_{xx}
σ_{yy}	ε_{yy}
σ_{zz}	ε_{zz}
σ_{xy}	ε_{xy}
σ_{yz}	ε_{yz}
σ_{xz}	ε_{xz}

For the verification of the code we use a simple tensile load case E11. In all other directions we impose no restrictions except PBC. As evaluated reaction we use σ_{xx} and the lateral strains ε_{yy} and ε_{zz}. The normal stress contains information about the Young's modulus and the plastic parameters. The lateral strains are necessary for the identification of the Poisson's ratio. Applying a strain in xx-direction will lead to decreasing

dimensions in yy- and zz-direction. This reaction is necessary to keep a state of minimum stress. Simultaneously this means that the lateral stresses do not contain any useful information, because they are numerically zero. The validation study is realized with the same load case. Similar to the verification study we take σ_{xx}, ε_{yy} and ε_{zz} to extract information about all material parameters. In the next step we handle load case E11, then G12 and finally combine them. Through the additional obtained information we try to improve the uniqueness of the determined material parameter values. As evaluated reaction for the load case G12 we use the stresses σ_{xy}. As a last study we investigate the application of cyclic loading as E11 load case. We perform this study with varying load parameters (see subsection 3.2.2).

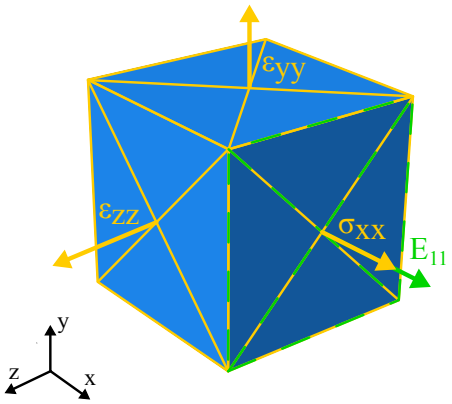


Figure 3.1: Illustration of load case and evaluated stress and strain reactions.

3.2.2 Load parameters and load reactions

For the optimisation process we use the data from MD simulations as input-file. This data are referenced as reference data in the following. They contain stress and strain values for all time steps during the loading process in all normal and shear directions. Thus, we can register different trends of loading together with the corresponding responses. We split the reference data into load parameters and reference load reactions. The load parameters define the quantitative values of the prescribed load case. Since we defined the load cases similar to the ones in the MD simulations, we can process the data from the load parameters directly. If we know the load case, we can easily extract the load parameters from the reference data and transfer them into the ABAQUS model. A detailed description of the load application in ABAQUS can be found in section 3.4. The RLR represent the material response during the MD simulation. From this, we extract the stress and strain values according to the chosen evaluated reaction. We neglect the other ones, since they probably contain little information about the material behaviour. Therefore, we exclude this useless data from our definition of the RLR. To perform the comparison of material behaviours we need analogous data from the FEM simulation. In the way described in section 3.5 we can read out stress and strain values in all directions. Similar to the reference load reactions we extract the values corresponding to the evaluated reaction. These values are called optimized load reactions.
Table 3.3 shows the investigated load cases and load parameters. In the verification and validation studies we apply linear strain up to a maximum value of 20%. In the validation

studies we use different mixing ratios which show different mechanical behaviours. In the next study we investigate a tensile strain following a sinus function over time with a maximum amplitude of 15 % strain. We only consider the first quarter of one period up to the maximum value as a preparation for studies with cyclic loading. In this preparing study we want to investigate how non-linear loadings are handled. Then we use the same load parameters but apply them as shear strain. In the next step we use the same load parameters but combine the load cases of E11 and G12. Important to notice is that the previously introduced load parameters proceed in a wide strain range. Assuming that the material starts to plastify quite fast, the majority of the loading steps are located in the plastic domain of the material. Conversely, the load parameters contain only little information about the elastic material behaviour. In section 4.1 the issue about this unequal distribution in the material domains becomes clear. As a last study we investigate a full period of a sinusoidal loading for a tensile load case in xx-direction. We use amplitudes of 1 %, 5 % and 8 %. Through the use of this load parameters we try to get a larger proportion of data points in the elastic domain.

Table 3.3: Overview of test series, load cases and load parameters.

Test series	**Load case**	**Load parameters**		**Mixing ratio**	**Evaluated reaction**
		Trajectory	**Amplitude**		
Verification	E11	Linear	20%	6:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
Validation I	E11	Linear	20%	4:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
Validation II	E11	Linear	20%	6:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
Validation III	E11	Linear	20%	8:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
Normal strain	E11	Sinus ($\frac{1}{2}\pi$)	15%	6:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
Shear strain	E11	Sinus ($\frac{1}{2}\pi$)	15%	6:3	σ_{xy}
Normal & Shear strain	E11 G12	Sinus ($\frac{1}{2}\pi$)	15%	6:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \sigma_{xy}$
Normal strain	E11	Sinus (2π)	1%	6:3	$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
			5%		$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$
			8%		$\sigma_{xx}, \varepsilon_{yy}, \varepsilon_{zz}$

3.3 Error calculation

As described in section 3.1 the numerical optimisation method requires a scalar function to minimize. Since the trend of the loading process should be represented, we need a method to condens the information of all load reactions into a single value. For a representative value we decide to build a root mean squared error (RMSE). NOCH MEHR DAZU THEORIE. First we extract the reference load reactions and the optimized load reactions in the way described in section 3.5. In the next step we have to build the difference between them. We iterate over all load steps and compute the difference between the load reactions at the current load step. Figure 3.2 displays this procedure for an

examplary set of reference load reactions and OLR. Here σ_{xx} is the selected evaluated reaction. For every load step i their corresponding reference load reactions (RLR) σ_i^{RLR} and optimized load reactions (OLR) σ_i^{OLR} is logged. The blue arrow highlights their difference $\Delta\sigma_i$ for one examplary load step, according to Equation 3.1. We square each of these differences to avoid negative values. As described in subsection 3.2.2, the distribution of the data points is unfavourable for the determination of the elastic parameters. To support the algorithm to find the elastic parameters anyway, we applied a weight of 100 at the data point in the elastic domain. In the next step we build the mean value of the weighted arrays. The resulting value is called mean squared error (MSE). We compute the MSE for one evaluated reaction according to Equation 3.2. Depending on the evaluated reaction we compute mse_σ or mse_ε. We have to compute this value for every selected evaluated reaction.

$$\Delta\sigma_i = \sigma_i^{RLR} - \sigma_i^{OLR} \qquad \Delta\varepsilon_i = \varepsilon_i^{RLR} - \varepsilon_i^{OLR} \tag{3.1}$$

$$\text{mse}_\sigma = \frac{\sum_{i=1}^{N_{LS}} w_i(\Delta\sigma_i)^2}{\sum_{i=1}^{N_{LS}} w_i} \qquad \text{mse}_\varepsilon = \frac{\sum_{i=1}^{N_{LS}} w_i(\Delta\varepsilon_i)^2}{\sum_{i=1}^{N_{LS}} w_i} \tag{3.2}$$

N_{LS} : Number of load steps $\qquad$ w_i : weight

For the tensile load case for example we must perform this for the evaluated reaction $\sigma_{xx}, \varepsilon_{yy}$ and ε_{zz}. If we now construct a single value out of these MSEs we must ensure a common scale. Otherwise, their influence on the overall error may vary significantly. Therefore, it is necessary to apply weights to the MSE of certain evaluated reaction. The exact weights depend on the load case and the used load parameter set. In general, the MSEs of evaluated strain reactions are much smaller than the ones from evaluated stress reactions, such that a weight of around 10e4 is necessary for mse_ε. After that we sum up the weighted MSE and calculate the mean value again. From this value we then compute the square root, as shown in Equation 3.3. Since our code is able to process multiple load cases in one optimisation process we can calculate the RMSE for every load case and apply weights depending on the load case. Then we sum up all these weighted RMSE values. Additionally, multiple load parameters sets can be processed which leads to a repetition of the described procedure for every load parameter set. Then we can apply weights for every load parameter set and sum it again, which results in a double sum according to Equation 3.4. This value is the one we return our minimization function. Through the adjustment of the material values this value should be minimized.
In the following sections we have a closer look at the implementation of this minimization process.

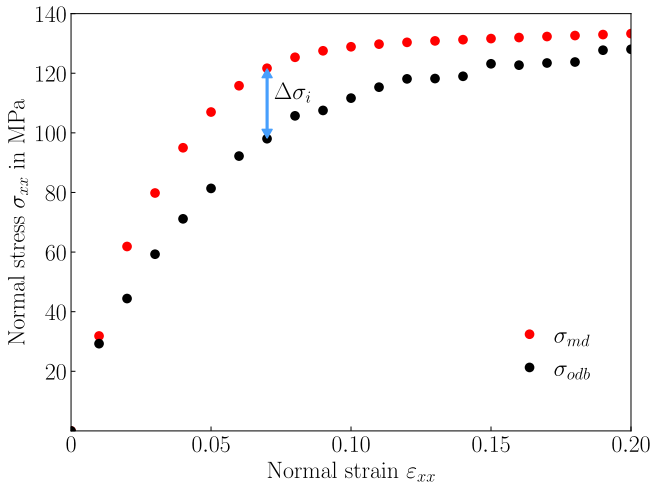


Figure 3.2: Error plot.

$$\text{rmse} = \sqrt{\frac{\sum_{\text{ESR}} w_\sigma \cdot \text{mse}_\sigma + \sum_{\text{EER}} w_\varepsilon \cdot \text{mse}_\varepsilon}{N_{\text{ESR}} + N_{\text{EER}}}} \tag{3.3}$$

$$\text{error} = \sum_{\text{LP}} \sum_{\text{LC}} w_{\text{LP}} w_{\text{LC}} \cdot \text{rmse}_{\text{LC,LP}} \tag{3.4}$$

N_{ESR} : Evaluated stress reactions

N_{EER} : Evaluated strain reactions

N_{LC} : Number of load cases

N_{LP} : Number of load parameter sets

3.4 Preprocessing

Table 3.4: Input paramters for optimisation process.

Input parameter	Directions	Category	Data format	Unit
Young's modulus	–	value	array	MPa
	–	minimum	scalar	MPa
	–	maximum	scalar	MPa
Poisson's ratio	–	value	array	–
	–	minimum	scalar	–
	–	maximum	scalar	–
Plastic Yield	–	value	array	MPa
	–	minimum	scalar	MPa
	–	maximum	scalar	MPa
Alpha, beta, gamma	–	value	array	–
	–	minimum	scalar	–
	–	maximum	scalar	–
Load parameters	–	filename	string	–
	–	weight	scalar	–
Load case	E11, E22, E33, G12, G23, G13	active	0/1	–
		weight	scalar	–
Stress evaluation	xx, yy, zz, xy, yz, xz	active	0/1	–
		weight	scalar	–
Strain evaluation	xx, yy, zz, xy, yz, xz	active	0/1	–
		weight	scalar	–
Load weighting	normal stress, normal strain, shear stress, shear strain	weight	scalar	–

As model we use a simple isotropic cube of size 1x1x1. element type

Before starting with the optimisation process, we need some preprocessing steps to prepare a working Abaqus model with the required properties. In picture XX the complete structure of the code is depicted. The upper part belongs to the preprocessing. In the first step the code extracts the values from the input file. Table **??** lists the input parameters relevant to the optimisation process. The whole input file is included in the Attachment XX. Here the user has multiple options to specify the optimisation process. It is possible to test multiple initial values for the material parameters calling the script once. This function is important to verify the optimisation results with varying input values. For every material parameter we can write an array of initial values. Then the code loops over all array entries at a time to extract one initial value for each parameter (see Table 3.5). As a consequence all arrays need to be of same length. For all the created initial value combinations the code creates a new ModeldataBase (mdb) in Abaqus and

a new folder structure to set the working directory and store the results. mean squared error (MSE)

Material Parameter	Combination 1	2	3	4	5
E	E_1	E_2	E_3	E_4	E_5
ν	ν_1	ν_2	ν_3	ν_4	ν_5
σ_{pl}	σ_{pl_1}	σ_{pl_2}	σ_{pl_3}	σ_{pl_4}	σ_{pl_5}
α	α_1	α_2	α_3	α_4	α_5
β	β_1	β_2	β_3	β_4	β_5
γ	γ_1	γ_2	γ_3	γ_4	γ_5

(a) Arrangement of initial value combination of material parameters.

Model	Load case	Load parameters
Model 0	E11	Data set 1
Model 1	E11	Data set 2
Model 2	E11	Data set 3
Model 3	G12	Data set 1
Model 4	G12	Data set 2
Model 5	G12	Data set 3

(b) Model creation for load case and parameter combinations.

Table 3.5: Loop conditions in preprocessing.

Afterwards we start to construct the model. As discussed in section XX we use a cube with size 1x1x1 as model. We mesh the cube with 6x6x6 XXXX elements. The number of elements is a compromise between a coarse mesh for fast computation and a minimum number to avoid convergence errors. Although we use the hyperelastic material law in our optimisation process, we first have to build the model with elastic material. This is necessary for the usage of EasyPBC in the next step. Now we use the load case defined in the input file to create a EasyPBC job to apply it on the cube. As discussed in chapter XXX we use EasyPBC for the automatic construction of periodic boundary conditions. We use this set up to simulate a small detail of a infinitely large area (SCHLECHT FROMULIERT). Aside from that we use the generated boundary conditions for the applied load case. Since they act at a reference point a homogeneous load contribution is ensured. –> vlt auch in basics teil.. However the settings from EasyPBC contain some default values, we have to adjust. EasyPBC applies for every load case a uniform displacement with a standard fixed value. In our optimisation we want to study cases with applied stresses as well. Additional we have to adapt the value of the load. For a correct comparison of the Abaqus data with the MD-data we have to create evaluation points at similar load increments. In Abaqus we can solve this issue by creating an amplitude. We register the evaluation points from the MD-data as steps and use this amplitude to apply the load. The value of the load is then set to 1 because it only defines the factor the amplitude is multiplied (see Figure 3.5). Afterwards we modify the increment settings. EasyPBC automatically creates increments with fixed size and without non-linear geometry effects. In order not to run into convergence errors we use automatic incrementation. Especially in the first load steps we observe large deformations. If we try to resolve such large deformations in one incrementation step Abaqus cannot resolve the step. With automatic incrementation Abaqus can adapt the number of increments per load step dynamically. The non-linear geometry effects have to be considered because of the material properties we use. As described before we build elastic material for the usage of EasyPBC. In the following the code removes this material and substitutes it with a hyper-elastic material which is suitable for high non-linear deformation. By using this material, Abaqus demands the inclusion of non-linear geometry effects. In the last step of preprocessing we store the model in a dictionary. We use this dictionary later to call the models for the optimisation. We perform the preprocessing for all prescribed load cases. This means for example if we define E11,

G12, and G23 as load cases, we create one model for each load case in the previous described manner. Furthermore, we loop over the load parameters and create separate models. In the end we have then for each combination of load case and load parameter one model.

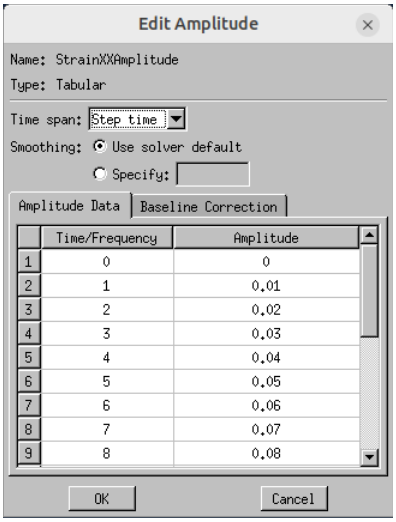


Figure 3.3: Definition of load amplitude in ABAQUS.

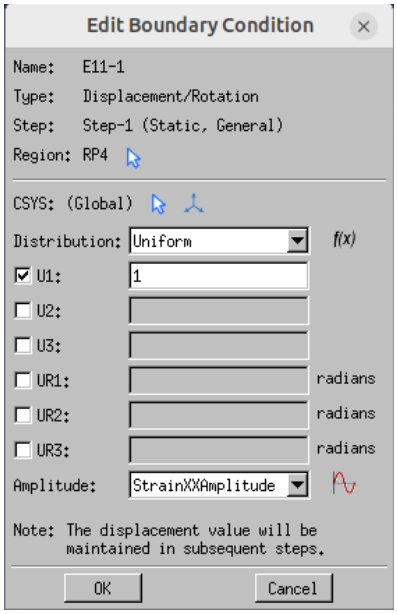


Figure 3.4: Boundary condition menu in ABAQUS.

Figure 3.5: Loop conditions in preprocessing.

3.5 Optimization process

Parameter	Content	Data format	Explanation
Objective function	Optimization function	–	Function whose scalar value should be minimized
Initial guess	Material values	array	Initial (scaled) values for the optimization parameters
Additional arguments	Cube parameters	object	Model information from input file
	Load parameters	dictionary	Load parameters from MD-simulations
	Work directory	string	Path to store results
	Evaluation counter	scalar	Counter for the performed function evaltions
method	Nelder mead	–	Mathematical algorithm to perform minimization
bounds	Minimal and maximal material values	array	Limits possible range of optimization parameters
maxiter	Number of maximum iterations	scalar	Limit for optimization iterations

Table 3.6: Input parameters for SciPy minimize function.

In the following section we describe the optimisation process. We start the processing by calling the scipy-minimize function. We pass this function various parameters to perform the optimisation listed in table XX. (MEHR ÜBER INPUT PARAMETER

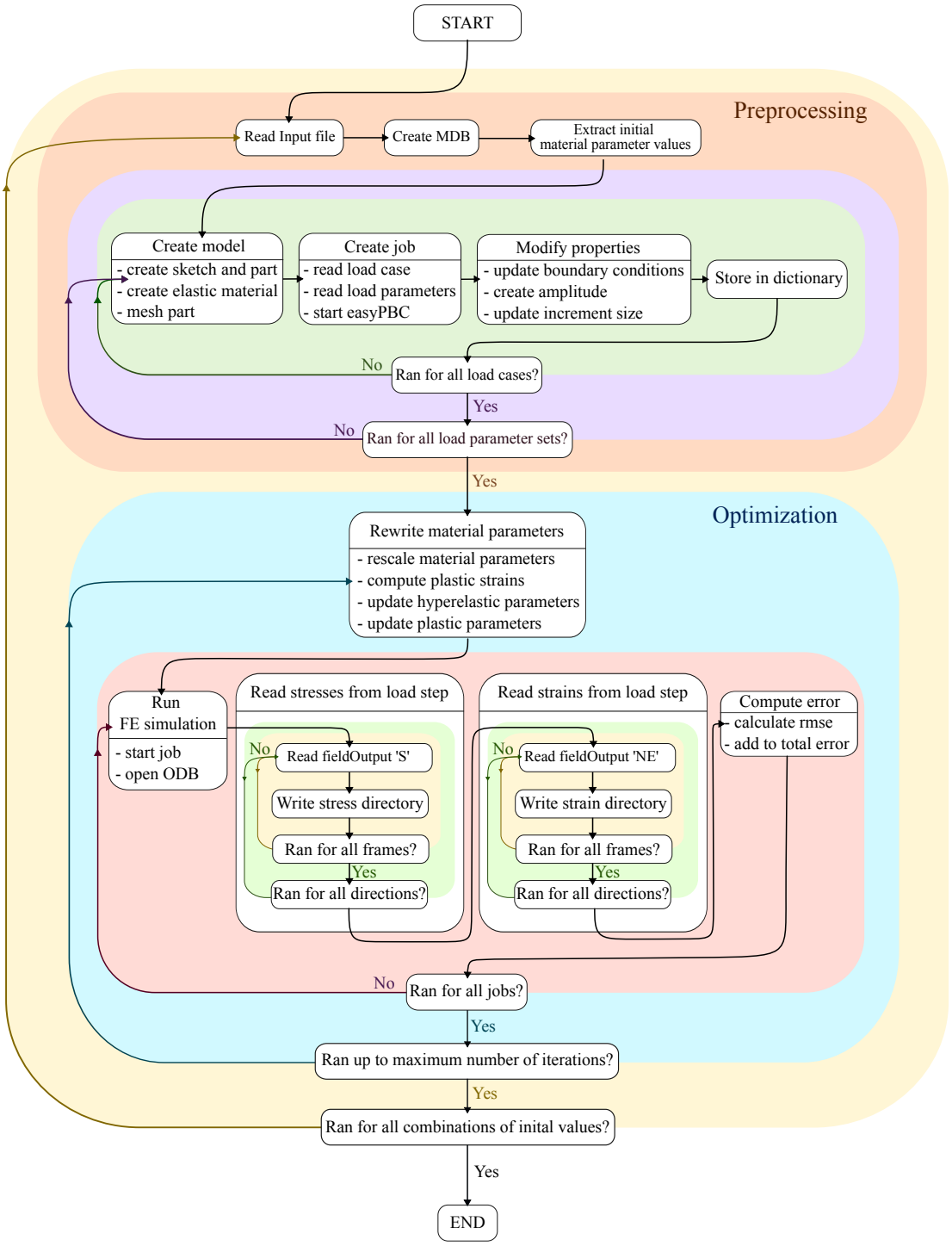


Figure 3.6: flowchart code.

INKL TABLEE) The minimize function itself calls our self-written optimisation function, where the evaluation takes place. As described before we create a model with a corresponding job for every combination of load case and load parameters and store them in a dictionary. Now we pass the whole dictionary to the optimisation function. All of the models describe now different test cases for the same material. We want to use them all to get as much information as possible, such that we have to include all of them into the optimisation process. To do so we have to calculate an error expression from all these analyses as described in section XX. We start the process with rewriting the material values in all models. Since they all describe the same material we write the same values for every model. For the minimization computation optimisation parameters are scaled in the bounds 0-1, that we have to rescale them first. Then we can use the rescaled parameters to compute the values for the plastic stress function with the formula for VOCE-hardening. Now we can update all material values. in the next step we handle the models successively. We start a job to perform the ABAQUS analysis and open the resulting output-data base. Afterwards we read the stresses from the odb. We do this by reading the fieldOutput variable 'S' and write the data in a stress directory. Since we need the stress-values at all the defined strain steps we read out every frame. One frame corresponds with one strain step. Additionally we loop over all directions (xx, yy, zz, xy, yz, xz). The same procedure is done for the strain values. Here it is important to read out the correct strain variable 'NE' (nominal strain). For hyperelastic materials ABAQUS uses as standard value the logarithmic strain ('LE'), which gives incorrect values in our studies. Then we store all values for all frames and directions in a dictionary again. Now we collected all required data to calculate the error. We do this in the way described in section XX. For a better structure of the code this part is outsourced in a separate function. We call this function and pass the stress and strain directory as well as the corresponding load parameters from the md-analysis. Then the computation runs and the function returns the rmse value for this job. Multiplied with its corresponding weights for load case and load parameters we add this value to the total error value. Now we restart the result reading and error computation for the next job. When all jobs are processed we have a total error value containing information from all jobs about the quality of the current material values. This value is the one we return our minimization function. It uses this values to compute internal the next material value combination to reduce the returned error value. Now one optimisation iteration is performed. The new combination of material values is passed to our optimisation function and it starts again. This process will run till our defined number of maximum iterations is reached.

4 Results

In this chapter the results from different test cases presented in section XX will be evaluated. First, we discuss the verification results to understand the general behavior of the optimization process. In the next step we validate the optimization performance using different data sets. Finally, we present the results of the cyclic load cases.

4.1 Verification

In this section, we discuss the results of the data set used for the verification of our optimization process. To evaluate the quality of the optimization process, we define characteristic quantities and investigate their evolution. Noch den load case kurz aufschreiben.

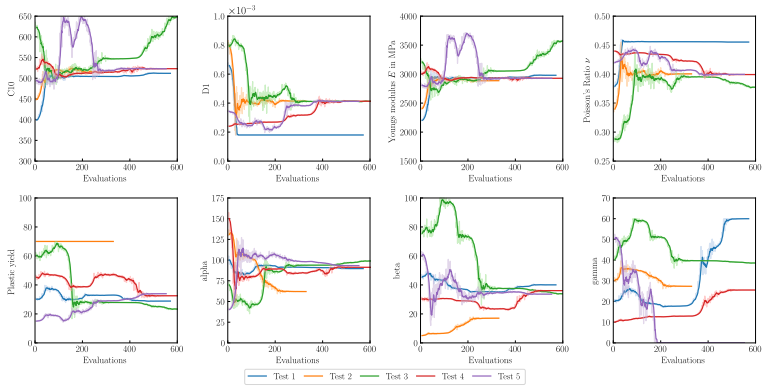
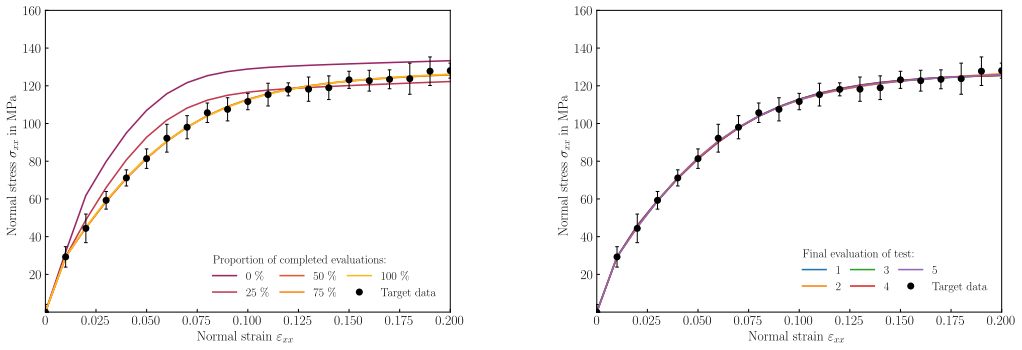


Figure 4.1: optimization progress of material parameters.

As process quantities we log the evolution of the material parameters during the optimization. Since these are our input parameters we performed multiple tests with varying parameter combinations to evaluate the stability of our program. The results are presented in 4.1. In the first row the elastic material parameters are presented. For a better understanding, we transformed the hyper-elastic parameters $C10$ and $D1$ into Young's modulus E and Poisson ratio ν. In the second row the plastic material parameters are presented. For elastic and plastic parameters we can observe convergence for every parameter combination. However, the converged solutions differ from each other for most of the combinations. For a detailed discussion of possible reasons we separate between elastic and plastic material behavior. Since our tested material shows an elastic response only up to the second data point, there might be not enough optimization points to find an unique solution for the elastic material parameters. Nevertheless, we have to investigate other characteristic quantities to ensure our assumption and understand the influence of the plastic parameters. In 4.2(a) the progress of the stress-strain curve in normal direction during one exemplary test together with the target curve from the MD simulation is presented. The optimized curve matches the target curve after only 25%

of the evaluations. Since the stress-strain curve is one of our target data this progress indicates a correct optimization behavior of our algorithm. To support this assumption the final stress-strain curves of the test series are depicted in 4.2(b). Despite the high variance of the final material parameters, the stress-strain curves all matches the target data for the stress-strain curve in normal direction. Because of this deviation we depicted the influence of the parameters on the trend of the VOCE-hardening curve shown in Figure 4.3. The parameter alpha has the greatest impact on the shape of the curve, while a variety of 50% in the parameter gamma has hardly any visible effect. This leads to a high flexibility in adjusting the shape of the curve and as a consequence to multiple possible parameter combinations to fit the target curve. To support our assumption we check the quality of the optimization result by plotting the progress of the root mean squared error (RSME) for all the tests in Figure 4.4. We observe that a common minimum RMSE value is reached in all optimization runs, indicating that the results are of equivalent quality. The results of this verification tests lead to some states about the quality of the optimization algorithm. The results of the stress-strain data show a good match of the optimized curve with the target data for every test which is confirmed by the RMSE. In contrast we observe a high variance in final the material parameters found by the algorithm. These results suggest that the algorithm can generally find parameter values to match the target data. However, the variance in these optimal parameters shows that multiple parameter combinations lead to the same quality of result. This behavior may be due to the relatively large number of optimization parameters compared to the dimension of the target data. To verify this assumption we reduced the number of material parameters. Since only the first point of the target data lies in the elastic domain, we fixed the elastic material behavior and computed them directly from the data of the first point. Then we tested this new configuration of the algorithm with the current target data and two other data sets.



(a) evolution of stress-strain curve

(b) final stress-strain curves

Figure 4.2: a) evolution of the stress-strain curves during optimization for exemplary test, b) final stress-strain curves for complete test study.

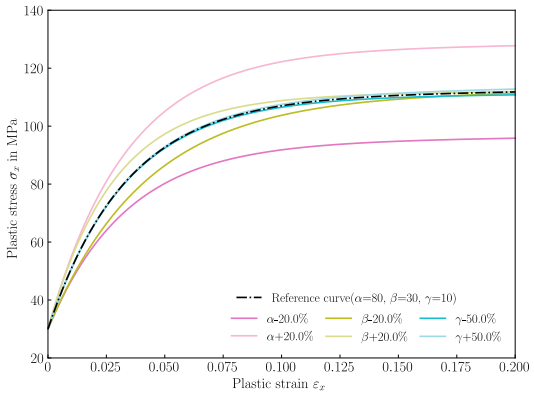


Figure 4.3: parameter influence on voce-hardening curve.

PICTURES with Krümmung und Steigung –> parameters to characterize curve

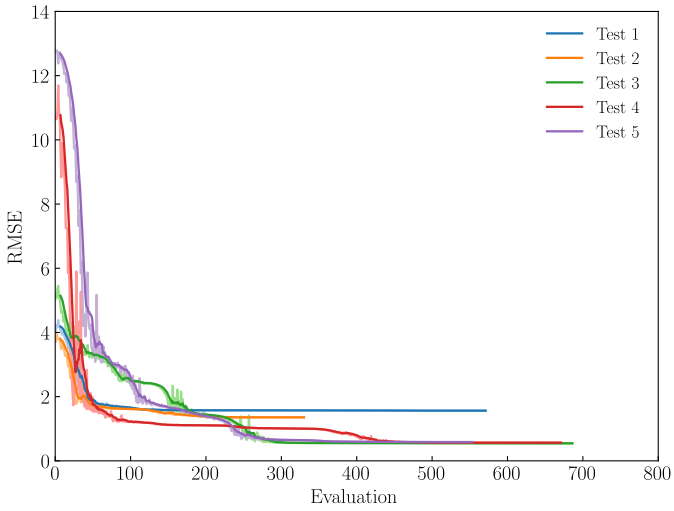


Figure 4.4: rmse for multiple tests.

4.2 Validation

To improve our algorithm we reduced the number of optimization parameters by fixing the elastic material parameters. The results of this implementation for three different data sets will be discussed in this section.

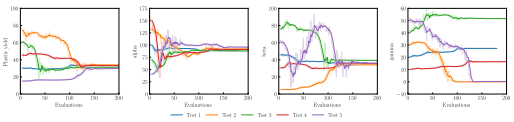
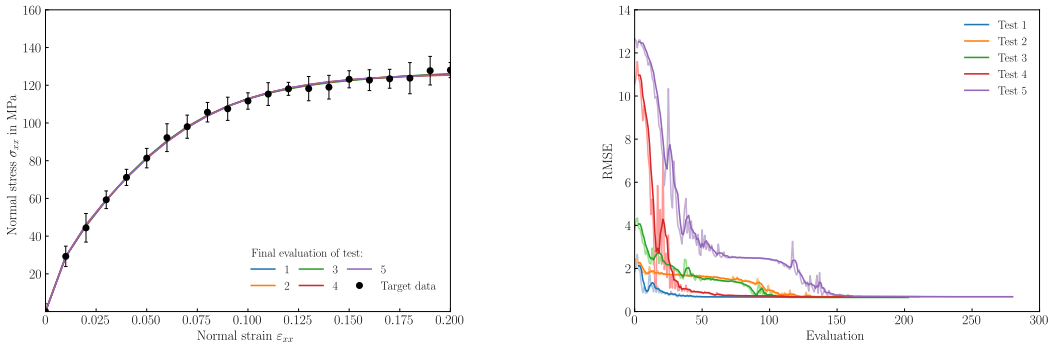


Figure 4.5: progress of material parameters for validation tests.

In the first step we used the same data set as in **??** to test the modified algorithm. The optimized plastic material parameters are shown in Figure 4.5. In all tests, the

values of the plastic yield, alpha and beta demonstrate a converging trend towards a singular solution. The only exception to this is gamma whose converged values vary for each individual test. As was outlined in the preceding discussion, gamma exerts minimal influence on the trend of the hardening curve. Consequently, the focus shall be directed towards the plastic yield, alpha and beta, which indicate an improvement in their optimization behavior. The quality of this optimized parameters is ensured through the match of the stress-strain curves with the target data. As demonstrated in Figure **??** the final stress-strain curves exhibit a strong correlation with the target data. The evolution of the RMSE XXX supports this results with small values for every test. A comparison of the results of the present study with those of the verification study reveals an equivalent level of optimization quality. Additionally, the results of the material parameters indicate a positive impact of the algorithm modification, showing a unique solution for the important parameters.

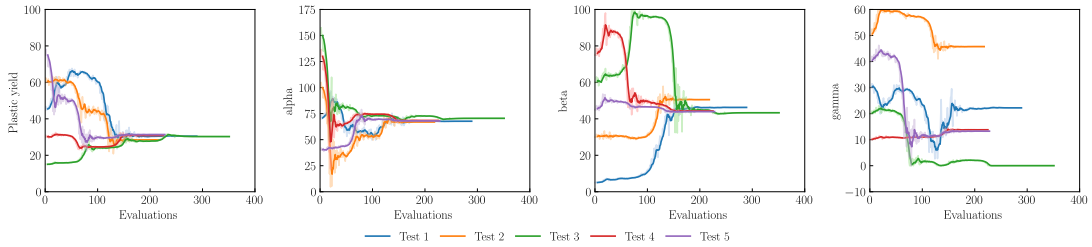


(a) Final stress-strain curves.

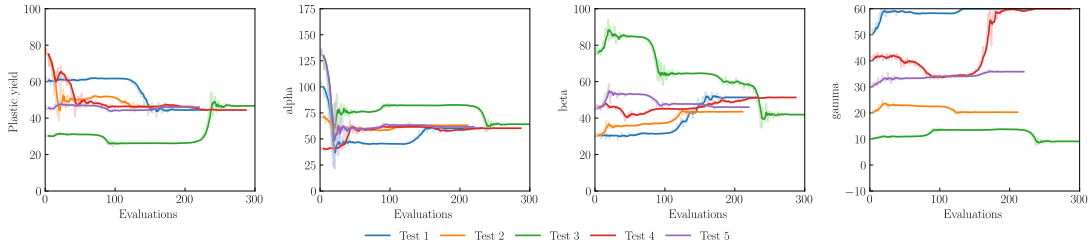
(b) RMSE evolution.

Figure 4.6: Results of validation tests with 6to3 dataset.

To verify our algorithm independent of the used target data set, we made the same tests with two additional data sets. In the following we present the results of studies for mixing ratio 4:3 and 8:3.



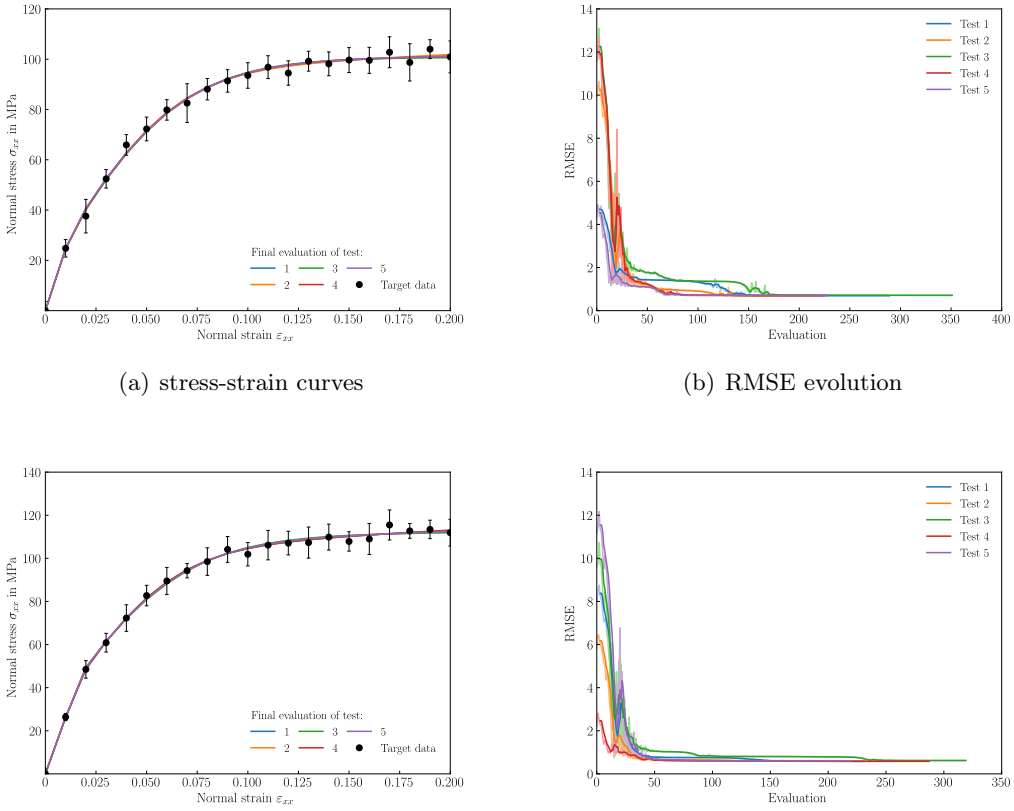
(a) evolution of material 4:3



(b) evolution of 8:4

Figure 4.7: Evolution of material parameters for a) mixing ratio 4:3 and b) mixing ratio 8:3.

The evolution of the plastic material parameters for the mixing ratios 4:3 and 8:3 in plotted in Figure 4.7. We can observe a similar convergence behaviour as in the validation study with mixing ratio 6:3. Only test case 3 for mixing ratio 8:3 shows a deviation provided that all values converge quite late. Since we chose the initial values randomly this might occur through an unfavourable combination of values. In Figure 4.8 we represent the optimized stress-strain curves and the evolution of the RMSE. For all tests the stress-strain values correlate with the target data. The equivalent level of the RMSE for the converged solutions indicate a similar quality of the optimization result for all tests. These results indicate an improvement of the solution results through determining the elastic parameters.



(a) stress-strain curves

(b) RMSE evolution

(c) Final stress-strain curves

(d) RMSE evolution

Figure 4.8: Results of validation tests with mixing ratios 4:3 and 8:3: a) final stress-strain curves for mixing ratio 4:3, b) RMSE for mixing ratio 8:3, c) final stress-strain curves for mixing ratio 4:3, d) RMSE for mixing ratio 8:3.

Overall these results demonstrate the reliability of the optimization algorithm for the load case of a single tensile strain in one direction with fixed elastic parameters. The specification of the elastic parameter values improves the optimization performance in a way that for the plastic yield, alpha and beta independent of the initial values a singular solution can be found. However, the manual specification of Youngs modulus and Poisson ratio is only possible for target data sets with exactly one data point in the elastic domain of the material. For data sets with multiple points in the elastic domain a manual specification becomes complicated quite fast. Additional, for materials with completely unknown material behaviour, the point of transition between elastic and plastic behaviour is still unknown. In order to process such data sets too, we need to integrate the elastic parameters in the optimization process. In doing so the singularity of the solution should be maintained. Therefore the algorithm needs additional information about the mechanical material behaviour. In the following step we tried to do so through the combination of two load cases. Additional to the already tested tensile strain we applied a shear strain. As described in section XX the shear modulus contains information about Youngs modulus and Poisson ratio what might improve the performance of the optimizatoin process. The information contained within the shear modulus about Youngs modulus and Poisson ratio might enclose the necessary restrictions to reduce the solution variability.

Warum sinusförmige belastung? Jz schon mit zyklischen versuchen kommen?

4.3 shear and normal strain tests combined

4.4 cyclic tests

5 Conclusion

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A Appendix

A.1 Section

B Appendix