Optimal error functional for parameter identification in anisotropic finite strain elasto-plasticity

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Abstract. A problem of parameter identification for a model of finite strain elasto-plasticity is discussed. The utilized phenomenological material model accounts for nonlinear isotropic and kinematic hardening; the model kinematics is described by a nested multiplicative split of the deformation gradient. A hierarchy of optimization problems is considered. First, following the standard procedure, the material parameters are identified through minimization of a certain least square error functional. Next, the focus is placed on finding optimal weighting coefficients which enter the error functional. Toward that end, a stochastic noise with systematic and non-systematic components is introduced to the available measurement results; a superordinate optimization problem seeks to minimize the sensitivity of the resulting material parameters to the introduced noise. The advantage of this approach is that no additional experiments are required; it also provides an insight into the robustness of the identification procedure. As an example, experimental data for the steel 42CrMo4 are considered and a set of weighting coefficients is found, which is optimal in a certain class.

1. Introduction
In the current study, a viscoplastic material model of Shutov and Kreißig is considered [6]. It is suitable for large strain metal forming applications.\textsuperscript{1} Within the model, the material properties are described by a set of material parameters. In general, the inverse problem of parameter identification is ill posed. For that reason, some regularized strategies of material parameter identification were presented in [10] for the considered material model. In this work we seek for an optimal parameter identification strategy which provides material parameters least dependent on the measurement errors.

2. Material model of finite strain viscoplasticity
Let us recall the constitutive equations of the model proposed by Shutov and Kreißig (cf. [6]), which accounts for nonlinear isotropic and kinematic hardening. We start with the classical multiplicative decomposition of the deformation gradient $\mathbf{F}$ into the inelastic and elastic parts

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_i,$$

(1)

Next, following [3], two nested multiplicative decompositions are introduced

$$\mathbf{F}_i = \mathbf{F}_{1e} \mathbf{F}_{1i}, \quad \mathbf{F}_i = \mathbf{F}_{2e} \mathbf{F}_{2i},$$

(2)

\textsuperscript{1} Further extensions of this model are reported in [11] and references cited therein.
where $F_{1i}$ and $F_{2i}$ are dissipative parts of the inelastic deformation gradient $F_i$; $F_{1e}$ and $F_{2e}$ are conservative parts of $F_i$. The local deformation history is described by the right Cauchy-Green tensor $C := F^T F$. The current state of the material is described by internal variables

$$ C_i := F_i^T F_i, \quad C_{1i} := F_{1i}^T F_{1i}, \quad C_{2i} := F_{2i}^T F_{2i}. $$

(3)

By definition, these tensors are symmetric and positive definite; due to the incompressibility condition, they are unimodular. Let $\psi$ be the Helmholtz free energy per unit mass. Assume

$$ \psi = \psi_{el}(CC_1^{-1}) + \psi_{kin1}(C_iC_1^{-1}) + \psi_{kin2}(C_iC_2^{-1}) + \psi_{iso}(s - s_d), $$

(4)

where functions $\psi_{el}(CC_1^{-1})$, $\psi_{kin1}(C_iC_1^{-1})$, $\psi_{kin2}(C_iC_2^{-1})$ and $\psi_{iso}(s - s_d)$ describe the energy storage due to macroscopic elastic strain as well as kinematic and isotropic hardening. The functions $\psi_{el}$, $\psi_{kin1}$, and $\psi_{kin2}$ are isotropic. To be definite, we employ the following ansatz:

$$ \rho_R \psi_{el}(A) = \frac{k}{2} (\ln \sqrt{\det A})^2 + \frac{\mu}{2} (\text{tr} \overline{A} - 3), $$

(5)

$$ \rho_R \psi_{kin1}(A) = \frac{c_1}{4} (\text{tr} \overline{A} - 3), \quad \rho_R \psi_{kin2}(A) = \frac{c_2}{4} (\text{tr} \overline{A} - 3), $$

(6)

$$ \rho_R \psi_{iso}(s_e) = \frac{\gamma}{2} (s_e)^2, \quad \overline{A} := (\det A)^{-1/3} A, $$

(7)

where $A$ is an arbitrary second rank tensor; $s_e$ is an arbitrary scalar; $k$, $\mu$, $c_1$, $c_2$, $\gamma$ are material parameters; $\rho_R$ is the mass density in the reference configuration. Using the Coleman-Noll procedure, the second Piola-Kirchhoff stress is computed through

$$ \overline{T} = 2\rho_R \frac{\partial \psi_{el}(CC_1^{-1})}{\partial C} \big|_{C_i=\text{const}}. $$

(8)

Partial backstresses $\overline{X}_1$, $\overline{X}_2$ and the overall backstress $\overline{X}$ are evaluated by

$$ \overline{X}_1 = 2\rho_R \frac{\partial \psi_{kin1}(C_iC_1^{-1})}{\partial C_i} \big|_{C_{1i}=\text{const}}, \quad \overline{X}_2 = 2\rho_R \frac{\partial \psi_{kin2}(C_iC_2^{-1})}{\partial C_i} \big|_{C_{2i}=\text{const}}, \quad \overline{X} = \overline{X}_1 + \overline{X}_2. $$

(9)

The isotropic hardening $R$ is defined by

$$ R = \rho_R \frac{\partial \psi_{iso}(s - s_d)}{\partial s} \big|_{s_d=\text{const}}. $$

(10)

A viscous overstress $f$, which depends on the loading rate, is given by

$$ f := \overline{\overline{f}} - \sqrt{\frac{2}{3}} (K + R), \quad \overline{\overline{f}} := \sqrt{\text{tr}[(\overline{C} \overline{T} - C_i \overline{X})^D]^2}, $$

(11)

where $K$ stands for the initial yield stress, $(\cdot)^D$ denotes a deviatoric part, $\overline{\overline{f}}$ is a driving force of the inelastic flow. The inelastic multiplier $\lambda_i$ equals the rate of the inelastic flow; it is computed using the Perzyna law

$$ \lambda_i = \frac{1}{\eta} \left( \frac{f}{k_0} \right)^m, \quad \langle x \rangle := \max(x, 0), $$

(12)

where $\eta$ and $m$ are viscous parameters; $k_0 = 1$ MPa is used to obtain a non-dimensional quantity in the bracket. The inelastic flow is governed by the following evolution equations

$$ \dot{C}_i = \frac{2\lambda_i}{3} (\overline{C} \overline{T} - C_i \overline{X})^D C_i, $$

(13)
\[
\dot{C}_1 = 2\lambda_1 \kappa_1 (C_1 \tilde{X}_1) D C_1, \quad \dot{C}_2 = 2\lambda_2 \kappa_2 (C_2 \tilde{X}_2) D C_2, \quad (14)
\]
\[
\dot{s} = \sqrt{\frac{2}{3}} \dot{\lambda}_1, \quad \dot{s}_d = \frac{\beta}{\gamma} \dot{s} R. \quad (15)
\]

Here, \(\kappa_1, \kappa_2\), and \(\beta\) are material parameters; \((\cdot)\) is a material time rate. If the initial state is isotropic, undeformed, and stress free, then we may assume the following trivial initial conditions:

\[
C_1|_{t=0} = C_2|_{t=0} = 1, \quad s|_{t=0} = s_d|_{t=0} = 0. \quad (16)
\]

This model is thermodynamically consistent, objective and \(\omega\)-invariant. It is free from nonphysical shear oscillations. Robust and efficient numerical algorithms are available [12].

3. Experimental data for the steel 42CrMo4

In the current study we use experimental data reported in [9] for the high-strength steel 42CrMo4. Torsion tests carried out on thin-walled tubular specimens are considered. In Figure 1, the shear stresses are plotted versus the prescribed shear strain for two different loading programs (see [9] for additional details). In the as-received state the material is isotropic. Figure 1 indicates that the material exhibits a distinct Bauschinger effect. Thus, the material model should employ the nonlinear kinematic hardening.

Figure 1. Experimental data and simulation results for torsion of thin-walled tubes made from 42CrMo4 steel: shear stresses versus shear strains for two different loading programs.

4. Classical strategy of material parameter identification

Some of the parameters can be identified by general considerations (cf. [9]). These pre-identified parameters are summarized in Table 1.

| \(k\) | \(\mu\) | \(\eta\) | \(m\) | \(K\) |
|-------|-------|-------|-------|-------|
| 135600 MPa | 52000 MPa | 500000 s | 2.26 | 335 MPa |

2 A general definition of the \(\omega\)-invariance is given in [7]. A proof of the \(\omega\)-invariance for the current model is provided in [8].
Now we need to identify six hardening parameters: $\gamma$, $\beta$ from the Voce isotropic hardening law and $c_1$, $c_2$, $\kappa_1$, $\kappa_2$ of the Armstrong-Frederick kinematic hardening rule. Since the mentioned hardening mechanisms are coupled, all the hardening parameters need to be identified simultaneously. Following the classical approach, we build an error functional

$$
\Phi(p) = \Phi(\gamma, \beta, c_1, c_2, \kappa_1, \kappa_2) = \sum_{i=1}^{N_{\text{exp}}} \omega_i [\text{Exp}_i - \text{Mod}_i(p)]^2, \quad (17)
$$

where $N_{\text{exp}}$ is the number of points on the experimental stress-strain curves, $\text{Exp}_i$ are measured shear stresses, $\text{Mod}_i$ are the corresponding simulation results (model response), $\omega_i \geq 0$ are the weighting coefficients. For this error functional, an optimal set of parameters is identified:

$$
p_*(\omega_1, \ldots, \omega_{N_{\text{exp}}}) = (\gamma, \beta, c_1, c_2, \kappa_1, \kappa_2) = \arg \min \Phi. \quad (18)
$$

The minimum of $\Phi$ is found using the gradient-based Levenberg-Marquard algorithm (cf. [4]).

Within the classical identification procedure, all data points are equally weighted ($\omega_i \equiv 1$).

The identified hardening parameters are presented in Table 2 and the corresponding simulation results are shown in Figure 1. One drawback of this approach is that it says nothing about the influence of the measurement errors on the resulting parameters.

### 5. Strategy with optimal choice of weighting coefficients

Let $p^*(\omega_i)$ be the solution of the optimization problem (17)–(18) with weighting coefficients $\omega_i$, $i = 1, 2, \ldots, N_{\text{exp}}$. In this section we formulate a problem of finding the weighting coefficients $\omega_i$ which are optimal in a certain sense.

#### 5.1. Introduction of noise to experimental data

Let us replace the experimental data $\text{Exp}_i$ by the noisy data $\text{Exp}_i + \text{Noise}_i$, where

$$
\text{Noise}_i = \text{Noise}_{i,\text{nonsyst}} + \varepsilon_1 \text{Mode}_{1i} + \varepsilon_2 \text{Mode}_{2i}, \quad (19)
$$

Here, $\text{Noise}_{i,\text{nonsyst}} \in \Phi(0, \sigma)$ is a non-systematic error; $\varepsilon_1, \varepsilon_2 \in \Phi(0, \sigma)$ and vectors $\text{Mode}_{1i}$ and $\text{Mode}_{2i}$ are known a priori and correspond to systematic measurement errors (see Figure 2).

#### 5.2. Analytical expression for material parameters corresponding to noisy data

First, consider the error functional (17) built from the noise-free data. The minimizing set of parameters and the Jacobian are

$$
p_* (\omega_1, \ldots, \omega_{N_{\text{exp}}}) = \arg \min \Phi, \quad J = \left. \frac{\partial \text{Mod}(p)}{\partial p} \right|_{p_*}. \quad (20)
$$

Next, the model prediction is linearized near $p_*$:

$$
\text{Mod}(p) \approx \text{Mod}^\text{lin}(p) = \text{Mod}(p_*) + J(p - p_*). \quad (21)
$$

The error functional, which corresponds to the $j$-th realisation of (19), takes the form

$$
\Phi^{(j)}(p) = \sum_{i=1}^{N_{\text{exp}}} \omega_i [\text{Exp}_i + \text{Noise}_i^{(j)} - \text{Mod}^\text{lin}_i(p_*)]^2. \quad (22)
$$

3 Obviously, the error functional (17) is related to the $L_2$ norm of the residual. The use of other norms for the identification of material parameters was discussed in [5].

4 The idea of introducing artificial errors in order to estimate the level of uncertainty was considered, among others, in [2]. Other engineering applications are given in [1].
Figure 2. Various modes of measurement errors: error due to false measurement of stresses (a); error due to a play in the testing assembly, which appears after load reversal (b).

Denote by $\mathbf{p}^{(j)}$ the solution corresponding to the $j$-th realisation of the stochastic model:

$$\mathbf{p}^{(j)} = \arg \min \Phi^{(j)}. \quad (23)$$

The set of vectors $\mathbf{p}^{(j)}$ for a sufficiently large number of realisations will be referred to as “cloud of parameters”. The size of the “cloud” is a measure for the parameter dependence on the measurement errors. In the following we seek for the weighting factors $w_i$, which minimize the size of the “cloud”. The advantages of this problems statement are as follows: (i) There is no need for additional experiments. (ii) The form of the “cloud” provides insight into the correctness of the parameter identification problem.

A closed form expression for $\mathbf{p}$ pertaining to the linearized model response $\text{Mod}^{\text{lin}}$ is available:

$$\mathbf{p} = -\frac{1}{2}(J^T W^2 J)^{-1}(J^T W^2 A + AW^2 J), \quad (24)$$

where $A := \text{Mod}(\mathbf{p}_s) - J\mathbf{p}_s - \text{Exp} - \text{Noise}$, $W = \text{diag}(\omega_1, \omega_2, ..., \omega_{N_{\text{exp}}})$.

Let us show that for the noise-free data ($\text{Noise} = 0$) the analytical solution (24) coincides with $\mathbf{p}_s$. Toward that end we consider the original problem (17)–(18) (for simplicity assume that all the weights are equal to 1):

$$\Phi(\mathbf{p}) = ||\text{Mod}(\mathbf{p}) - \text{Exp}||^2, \quad \mathbf{p}_s = \arg \min \Phi \quad \Rightarrow \quad \frac{\partial \Phi}{\partial \mathbf{p}}_{|\mathbf{p}_s} = 0. \quad (25)$$

$$\frac{\partial \Phi}{\partial \mathbf{p}} = 2(\text{Mod}(\mathbf{p}) - \text{Exp})^T \frac{\partial \text{Mod}(\mathbf{p})}{\partial \mathbf{p}} = 2(\text{Mod}(\mathbf{p}) - \text{Exp})^T J, \quad \text{Mod}_s = \text{Mod}(\mathbf{p}_s), \quad (26)$$

$$2(\text{Mod}_s - \text{Exp})^T J = 0. \quad (27)$$

On the other hand, for the linearized problem (22) with $\text{Noise} = 0$ we have

$$\Phi^{\text{lin}}(\overline{\mathbf{p}}) = ||\text{Mod}_s + J(\overline{\mathbf{p}} - \mathbf{p}_s) - \text{Exp}||^2, \quad \Phi^{\text{lin}}(\overline{\mathbf{p}}_s) = \Phi(\overline{\mathbf{p}}_s). \quad (28)$$

Recalling (27), we arrive at

$$\frac{\partial \Phi^{\text{lin}}}{\partial \overline{\mathbf{p}}}_{|\overline{\mathbf{p}}_s} = 2(\text{Mod}_s - \text{Exp})^T J = 0. \quad (29)$$
Thus, in the noise-free case ($\text{Noise} = 0$), the linearized problem (29) has the same solution $\bar{p}_s$ as the original problem (27). This justifies the linearization of $\text{Mod}$.

Let $N_{\text{noise}}$ be the number of realizations of (19). The size of the “cloud” is defined as

$$\text{Size}(\omega_1, \ldots, \omega_{N_{\text{exp}}}) := \frac{1}{N_{\text{noise}}} \sum_{j=1}^{N_{\text{noise}}} \left( \frac{\sum_{k=1}^{6} (p_j^{(k)} - p_k^*)}{\sum_{k=1}^{6} p_k^*} - 1 \right)^2, \quad \bar{p}_s = \bar{p}_s(\omega_1, \ldots, \omega_{N_{\text{exp}}}). \quad (30)$$

### 5.3. Strategies with non-trivial weighting coefficients

The material under consideration exhibits a clear Bauschinger effect. Thus, on the stress-strain curve there is a zone of a smooth re-plastification, which we call “plastic knee”, Figure 3. In other words, the “knee” corresponds to the transient hardening, occurring shortly after load reversals. Experimental data near the “knee” are very important for identification of parameters of kinematic hardening. This motivates an identification strategy where the experimental data near the “knee” are given a larger weight than the remaining experimental data.

By “knee 9/4” and “knee 4” denote identification strategies, where the weighting coefficients in the “knee” region equal $\omega_i = 9/4$ and $\omega_i = 4$, respectively. The identified material parameters for different strategies are summarized in Table 2. Computations of the size of the “cloud” (cf. Table 3) using $N_{\text{noise}} = 1000$ realisations reveal that the strategy “knee 4” yields results, which are least sensitive to the introduced noise.

![Figure 3.](image)

**Figure 3.** A domain called “plastic knee” on the stress-strain curve.

| parameter | classical ($\omega_i = 1$) | “knee 4” | “knee 9/4” |
|-----------|--------------------------|-----------|-------------|
| $\gamma$  | 141.18 MPa | 165.29 MPa | 157.81 MPa  |
| $\beta$   | 0.0375 [-] | 0.2569 [-] | 0.1832 [-] |
| $c_1$     | 1692.6 MPa | 1985.8 MPa | 1875.7 MPa  |
| $c_2$     | 23255.1 MPa | 23386.9 MPa | 23481.1 MPa |
| $\kappa_1$ | 0.0038419 1/MPa | 0.0038660 1/MPa | 0.0038567 1/MPa |
| $\kappa_2$ | 0.0045175 1/MPa | 0.0047926 1/MPa | 0.0046769 1/MPa |
6. Conclusion

A new method is suggested, which allows one to choose optimal strategies of material parameter identification. The method is based on the two-scale approach: on the lower scale, the material parameters are identified by minimizing the error functional $\Phi$; on the upper scale, optimal weighting coefficients are found by minimizing the size of the “parameter cloud”. For the material under consideration, an optimal identification strategy is found, among the three considered possibilities. As an alternative to (19), other stochastic models of noise can be used depending on the specific application. In the follow-up research, a broader class of identification strategies will be analyzed. The method is especially promising when experiments of different types are to be efficiently combined within a single error functional.

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