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Abstract

In this paper we discuss the identification of parameter functions in material models for elastic large deformations. A model of the the forward problem is given, where the displacement of a deformed material is found as the solution of a nonlinear PDE. Here, the crucial point is the definition of the 2nd Piola-Kirchhoff stress tensor by using several material laws including a number of material parameters. In the main part of the paper we consider the identification of such parameters from measured displacements, where the inverse problem is given as an optimal control problem. We introduce a solution of the identification problem with Lagrange and SQP methods. The presented algorithm is applied to linear elastic material with large deformations.

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1 Introduction

In mechanical engineering the simulation of deformations and stresses is an important application of FEM software. For given geometry and loads the displacement of a body has to be calculated as the solution of an elliptic partial differential equation. In this context, the stress tensor needs to be defined with an adequate material law, depending on the considered material. A wide variety of such material laws exists. Common for all of them is, that several material properties are involved via material parameters. In the following we want to deal with the identification of these material parameters from given displacement data. This denotes an inverse identification problem in contrast to the direct simulation problem.

While solving identification problems for large deformations, difficulties emerge due to several facts. At one hand, the governing equation denotes a nonlinear PDE even for linear material laws. This results from nonlinear terms in the strain tensor, that cannot be omitted in the case of large deformations. See [11] and [12] for details on the nonlinear PDE model. Additionally, nonlinearity arises from nonlinear material laws, such as Neo-Hooke and Mooney-Rivlin (basing on the fundamental papers [14] and [16]), or Modified Fung material [3]. On the other hand, we are interested in the identification of parameter functions and thus the inverse problem may turn out to be ill-posed. Therefore, a stable solution of the identification problem needs to involve regularization methods. For a survey on regularization theory see e. g. [4] and [9].

In the last years the theory on the identification of material parameters made considerable progress. Thus, for the linear theory with small deformations and linear elasticity the identification of scalar parameters as well as parameter functions is well known. See in the linear context e. g. the survey paper [1] and the references therein or the numerical study [8]. Results for the identification of scalar parameters in nonlinear material laws with large deformations can be found in [6]. A recent study on identification problems for Neo-Hooke material with large deformations is presented in the paper [5].

In our work we will focus on the identification of parameter functions for compressible material with large deformations. Therefore, the identification problem will be formulated as an optimal control problem as suggested in the paper [2]. For the solution of the resulting constrained minimization problem Lagrange and SQP methods will be implemented following the results of [7].

The paper is organized in the following manner. In section 2 a survey on the large deformation theory is presented. We introduce a nonlinear PDE model for the direct problem and focus on the material-depending definition of the 2nd Piola-Kirchhoff stress tensor. The derivation of the stress tensor from special energy density functions - referring to the material laws - is explained. In the next section we deal with the inverse problem. Thereby, we discuss the variety of arising identification problems and present a general solution framework with SPQ methods. Concluding this section, the identification algorithm is applied to linear elastic material with large deformations. Finally, an outlook on future work and open questions is given.

2 Elastic large deformations

In the following section we sketch the PDE model for elastic large deformations as it was presented in detail in the papers [11] and [12]. Thereby the considered differential equations are derived in terms of tensor calculus. An extensive survey on tensor analysis is given e. g. in the monograph [17]. In this study we assume dealing with compressible material. For incompressible material additional equations have to be introduced, see e.g. [6] and [11].

2.1 PDE model for the direct problem

The deformation of a body Ω_0 is quantified by the displacement, which is defined as follows.

Definition 2.1 (Displacement U of a body Ω_0)**.** *Let $\Omega_0 \subset \mathbb{R}^3$ be an undeformed body and let $\Omega_t \subset \mathbb{R}^3$ be the same body after a deformation. A mass point at position $X \in \Omega_0$ is moved by the displacement to a position $x \in \Omega_t$. Thus we define*

$$x = X + U(X)$$

with the displacement $U(X) \in \mathbb{R}^3$.

Note, that for elastic material behavior the body returns to state Ω_0 after removing loads. Throughout the paper we distinguish the deformed and undeformed state by using capital letters for variables in undeformed state and lower case letters in deformed state.

The governing equation describing the equilibrium of forces in a deformed body is given by the elliptic PDE

$$\operatorname{div} \sigma + \rho \vec{f} = \vec{0} \qquad \forall x \in \Omega_t \, . \tag{1}$$

The complete boundary value problem additionally contains force loads referring to Neumann boundary conditions and Dirichlet boundary conditions in the case of fixed displacements at the boundary. In equation (1), $\sigma = \sigma(x, U)$ denotes an appropriately chosen stress tensor, which is depending on x and U. Further variables are the density $\rho = \rho(x)$ and the vector of volume forces $\vec{f} = \vec{f}(x)$.

As derived in [11], the weak solution of (1) is found as the solution of the following variational problem.

Definition 2.2 (Variational problem for equation (1))**.** *Find a displacement vector U (fulfilling Dirichlet boundary conditions on Γ_{D_0}) as the solution of*

$$\int_{\Omega_0} \overset{2}{T} : E(U;V)\, d\Omega_0 = \int_{\Omega_0} \rho_0 \vec{f} \cdot V\, d\Omega_0 + \int_{\Gamma_{N_0}} \vec{g} \cdot V\, dS_0 \quad \forall V \in (H_0^1(\Omega_0))^3 \tag{2}$$

with the variables:

- $\overset{2}{T} = \overset{2}{T}(U)$*: 2nd Piola-Kirchhoff stress tensor*
- $E(U;V)$*: Fréchet derivative of the strain tensor* $E(U)$
- ρ_0*: initial density field*
- $\vec{g}$*: given tractions on Neumann boundary* Γ_{N_0}
- V*: test functions with* $V|_{\Gamma_{D_0}} = \vec{0}$ *on Dirichlet boundary* Γ_{D_0}

The tensors $E(U)$*,* $E(U;V)$*, and* $\overset{2}{T}$ *are symmetric tensors of second order.*

Note, that (2) is defined in Ω_0 and therefore the model can be reduced to the undeformed state. Thus, in contradiction to the general case, where curvilinear coordinates, covariant and contravariant tensor basis have to be taken into account, we can simplify our problem to orthonormal coordinates in Ω_0. Then the covariant and contravariant tensor basis coincide with the standard basis.

We consider details of equation (2). The strain tensor $E(U)$ for large deformations is defined as

$$2E(U) = \text{Grad}U + \text{Grad}U^T + \text{Grad}U \cdot \text{Grad}U^T \;, \tag{3}$$

with $A \cdot B$ denoting the contraction of tensors. Thus, the Fréchet derivative $E(U;V)$ as a linearization of the strain tensor has to fulfill

$$E(U+V) = E(U) + E(U;V) + \mathcal{O}(\|V\|^2) \;,$$

which eventually leads to

$$2E(U;V) = \text{Grad}V + \text{Grad}V^T + \text{Grad}U \cdot \text{Grad}V^T + \text{Grad}V \cdot \text{Grad}U^T \;. \tag{4}$$

Due to (3) and (4), the PDE (1) is nonlinear in U even for linear material behavior.

In deformed state Ω_t a Neumann boundary condition means

$$\vec{n}_t \cdot \sigma = \vec{g}_t \quad \text{on} \quad \Gamma_{N_t}$$

with given tractions $\vec{g}_t$ and outer normal vector $\vec{n}_t$. Transforming this to the undeformed state, we derive

$$\vec{n}_0 \cdot \overset{1}{T} = \vec{g} \quad \text{on} \quad \Gamma_{N_0} \tag{5}$$

with the 1st Piola-Kirchhoff stress tensor $\overset{1}{T} = \overset{2}{T} \cdot F^T$. The tensor $\overset{1}{T}$ is an unsymmetrical, second order tensor and $F = I + \text{Grad}\, U^T$ denotes the deformation gradient.

The crucial point of the above equations is the definition of the 2nd Piola-Kirchhoff stress tensor $\overset{2}{T}$. With an appropriate choice of this tensor, the stress tensor σ in (1) is replaced respecting specific material properties.

2.2 Material laws and the 2nd Piola-Kirchhoff stress tensor

For defining the 2nd Piola-Kirchhoff stress tensor we follow a quite abstract ansatz as explained in [11]. Thus, with an energy density function Ψ we set the energy functional

$$\Phi(U) = \int_{\Omega_0} \Psi(G) \mathrm{d}\Omega_0 - f(U) \ ,$$

where f denotes the linear functional

$$f(U) = \int_{\Omega_0} \rho_0 \vec{f} \cdot U \mathrm{d}\Omega_0 + \int_{\Gamma_{N_0}} \vec{g} \cdot U \mathrm{d}S_0$$

and G is the right Cauchy-Green tensor

$$G = F^T \cdot F = I + 2E(U) \ . \tag{6}$$

Then minimizing Φ over U yields

$$\Phi(U; V) := \frac{\partial \Phi}{\partial U}(V) = 0 \quad \forall V \ ,$$

which is in fact the variational problem (2) with

$$\overset{2}{T} = 2 \frac{\partial \Psi(G)}{\partial G} \ . \tag{7}$$

Note, that induced by this ansatz the stress tensor $\overset{2}{T} = \overset{2}{T}(E(U))$ depends on $E(U)$. The energy density function Ψ includes material laws and has to be appropriately chosen according to the considered material. Following the notation of [11] and [12] we define

$$\Psi(G) = \Psi(a_1, a_2, a_3) \ , \tag{8}$$

where the dependence on G is formulated in terms of the invariants of G by using

$$a_k = a_k(G) = \frac{1}{k}\mathrm{tr}\ G^k,\ \ k = 1, 2, 3 \ .$$

Hence, for the invariants holds (see e. g. [17, p. 186]):

- 1st invariant: $I = \mathrm{tr}\ G = a_1$
- 2nd invariant: $II = \frac{1}{2}(a_1^2 - 2a_2)$
- 3rd invariant: $III = \det G = \frac{1}{6}(a_1^3 - 6a_1a_2 + 6a_3)$

For calculating $\overset{2}{T}$ via (7) we apply the chain rule and derive

$$\overset{2}{T} = 2\frac{\partial\Psi(G)}{\partial G} = 2\sum_{k=1}^{3}\left(\frac{\partial\Psi}{\partial a_k}\right)\frac{\partial a_k}{\partial G} \ .$$

Obviously, $\frac{\partial a_k}{\partial G}$ denotes a second order tensor with

$$a_k(G + \Delta G) = a_k(G) + \left(\frac{\partial a_k}{\partial G}\right) : \Delta G + \mathcal{O}(\|\Delta G\|^2) \ ,$$

which means in detail

$$\begin{aligned} a_k(G + \Delta G) &= \frac{1}{k}\mathrm{tr}(G + \Delta G)^k \\ &= \frac{1}{k}\mathrm{tr}(G)^k + \frac{1}{k}\mathrm{tr}(k\, G^{k-1} \cdot \Delta G) + \mathcal{O}(\|\Delta G\|^2) \\ &= a_k(G) + G^{k-1} : \Delta G + \mathcal{O}(\|\Delta G\|^2) \ . \end{aligned}$$

Here we used the fact, that the trace operator can be written as a tensor contraction. Consequently

$$\frac{\partial a_k}{\partial G} = G^{k-1}$$

holds and hence

$$\overset{2}{T} = 2\sum_{k=1}^{3}\left(\frac{\partial\Psi}{\partial a_k}\right)G^{k-1} \ . \tag{9}$$

Note, that in (9) for varying material laws only the derivatives $\frac{\partial\Psi}{\partial a_k}$ have to be adapted with respect to the chosen energy density function Ψ.

Several functions Ψ can be found in literature. Well known is the linear material law of linear elasticity.

Definition 2.3 (Linear elastic material)**.** *For linear elasticity the function* Ψ *is defined as*

$$\Psi = \frac{\mu}{2}\left(a_2 - a_1 + \frac{3}{2}\right) + \frac{\lambda}{8}\left(a_1^2 - 6a_1 + 9\right) \tag{10}$$

with material parameters λ *and* μ *(Lame's constants).*

The material law (10) is valid for small as well as for large deformations. The formulation (10) is equivalent to

$$\overset{2}{T} = 2\mu E(U) + \lambda((\mathrm{tr}\, E(U))I) = \mathbb{C} : E(U) \tag{11}$$

with a 4th-order material tensor $\mathbb{C} = \mathbb{C}(\lambda, \mu)$. Here, $A : B$ denotes a double contraction of tensors. Expanding the linear theory, for hyperelastic materials exist also nonlinear material laws. The following two energy density functions originally base on the papers [14] and [16] and are widely used in recent studies on hyperelasticity.

Definition 2.4 (Neo-Hooke and Mooney-Rivlin material)**.** *The Neo-Hooke material is defined via*

$$\Psi = c_{10}(a_1 - \ln(\det G) - 3) + D_2 \ln^2(\det G) \tag{12}$$

with parameters c_{10} *and* D_2*. This is a simplification of the more general energy density function for Mooney-Rivlin material*

$$\Psi = c_{10}(a_1 - 3) + c_{01}\left[\frac{1}{2}(a_1^2 - 2a_2)\right] - (c_{10} + 2c_{01})\ln(\det G) + D_2 \ln^2(\det G) \tag{13}$$

with the additional parameter c_{01}*.*

The last nonlinear material we want to mention here, is the so called Modified Fung material [3].

Definition 2.5 (Modified Fung material)**.** *For the Modified Fung material law, the function* Ψ *is defined as*

$$\Psi = \frac{c_{10}}{\alpha}\left[e^{\alpha(a_1 - \ln(\det G) - 3)} - 1\right] + D_2 \ln^2(\det G) \tag{14}$$

with parameters c_{10}*,* α*, and* D_2*.*

2.3 The 2nd Piola-Kirchhoff stress tensor for linear elasticity

In the following we give a detailed view on the explicit derivation of the 2nd Piola-Kirchhoff stress tensor via formula (9). Hence, we have to calculate the derivatives $\frac{\partial\Psi}{\partial a_1}$ and $\frac{\partial\Psi}{\partial a_2}$ of the real function (10), which is not depending on a_3. We derive

$$\begin{aligned}\frac{\partial\Psi}{\partial a_1} &= -\frac{\mu}{2}+\frac{\lambda}{4}(a_1-3)\\ \frac{\partial\Psi}{\partial a_2} &= \frac{\mu}{2}\end{aligned}$$

and consequently

$$\overset{2}{T}=\left[-\mu+\frac{\lambda}{2}(a_1-3)\right]I+\mu G=\mu(G-I)+\frac{\lambda}{2}(\operatorname{tr}G-3)I\ .$$

Replacing $G=I+2E(U)$ and $\operatorname{tr}G=\operatorname{tr}(I+2E(U))=3+2\operatorname{tr}E(U)$ in the last equation leads to

$$\overset{2}{T}=2\mu E(U)+\lambda(\operatorname{tr}E(U))\,I\ ,$$

which is exactly the well known formulation (11).

2.4 The 2nd Piola-Kirchhoff stress tensor for nonlinear material laws

The definition of the 2nd Piola-Kirchhoff stress tensor via (9) can be applied in an analogous way for all choices of energy density functions $\Psi=\Psi(a_1,a_2,a_3)$. For the Neo-Hooke material law the function (12) is written as

$$\Psi=c_{10}\left(a_1-\ln\left[\frac{1}{6}(a_1^3-6a_1a_2+6a_3)\right]-3\right)+D_2\ln^2\left[\frac{1}{6}(a_1^3-6a_1a_2+6a_3)\right]$$

by using

$$\det G=\frac{1}{6}(a_1^3-6a_1a_2+6a_3)\ .$$

Thus, the derivatives are

$$\begin{aligned}\frac{\partial\Psi}{\partial a_1} &= c_{10}\left(1-\frac{3a_1^2-6a_2}{6\det G}\right)+2D_2\ln(\det G)\left(\frac{3a_1^2-6a_2}{6\det G}\right)\\ \frac{\partial\Psi}{\partial a_2} &= (c_{10}-2D_2\ln(\det G))\left(\frac{a_1}{\det G}\right)\\ \frac{\partial\Psi}{\partial a_3} &= (-c_{10}+2D_2\ln(\det G))\left(\frac{1}{\det G}\right)\ ,\end{aligned}$$

which completely defines $\overset{2}{T}$. In the case of Mooney-Rivlin material the function Ψ emerges from an extension of the Neo-Hook function (12) with the additional term

$$\Psi_2=c_{01}\left[\frac{1}{2}(a_1^2-2a_2)-2\ln(\det G)\right]\ .$$

Therefore, additional terms appear in the derivatives of Ψ and the calculation of $\overset{2}{T}$ is straight forward.

Remark 2.1. We mention, that alternative formulations of the Tensor $\overset{2}{T}$ exist, which are equivalent to (9). E. g. for Neo-Hook material the 2nd Piola-Kirchhoff stress tensor can be written as

$$\overset{2}{T}(G) := 2\Big[c_{10}(I - G^{-1}) + D_2 2\ln[\det G]G^{-1}\Big] .$$

Note, that for the above result we have to guarantee the existence of G^{-1} and that G^{-1} is bounded, i.e.

$$\left\|G^{-1}\right\| \leq C < \infty .$$

An alternative representation of the 2nd Piola-Kirchhoff stress tensor for Mooney-Rivlin material is

$$\overset{2}{T}(G) := 2\Big[c_{10}(I - G^{-1}) + c_{01}((\operatorname{tr} G)I - G - 2G^{-1}) + D_2 2\ln[\det G]G^{-1}\Big] .$$

2.5 Solution of the direct problem

We are interested in finding a solution U of the variational problem (2), which denotes a weak solution of the corresponding PDE (1). In the following we reformulate (2) as

$$a(U; V|p) = f(V) \quad \forall V \in (H_0^1(\Omega_0))^3 \tag{15}$$

with the functionals

$$a(U; V|p) := \int\limits_{\Omega_0} \overset{2}{T} : E(U; V)\mathrm{d}\Omega_0 \tag{16}$$

and

$$f(V) = \int\limits_{\Omega_0} \rho_0 \vec{f} \cdot V \mathrm{d}\Omega_0 + \int\limits_{\Gamma_{N_0}} \vec{g} \cdot V \mathrm{d}S_0 . \tag{17}$$

Solving (15) leads in general to a nonlinear system, due to the fact, that $a(U; V|p)$ is only a semilinear functional, being nonlinear in U and linear in V. The functional $a(U; V|p)$ additionally depends on the material parameter vector p via the definition of the 2nd Piola-Kirchhoff stress tensor. In the case of linear elastic material, we set e. g.

$$p = \begin{pmatrix} \lambda \\ \mu \end{pmatrix} .$$

Note, that the dependence of $a(U; V|p)$ from p is also nonlinear for nonlinear material laws.

In order to overcome the nonlinearity of (15), a Newton iteration with incremental applying of loads is adapted (see e. g. [5] or [11]). We introduce a linearization $a_0(U; V, W|p)$ of $a(U; V|p)$ such that

$$a(U + W; V|p) = a(U; V|p) + a_0(U; V, W|p) + \mathcal{O}(\|W\|^2) \, . \tag{18}$$

The idea presented in [11] is, to solve for $t \in [0, 1]$ the auxiliary problem

$$a(U_t; V|p) = tf(V) \; \forall V$$

via a Newton iteration with initial guess $U_{t-\Delta t}$ and appropriately defined time step $\Delta t \ll 1$. This means, that instead the full load (referring to $f(V)$ or $t = 1$, resp.), only a load step is applied as a boundary condition of the PDE. Then continue with setting $t := t + \Delta t$ and repeating the Newton iteration. This iteration process is done until $t = 1$, such that in the last load step the original equation (15) is solved.

Algorithm 2.1 (Newton linearization with stepwise applied loads)**.** The algorithm for solving the variational problem (15) holds the following scheme:

START		define $\Delta t \ll 1$ and $\varepsilon \ll 1$ set $t = \Delta t$ and $U = \vec{0}$
DO WHILE t $\leq$ 1		
NEWTON ITERATION		
	a)	calculate a solution ΔU of $a_0(U; \Delta U, V|p) = tf(V) - a(U; V|p) \quad \forall V$
	b)	set $U := U + \Delta U$
	c)	if $\|\Delta U\|/\|U\| < \varepsilon$: set $t = t + \Delta t$
	d)	go to **a)**
END WHILE		

Note, that for $t = 0$ we choose $U_0 = \vec{0}$ and thus $E(\vec{0}, V) = \varepsilon(V)$ denotes the strain tensor for linear elastic small deformations, i.e. the Newton iteration starts with linear elastic small deformations. The algorithm described above is used in the nonlinear PDE solver of the MATLAB PDE toolbox [18]. The authors of [5] mention, that in their study approximately 80 load steps with 6 Newton iterations for each step were necessary for obtaining convergence of the algorithm. At one hand, if Δt is chosen too large, the iteration process may diverge, but on the other hand a considerable amount of numerical costs results from the repeated call of the forward problem solver.

3 Identification of material parameters

3.1 Discussion of identification problems

For an application of the material laws (10)–(14) the parameters λ, μ, c_{01}, c_{10}, D_2, and α need to be known. Due to the fact, that these parameters cannot be measured directly, we have to solve an appropriate inverse identification problem, where the material parameters are identified from given data. In particular for mechanical inverse problems, the measurement data will denote given displacements or forces at some measuring points.

In literature a wide range of studies on the identification of material parameters can be found. In this context the full linear theory for small deformations and linear elastic material behavior is well known even for the identification of parameter functions. We refer to the extensive survey [1] and the references therein and additionally to the numerical study [8]. For large deformation material parameter identification we mention e. g. the paper [6], where the identification of the scalar parameters $c_{10}, c_{01}, D_2, \alpha$ for the material laws (12)–(14) was considered. In this study a least square minimization with Gauss-Newton (Levenberg-Marquardt) and without any regularization was used (multi parameter regularization was mentioned as option). The identification based on simulated data with and without noise and single as well as simultaneous identification of parameters is discussed. The examined model situations (compressible material) were a cylindric tie bar and the 2D Cook membrane. Several measurement situations, e. g. single measurements and measured stress-strain curves were presented. For the numerical solution of the forward PDE the FE-code SPC-PM2AdNlMix was applied. The results of the study were, that identification was possible and exact in the noiseless and in the noisy case. Best results were reached for Neo-Hook and some small problems arose for Mooney-Rivlin due to the increasing nonlinearity. The recent paper [5] is devoted to the identification of parameter functions for a modified Neo-Hook material law with large deformations. The authors describe an algorithm using Quasi-Newton methods with BFGS. Here, the objective functional is defined as a residual norm with special weights. Additionally, methods for improving the efficiency of the minimization algorithm are suggested. An adaptive FE method is not used.

Up to now, only less studies on the identification of parameter functions for nonlinear material and large deformations can be found in literature. One reason may be, that despite the fact, that almost all presented results were obtained in a simplified 2D framework, the computational cost turn out to be considerable. This results from the nonlinearity of the PDE, which has to be eliminated by an additional Newton linearization. Besides questions concerning the efficiency of solution methods, it is a quite hard and currently not solved question, under what circumstances the large deformation identification problems can be solved uniquely.

3.2 The inverse problem as a minimization problem

Let $p = p(X)$ denote a spatially varying vector of n_{par} material parameters

$$p(X) := \begin{pmatrix} p_1(X) \\ \vdots \\ p_{n_{par}}(X) \end{pmatrix} , \quad X \in \Omega_0 ,$$

with bounded parameter functions $p_i \in L^\infty(\Omega_0)$, $i = 1, \ldots, n_{par}$. For estimating an unknown parameter p, we have to solve the following inverse problem.

Definition 3.1 (Inverse parameter identification problem (IP))**.** *Find for given displacement data U_{data} a parameter $p(X)$ referring to the chosen material law, such that U_{data} and $p(X)$ fulfill the direct problem (15).*

We mention, that often the inverse problem (IP) is formulated as finding a solution of the operator equation

$$\mathcal{F}(p) = U .$$

Here, $\mathcal{F}$ denotes the explicit form of the nonlinear forward operator, assigning the corresponding weak solution U of (15) to a given parameter p.

Additionally, force measurements at a part of the Dirichlet boundary $\tilde{\Gamma}_D \subset \Gamma_D$ can be introduced. Thus, we assume the existence of a force density function $\vec{h}$ and define the force measuring operator

$$\mathcal{G}(U|p) = \vec{h} = \vec{n}_0 \cdot \overset{1}{T}(U)|_{\tilde{\Gamma}_{D_0}} , \tag{19}$$

where U is the solution of (15). Note, that for the numerical solution of [IP] we will not need the explicit existence of $\vec{h}$, due to the fact, that in practice only integrals over $\vec{h}$ at some part of the Dirichlet boundary are of interest.

Remark 3.1. The operator $\mathcal{G}$ is strongly related to the so called Dirichlet-to-Neumann map, which assigns the corresponding boundary loads to a given boundary displacement. In the paper [15] it is shown, that knowledge of the Dirichlet-to-Neumann map is sufficient for the unique solvability of the inverse problem (IP) in the case of linear elastic small deformations. See also [2] for a survey on uniqueness results, derived by analyzing the Dirichlet-to-Neumann map.

A weak formulation of $\mathcal{G}$ can be derived, if we interpret (19) as a Neumann boundary condition, being equivalent to the given Dirichlet boundary condition on $\tilde{\Gamma}_D$. Thus, we find that a solution of

$$a(U;V|p) = f(V) + \int\limits_{\tilde{\Gamma}_{D_0}} \vec{h} \cdot V \mathrm{d}S_0 \qquad \forall V \in (H^1(\Omega_0))^3 \text{ with } V|_{\Gamma_{D_0} \setminus \tilde{\Gamma}_{D_0}} = 0$$

will be equivalent to a solutuion of (15), if $\vec{h}$ is appropriately defined. Note the crucial point in the last equation, that contrary to (15) the space of test functions is slightly changed and consequently the Dirichlet boundary condition at $\tilde{\Gamma}_{D_0}$ is removed.

In other words, for given U and p solving (15), $\vec{h}$ is defined as the solution of the variational problem

$$\int\limits_{\tilde{\Gamma}_{D_0}} \vec{h} \cdot V \mathrm{d}S_0 = a(U;V|p) - f(V) \qquad \forall V \in (H^1(\Omega_0))^3 \text{ with } V|_{\Gamma_{D_0} \setminus \tilde{\Gamma}_{D_0}} = 0 \,. \tag{20}$$

The numerical solution of (20) is easy, due to the fact, that for given U it denotes a postprocessing calculation and in the discrete case the right hand side turns out to be the difference of two already known vectors.

The displacement data may denote a single displacement field, but it is also possible to measure multiple displacement data for differing boundary conditions. Thus, in general we assume

$$U_{data} = (U^1_{data}, \ldots, U^{n_{data}}_{data}) \,. \tag{21}$$

While stepwise applying loads, one can e. g. derive stress-strain curve multiple measurements. In the following, the use of multiple measurements will be indicated by a superscript i and according to (21) we suppose for the displacement

$$U := (U^1, \ldots, U^{n_{data}}) \,.$$

Several strategies for solving (IP) may be of interest. Without claiming completeness we mention three different approaches:

- least squares minimization with Gauss-Newton (Levenberg-Marquardt), studied for the identification of scalar λ, μ in the case of linear elastic small deformations in [8]
- multi parameter regularization strategies (theory [9], numerical studies [8])
- application of optimal control strategies [19], solving a constrained minimization problem with sequential quadratic programming and Lagrange techniques as discussed in [2], [7]

Following the simple least squares minimization approach as discussed in [8], (IP) can be formulated as an unconstrained minimization problem.

Definition 3.2 (Least squares minimization problem)**.** *The least squares minimization problem referring to (IP) is defined as*

$$J_{ls}(p) := \frac{1}{2} \sum_{i=1}^{n_{data}} \left[\omega^i \| \mathcal{P}^i \mathcal{F}^i(p) - U^i_{data} \|^2_{L^2(\Omega_0)} + \vartheta^i \| \mathcal{G}^i(U|p) - \vec{h}^i_{data} \|^2_{L^2(\tilde{\Gamma}_{D_0})} \right] \to \min_p \ . \tag{22}$$

Here, U is eliminated in the objective functional by using the explicit forward operator $\mathcal{F}$. The operator $\mathcal{P}$ denotes a linear projection operator. The weights ω^i and ϑ^i should be chosen, such that all measurements contribute to J_{ls} in the same order of magnitude. As mentioned in [5], additional measurement tensors could be introduced in order to emphasize more accurate measurements over inaccurate ones (if this is known). We omit such measurement tensors here.

The unregularized minimization problem (22) may have no stable solution in the case of parameter function identification, due to an expected ill posedness of the problem (IP). To overcome ill posedness, regularization terms can be added to (22) (e. g. Tikhonov regularization). Another well known regularization strategy in the case of multiple measurements is given by the multi parameter regularization. See e. g. [9] for theory. A numerical study on multi parameter regularization for (IP) with linear elastic small deformations is discussed in [8].

Definition 3.3 (Multi parameter regularization approach)**.** *For a multi parameter regularization approach the inverse problem (IP) is formulated as the constrained minimization problem*

$$\begin{aligned} J_{mp}(p) \quad &:= \quad \frac{1}{2} \| p - \hat{p} \|^2_{L^2(\Omega_0)} \to \min_p \\ s.t. \quad & \left\{ \begin{array}{l} \| \mathcal{P}^i \mathcal{F}^i(p) - U^i_{data} \|_{L^2(\Omega_0)} \leq \delta^i_1 \\ \| \mathcal{G}^i(U|p) - \vec{h}^i_{data} \|_{L^2(\tilde{\Gamma}_{D_0})} \leq \delta^i_2 \\ i = 1, \ldots, n_{data} \end{array} \right. \end{aligned} \tag{23}$$

with an initial guess $\hat{p}$ for the unknown material parameter.

In the following we will focus on a solution approach, which is widely used in optimal control. We assume, that the explicit operator $\mathcal{F}$ is defined by the implicit equation

$$\mathcal{A}(U|p) = 0$$

with $\mathcal{A}(U|p)$ fulfilling

$$\langle \mathcal{A}(U|p), V \rangle_{Z^*,Z} = a(U; V|p) - f(V) \ . \tag{24}$$

In this context, the notation $\langle .,. \rangle_{Z^*,Z}$ stands for the duality product in the space of test functions $Z = (H^1_0(\Omega_0))^3$ and its dual space Z^*. Thus, $\mathcal{A}(U|p) \in Z^*$ is a linear functional in Z. Note, that the definition (24) is natural, since $\mathcal{F}$ is implicitly defined via the variational problem (15). Then we formulate (IP) as a minimization problem with U and p denoting the variables to be optimized and the state equation (1) is considered as a constraint.

Definition 3.4 (Optimal control constrained optimization problem)**.** *With the objective functional*

$$J_{SQP}(U,p) := \frac{1}{2}\sum_{i=1}^{n_{data}} \left[\omega^i \|\mathcal{P}^i U^i - U^i_{data}\|^2_{L^2(\Omega_0)} + \vartheta^i \|\mathcal{G}^i(U|p) - \vec{h}^i_{data}\|^2_{L^2(\tilde{\Gamma}_{D_0})}\right] + R_\alpha(p)\ ,$$

the inverse identification problem (IP) is formulated as the constrained minimization problem

$$\begin{aligned} J_{SQP}(U,p) \quad &\rightarrow \quad \min_{U^i,p} \\ s.t. \qquad & \begin{cases} U^i(p) \text{ fulfill (15)} \ \Leftrightarrow \ \mathcal{A}(U^i|p) = 0 \\ i = 1, \ldots, n_{data} \end{cases} . \end{aligned} \tag{25}$$

Optionally, we can add in (25) the quite natural box constraints

$$0 < C_l \le p(X) \le C_u < \infty\ , \tag{26}$$

if a priori information about lower and upper bounds $C_l, C_u \in \mathbb{R}^{n_{par}}$ of the parameter p is known. Similar to the implicit forward operator $\mathcal{A}(U|p)$, the explicit operator $\mathcal{G}$ can be replaced by setting $\vec{h} := \mathcal{G}(U|p)$ as a variable and optimizing $U, p, \vec{h}$ under the additional constraint

$$\mathcal{H}(U;\vec{h}|p) = 0 \tag{27}$$

with

$$\langle \mathcal{H}(U;\vec{h}|p), V\rangle_{\tilde{Z}^*,\tilde{Z}} = \int\limits_{\tilde{\Gamma}_{D_0}} \vec{h}\cdot V \mathrm{d}S_0 - a(U;V|p) + f(V)\ .$$

Note, that according to (20) here V refers to the space

$$\tilde{Z} = \left\{ V \in (H^1(\Omega_0))^3 \ : \ V|_{\Gamma_{D_0}\setminus\tilde{\Gamma}_{D_0}} = 0 \right\}\ .$$

The term $R_\alpha(p)$ denotes a regularization term with corresponding regularization parameter α. Specific choices of $R_\alpha(p)$ we will discuss later.

3.3 Solution of the constrained minimization problem

In this study we focus on the regularized solution of (IP) via the optimal control minimization problem (25). Here, the idea is as follows: We apply a formal

Lagrange principle for deriving the first order optimality conditions, which leads to a nonlinear system. Then the resulting nonlinear system is solved iteratively by using a Newton method and including regularization terms.

This method denotes a SQP method (sequential quadratic programming) as it is well known in nonlinear optimization. See e. g. [10] for a convergence theory on infinite dimensional optimization with SQP methods. The application of SQP methods as a regularization method for identification problems was presented in [2]. In [7] details on the implementation of SQP methods for implicitly defined inverse problems can be found. Since (IP) can also be seen as an optimal control problem for partial differential equations, we additionally refer to the book [19] for details on optimal control and the formal Lagrange principle for such problems.

For simplicity we start with a single measurement ($n_{data} = 1$) and omit the force measurements $\vec{h}_{data}$ ($\vartheta = 0$). Then w. l. o. g. the weight ω my be assumed as $\omega = 1$. Following the direct Lagrange approach in [7] we define the Lagrange function referring to (25) as

$$L(U; \xi|p) := \frac{1}{2}\|\mathcal{P}U - U_{data}\|^2_{L^2(\Omega_0)} + \langle \mathcal{A}(U|p), \xi\rangle_{Z^*,Z} \; . \tag{28}$$

Note, that in the formal Lagrange principle the Lagrange multiplier $\xi \in Z$ is identified with a test function $V \in Z$ and thus

$$L(U; \xi|p) = \frac{1}{2}\|\mathcal{P}U - U_{data}\|^2_{L^2(\Omega_0)} + a(U; \xi|p) - f(\xi) \; .$$

The first order optimality condition for a minimizer (U^*, ξ^*, p^*) of (25) corresponds in weak formulation to the nonlinear system

$$\begin{aligned} \langle L_p, q\rangle_{Q^*,Q} &= 0 \qquad \forall q \in Q \\ \langle L_U, V\rangle_{Z^*,Z} &= 0 \qquad \forall V \in Z \\ \langle L_\xi, W\rangle_{Z^*,Z} &= 0 \qquad \forall W \in Z \; , \end{aligned} \tag{29}$$

where the space of parameters is set as $Q = (L^\infty(\Omega_0))^{n_{par}}$. In this context we assumed, that all Dirichlet boundary conditions are homogenous and hence $U \in Z$. Consequently, the directional derivatives of the Lagrange function hold

$$\begin{aligned} \langle L_p, q\rangle_{Q^*,Q} &= \langle [\mathcal{A}_p(U^*|p^*)]q, \xi^*\rangle_{Z^*,Z} \\ \langle L_U, V\rangle_{Z^*,Z} &= \langle [\mathcal{A}_U(U^*|p^*)]V, \xi^*\rangle_{Z^*,Z} + \langle \mathcal{P}V, \mathcal{P}U^* - U_{data}\rangle_{L^2(\Omega_0)} \\ \langle L_\xi, W\rangle_{Z^*,Z} &= \langle \mathcal{A}(U^*|p^*), W\rangle_{Z^*,Z} \end{aligned}$$

with the standard scalar product in $L^2(\Omega_0)$

$$\langle a, b\rangle_{L^2(\Omega_0)} = \int\limits_{\Omega_0} ab \, \mathrm{d}\Omega_0 \; .$$

The nonlinear system (29) is solved via a Newton iteration. Thus, the system (29) is linearized for a given iterate (U_k, ξ_k, p_k) and in each Newton step a resulting linear system is solved to calculate an iteration update $(\Delta U, \Delta\xi, \Delta p)$. Due to the Newton linearization, the second order directional derivatives of the Lagrange functional at the iterate (U_k, ξ_k, p_k) have to be calculated. We define the functionals

$$\begin{array}{rcll} L_{pp} & : & Q \to Q^* & \\ L_{UU} & : & Z \to Z^* & \\ L_{pU} & : & Z \to Q^* & \\ L_{Up} & : & Q \to Z^* & \Rightarrow L_{Up} = L_{pU}^{\star} \text{ (dual operator)} \end{array}$$

which holds the weak formulation

$$\begin{array}{lll} \langle L_{pp}q, r\rangle_{Q^*,Q} & = \langle [\mathcal{A}_{pp}(U_k|p_k)](q,r), \xi_k\rangle_{Z^*,Z} & \forall q, r \in Q \\ \langle L_{UU}V, W\rangle_{Z^*,Z} & = \langle [\mathcal{A}_{UU}(U_k|p_k)](V,W), \xi_k\rangle_{Z^*,Z} + \langle \mathcal{P}V, \mathcal{P}W\rangle_{L^2(\Omega_0)} & \forall V, W \in Z \\ \langle L_{pU}V, q\rangle_{Q^*,Q} & = \langle [\mathcal{A}_{pU}(U_k|p_k)](V,q), \xi_k\rangle_{Z^*,Z} & \forall V \in Z, \forall q \in Q \\ \langle L_{Up}q, V\rangle_{Z^*,Z} & = \langle [\mathcal{A}_{Up}(U_k|p_k)](q,V), \xi_k\rangle_{Z^*,Z} & \forall V \in Z, \forall q \in Q\ . \end{array}$$

In the following we simplify the notation and use the abbreviation

$$\mathcal{A}_{(.)} := [\mathcal{A}_{(.)}(U_k|p_k)]$$

for all derivatives. The second derivative of the operator $\mathcal{A}(U|p)$ at the point (U_k, p_k) is defined as

$$[\mathcal{A}''(U_k|p_k)]((V,q),(W,r)) := \mathcal{A}_{pp}(q,r) + \mathcal{A}_{pU}(V,q) + \mathcal{A}_{Up}(q,V) + \mathcal{A}_{UU}(V,W)$$

for $q, r \in Q$ and $V, W \in Z$. As discussed e. g. in [2] and [7], the Newton iteration for solving (29) can be written as

$$U_{k+1} = U_k + \Delta U,\ p_{k+1} = p_k + \Delta p,\ \xi_{k+1} = \xi$$

with an iteration update $(\Delta U, \Delta p)$ solving the quadratic minimization problem

$$\begin{array}{rcl} J_{iter}(\Delta U, \Delta p) & = & \frac{1}{2}\|\mathcal{P}(U_k + \Delta U) - U_{data}\|^2_{L^2(\Omega_0)} \\ & + & \langle [\mathcal{A}''(U_k|p_k)]((\Delta U, \Delta p), (\Delta U, \Delta p)), \xi_k\rangle_{Z^*,Z} + R_{\alpha_k}(p_k) \to \min\limits_{\Delta U, \Delta p} \\ \text{s.t.} & & \mathcal{A}(U_k|p_k) + \mathcal{A}_p\Delta p + \mathcal{A}_U\Delta U = 0 \end{array} \qquad (30)$$

with the Lagrange multiplier ξ referring to the linearized constraint. In (30) the regularization term

$$R_{\alpha_k}(p_k) = \frac{\alpha_k}{2}\|\Delta p - \hat{p}_k\|^2$$

is added. Depending on the choice of the regularization parameter α_k and the initial guess $\hat{p}$, several regularization methods may be implemented, e. g.

- $\hat{p}_k := 0$: Levenberg-Marquardt algorithm
- $\hat{p}_k := \hat{p} - p_k$, $\alpha_k := \alpha = const$: classical Tikhonov regularization
- $\hat{p}_k := \hat{p} - p_k$, $\alpha_k \leq \alpha_{k-1}$: iteratively regularized Gauss-Newton method .

Then the solution of (30) is found as a solution of the linear system

$$\begin{array}{rcll} \langle \mathcal{A}_{pp}(\Delta p, q) + \mathcal{A}_{pU}(\Delta U, q), \xi_k \rangle_{Z^*,Z} & & & \\ +\alpha_k \langle \Delta p, q \rangle_{L^2(\Omega_0)} + \langle \mathcal{A}_p q, \xi \rangle_{Z^*,Z} & = & \alpha_k \langle \hat{p}_k, q \rangle_{L^2(\Omega_0)} & \forall q \in Q \\ \langle \mathcal{A}_{Up}(\Delta p, V) + \mathcal{A}_{UU}(\Delta U, V), \xi_k \rangle_{Z^*,Z} & & & \\ +\langle \mathcal{P}\Delta U, \mathcal{P}V \rangle_{L^2(\Omega_0)} + \langle \mathcal{A}_U V, \xi \rangle_{Z^*,Z} & = & \langle U_{data} - \mathcal{P}U_k, \mathcal{P}V \rangle_{L^2(\Omega_0)} & \forall V \in Z \\ \langle \mathcal{A}_p \Delta p + \mathcal{A}_U \Delta U, W \rangle_{Z^*,Z} & = & \langle \mathcal{A}(U_k|p_k), W \rangle_{Z^*,Z} & \forall W \in Z \end{array} \tag{31}$$

which denotes the first order optimality conditions for (30). We calculate derivatives of the implicit forward operator by linearizing the weak formulation (24). Analogously to the first order linearization $a_0(U; W, V|p)$ of $a(U; V|p)$ (with respect to U) we define the first order linearization (with respect to p) $a_0(U; V|p; \Delta p)$, such that

$$a(U; V|p + \Delta p) = a(U; V|p) + a_0(U; V|p; \Delta p) + \mathcal{O}(\|\Delta p\|^2) \tag{32}$$

and the second order linearizations $a_1(U; \Delta U, W, V|p)$, $a_1(U; W, V|p; \Delta p)$, and $a_1(U; V|p; \Delta p, q)$ via

$$\begin{array}{rcl} a_0(U + \Delta U; W, V|p) & = & a_0(U; W, V|p) + a_1(U; \Delta U, W, V|p) + \mathcal{O}(\|\Delta U\|^2) \\ a_0(U; W, V|p + \Delta p) & = & a_0(U; W, V|p) + a_1(U; W, V|p; \Delta p) + \mathcal{O}(\|\Delta p\|^2) \\ a_0(U + \Delta U; V|p; q) & = & a_0(U; V|p; q) + a_1(U; \Delta U, V|p; q) + \mathcal{O}(\|\Delta U\|^2) \\ a_0(U; V|p + \Delta p; q) & = & a_0(U; V|p; q) + a_1(U; V|p; \Delta p, q) + \mathcal{O}(\|\Delta p\|^2) \ . \end{array} \tag{33}$$

Thus, the derivatives of $\mathcal{A}$ hold the weak formulation

$$\begin{array}{rcl} \langle \mathcal{A}_p q, V \rangle_{Z^*,Z} & = & a_0(U_k; V|p_k; q) \\ \langle \mathcal{A}_U W, V \rangle_{Z^*,Z} & = & a_0(U_k; W, V|p_k) \\ \langle \mathcal{A}_{pp}(q, r), V \rangle_{Z^*,Z} & = & a_1(U_k; V|p_k; q, r) \\ \langle \mathcal{A}_{UU}(W_1, W_2), V \rangle_{Z^*,Z} & = & a_1(U_k; W_1, W_2, V|p_k) \\ \langle \mathcal{A}_{pU}(W, q), V \rangle_{Z^*,Z} & = & a_1(U_k; W, V|p_k; q) \\ \langle \mathcal{A}_{Up}(q, W), V \rangle_{Z^*,Z} & = & a_1(U_k; W, V|p_k; q) \ . \end{array}$$

Referring to the above calculations and using the abbreviations

$$\begin{array}{rcl} b_p(q, r) & := & \langle q, r \rangle_{L^2(\Omega_0)} = \displaystyle\int_{\Omega_0} qr \, \mathrm{d}\Omega_0 \quad q, r \in Q \\ b_U(V, W) & := & \langle \mathcal{P}V, \mathcal{P}W \rangle_{L^2(\Omega_0)} = \displaystyle\int_{\Omega_0} (\mathcal{P}V)(\mathcal{P}W) \mathrm{d}\Omega_0 \quad V, W \in Z \ , \end{array}$$

the linear system (31) is finally formulated as

$$\begin{array}{rcll}
\alpha_k b_p(\Delta p, q) + a_1(U_k; \xi_k | p_k; \Delta p, q) & & & \forall q \in Q \\
+a_1(U_k; \Delta U, \xi_k | p_k; q) + a_0(U_k; \xi | p_k; q) & = & \alpha_k b_p(q, p_k^*) & \\
a_1(U_k; \xi_k, V | p_k, \Delta p) + b_U(\Delta U, V) & & & \forall V \in Z \\
+a_1(U_k; \Delta U, \xi_k, V | p_k) + a_0(U_k; \xi, V | p_k) & = & \langle U_{data} - \mathcal{P}U_k, \mathcal{P}V \rangle_{L^2(\Omega_0)} & \\
a_0(U_k; W | p_k; \Delta p) + a_0(U_k; \Delta U, W | p_k) & = & f(W) - a(U_k; W | p_k) & \forall W \in Z
\end{array} \tag{34}$$

Remark 3.2. For a linear material law the functional $a(U; V|p)$ is linear in p and thereby the derivatives of $\mathcal{A}$ with respect to p can be simplified to

$$\begin{array}{rcl}
\langle \mathcal{A}_p q, V \rangle_{Z^*,Z} & = & a(U_k; V|q) \\
\langle \mathcal{A}_{pp}(q, r), V \rangle_{Z^*,Z} & = & 0 \\
\langle \mathcal{A}_{pU}(W, q), V \rangle_{Z^*,Z} & = & a_0(U_k; W, V|q) \\
\langle \mathcal{A}_{Up}(q, W), V \rangle_{Z^*,Z} & = & a_0(U_k; W, V|q) \,.
\end{array}$$

Remark 3.3. The calculation of $a(U_k; V|p_k)$ is equivalent to the solution of a nonlinear PDE. According to the linearization (18), a stepwise updating of $a(U_k; V|p_k)$ could be introduced, where we assume, that $a(U_k; V|p_k)$ is known (e. g. $U_0 = 0 \Rightarrow a(0; V|p_0) = 0$) and

$$\begin{array}{rcl}
a(U_k + \Delta U; V|p_k + \Delta p) & = & a(U_k; V|p_k) + a_0(U_k; \Delta U, V|p_k) + a_0(U_k; V|p_k; \Delta p) \\
& + & a_1(U_k; \Delta U, V|p_k; \Delta p) + \mathcal{O}(\|\Delta U\|^2) + \mathcal{O}(\|\Delta p\|^2) \,.
\end{array}$$

Consequently, we set the update formula

$$a(U_k+\Delta U; V|p_k+\Delta p) \approx a(U_k; V|p_k)+a_0(U_k; \Delta U, V|p_k)+a_0(U_k; V|p_k; \Delta p) \,. \tag{35}$$

Thus, by this linearization strategy, the additional explicit calculation of the functional $a(U_k; V|p_k)$ may be omitted. Note, that this improves efficiency, but an additional error arises as well, because formula (35) denotes an approximation. For the forward operator calculation it works well, if the stepsize parameter Δt is chosen appropriately. For the inverse problem this might be realized by using a stepsize control in the SQP iteration, such that ΔU and Δp are small enough.
Remark 3.4. Often, the linear system (31) or (34), resp., is simplified by removing all the second order derivative terms.

In (28) we ignored additional force measurements, multiple measurements and box constraints. Now we consider, how the systems (31) and (34) have to be completed referring to these extensions. Let us first assume, that an additional force measurement is introduced and thus the Lagrange function (28) is extended by the term

$$L_{\mathcal{G}}(U|p) := \frac{1}{2} \|\mathcal{G}(U|p) - \vec{h}_{data}\|^2_{L^2(\tilde{\Gamma}_{D_0})} \,.$$

For calculating the SQP iteration update via (30) we have to find derivatives of

$$J_{\mathcal{G}}(U_k + \Delta U, p_k + \Delta p) := \frac{1}{2}\|\mathcal{G}(U_k + \Delta U|p_k + \Delta p) - \vec{h}_{data}\|^2_{L^2(\tilde{\Gamma}_{D_0})}$$

with respect to ΔU and Δp. These derivatives can be deduced from linearizing

$$\begin{aligned} \frac{1}{2}\|\mathcal{G}(U|p) - \vec{h}_{data}\|^2_{L^2(\tilde{\Gamma}_{D_0})} &= \frac{1}{2}\sum_{W\in\mathbb{W}} \langle \mathcal{G}(U|p) - \vec{h}_{data}, W\rangle^2_{L^2(\tilde{\Gamma}_{D_0})} \\ &= \frac{1}{2}\sum_{W\in\mathbb{W}} \Big[a(U;W|p) - f(W) - \langle \vec{h}_{data}, W\rangle_{L^2(\tilde{\Gamma}_{D_0})}\Big]^2 \end{aligned} \tag{36}$$

where the set $\mathbb{W}$ has to fulfill

$$\begin{aligned} \mathbb{W} = \Big\{ & W_i \in (H^1(\Omega_0))^3 \ : \ W_i|_{\Gamma_{D_0}\setminus\tilde{\Gamma}_{D_0}} = 0, \\ & \{W_i|_{\tilde{\Gamma}_{D_0}}\}_{i\in\mathbb{N}} \text{ is an orthonormal basis of } L^2(\tilde{\Gamma}_{D_0}) \Big\} . \end{aligned}$$

Note, that the W_i are not an elements of the space of test functions $Z = (H^1_0(\Omega_0))^3$. We set

$$f_{\mathcal{G}}(W) := f(W) + \langle \vec{h}_{data}, W\rangle_{L^2(\tilde{\Gamma}_{D_0})}$$

and consequently for all $V \in Z$ and $q \in Q$ a linearization of each summand in (36) holds

$$\begin{aligned} \frac{1}{2}\big[a(U+V;W|p) - f_{\mathcal{G}}(W)\big]^2 &\approx \frac{1}{2}\big[a(U;W|p) + a_0(U;V,W|p) - f_{\mathcal{G}}(W)\big]^2 \\ &= \frac{1}{2}\Big[\big(a(U;W|p) - f_{\mathcal{G}}(W)\big)^2 + a_0(U;V,W|p)^2\Big] \\ &\quad + \big[a(U;W|p) - f_{\mathcal{G}}(W)\big]a_0(U;V,W|p) \\ \frac{1}{2}\big[a(U;W|p+q) - f_{\mathcal{G}}(W)\big]^2 &\approx \frac{1}{2}\big[a(U;W|p) + a_0(U;W|p;q) - f_{\mathcal{G}}(W)\big]^2 \\ &= \frac{1}{2}\Big[\big(a(U;W|p) - f_{\mathcal{G}}(W)\big)^2 + a_0(U;W|p;q)^2\Big] \\ &\quad + \big[a(U;W|p) - f_{\mathcal{G}}(W)\big]a_0(U;W|p;q) , \end{aligned}$$

with

$$a_0(U;V,W|p)^2 = \mathcal{O}(\|V\|^2) \quad \text{and} \quad a_0(U;W|p;q)^2 = \mathcal{O}(\|q\|^2) .$$

Due to the definition of $J_{\mathcal{G}}(\Delta U, \Delta p)$ we replace $U := U_k + \Delta U$ and $p := p_k + \Delta p$ in the above equations and get

$$\frac{\partial J_{\mathcal{G}}}{\partial \Delta U} \quad \Rightarrow \quad \big[a(U_k + \Delta U; W|p_k + \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k + \Delta U; V, W|p_k + \Delta p)$$
$$\frac{\partial J_{\mathcal{G}}}{\partial \Delta p} \quad \Rightarrow \quad \big[a(U_k + \Delta U; W|p_k + \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k + \Delta U; W|p_k + \Delta p; q)$$

As mentioned in remark 3.3, these terms are still nonlinear in ΔU and Δp. We continue for the derivative with respect to ΔU

$$\begin{aligned}
&\big[a(U_k + \Delta U; W|p_k + \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k + \Delta U; V, W|p_k + \Delta p) \\
&\quad \approx \Big(\big[a(U_k; W|p_k) + a_0(U_k; \Delta U, W|p_k) + a_0(U_k; W|p_k; \Delta p) - f_{\mathcal{G}}(W)\big] \\
&\qquad \big[a_0(U_k; V, W|p_k) + a_1(U_k; \Delta U, V, W|p_k) + a_1(U_k; V, W|p_k; \Delta p)\big]\Big) \\
&\quad \approx \big[a(U_k; W|p_k) + a_0(U_k; \Delta U, W|p_k) + a_0(U_k; W|p_k; \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k; V, W|p_k) \\
&\qquad + \big[a(U_k; W|p_k) - f_{\mathcal{G}}(W)\big] \big[a_1(U_k; \Delta U, V, W|p_k) + a_1(U_k; V, W|p_k; \Delta p)\big]
\end{aligned} \tag{37}$$

and analogously for the derivative with respect to Δp

$$\begin{aligned}
&\big[a(U_k + \Delta U; W|p_k + \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k + \Delta U; W|p_k + \Delta p; q) \\
&\quad \approx \big[a(U_k; W|p_k) + a_0(U_k; \Delta U, W|p_k) + a_0(U_k; W|p_k; \Delta p) - f_{\mathcal{G}}(W)\big] a_0(U_k; W|p_k; q) \\
&\qquad + \big[a(U_k; W|p_k) - f_{\mathcal{G}}(W)\big] \big[a_1(U_k; \Delta U, W|p_k, q) + a_1(U_k; W|p_k; \Delta p, q)\big] .
\end{aligned} \tag{38}$$

Finally, we have to add terms referring to (37) and (38) in the first ($\Rightarrow \partial/\partial \Delta p$) and in the second ($\Rightarrow \partial/\partial \Delta U$) equation of the linear system (34):

- 1st equation, left hand side

$$\sum_{W \in \mathbb{W}} \Big\{ \big[a_0(U_k; \Delta U, W|p_k) + a_0(U_k; W|p_k; \Delta p)\big] a_0(U_k; W|p_k; q)$$
$$+ \big[a(U_k; W|p_k) - f_{\mathcal{G}}(W)\big] \big[a_1(U_k; \Delta U, W|p_k, q) + a_1(U_k; W|p_k; \Delta p, q)\big] \Big\}$$

- 1st equation, right hand side

$$\sum_{W \in \mathbb{W}} \Big\{ - \big[a(U_k; W|p_k) - f_{\mathcal{G}}(W)\big] a_0(U_k; W|p_k; q) \Big\}$$

- 2nd equation, left hand side

$$\sum_{W \in \mathbb{W}} \Big\{ \big[a_0(U_k; \Delta U, W|p_k) + a_0(U_k; W|p_k; \Delta p)\big] a_0(U_k; V, W|p_k)$$
$$+ \big[a(U_k; W|p_k) - f_{\mathcal{G}}(W)\big] \big[a_1(U_k; \Delta U, V, W|p_k) + a_1(U_k; V, W|p_k; \Delta p)\big] \Big\}$$

- 2nd equation, right hand side

$$\sum_{W\in\mathbb{W}} \Big\{ - \big[a(U_k;W|p_k) - f_{\mathcal{G}}(W)\big] a_0(U_k;V,W|p_k) \Big\}$$

Remark 3.5. If $\mathcal{G}$ is considered implicitly in (25) via the added constraint (27), we have to introduce a Lagrange multiplier $\xi_{\mathcal{G}}$ referring to this constraint. Then the linear system (34) is extended by a fourth equation, which results from the linearization with respect to $\xi_{\mathcal{G}}$.

Now we discuss the implementation of box conditions (26). The idea (see e. g. [19]) is the following: in the Lagrange functional (28) for the minimization problem (25) with box constraints (26) we add the term

$$L_{box}((\xi_l,\xi_u)|p) := \int\limits_{\Omega_0} \xi_l(C_l - p) + \xi_u(p - C_u)\mathrm{d}\Omega_0 \ ,$$

with Lagrange multipliers ξ_l and ξ_u referring to the lower and the upper bounds C_l and C_u. Note, that for the components $\xi_l^*, \xi_u^*, p_{box}^*$ of an optimal solution of (25) with box conditions the complementary slackness conditions

$$(\xi_l^*)_j(p_{box}^* - C_l)_j = 0, \quad j = 1,\dots,n_{par}$$

$$(\xi_u^*)_j(C_u - p_{box}^*)_j = 0, \quad j = 1,\dots,n_{par}$$

have to be fulfilled, i.e. for the lower bound constraint

- the lower bound for the jth component of p is active:

$$(p_{box}^*)_j = (C_l)_j \quad \Rightarrow \quad (\xi_l^*)_j \text{ variable}$$

- the lower bound for the jth component of p is inactive:

$$(p_{box}^*)_j > (C_l)_j \quad \Rightarrow \quad (\xi_l^*)_j := 0$$

(if the box constraint is inactive, it can be omitted).

The distinction between active and inactive upper bounds is analogously. Thus, the box constraints have only to be taken into account, if they are active and therefore the Lagrange functional $L_{box}((\xi_l^*,\xi_u^*)|p_{box}^*)$ is only defined over the so called active set.

We calculate derivatives of L_{box} with respect to ξ_l, ξ_u, and p (all other derivatives and second order derivatives are zero) and modify the linear system (34) for a given iterate (U_k, p_k, ξ_k) in the following way:

- introduce variables $\xi_l, \xi_u \in Q$ and set

$$(\xi_l(X))_j := 0 \quad \text{for} \quad (p_k(X))_j > (C_l)_j \tag{39}$$
$$(\xi_u(X))_j := 0 \quad \text{for} \quad (p_k(X))_j < (C_u)_j \tag{40}$$

  (minimization only over the active set)

- add in the first equation at the left hand side ($\Rightarrow \frac{\partial}{\partial \Delta p} L_{box}((\xi_l, \xi_u)|p_k + \Delta p)$)

$$\int_{\Omega_0} (-\xi_l + \xi_u) q \mathrm{d}\Omega_0$$

- add an equation referring to the lower bound ($\Rightarrow \frac{\partial}{\partial \xi_l} L_{box}((\xi_l, \xi_u)|p_k + \Delta p)$)

$$-\int_{\Omega_0} \Delta p \, q_l \mathrm{d}\Omega_0 = \int_{\Omega_0} (p_k - C_l) q_l \mathrm{d}\Omega_0 \quad \forall q_l \in Q \text{ fulfilling (39)}$$

- add an equation referring to the upper bound ($\Rightarrow \frac{\partial}{\partial \xi_u} L_{box}((\xi_l, \xi_u)|p_k + \Delta p)$)

$$\int_{\Omega_0} \Delta p \, q_u \mathrm{d}\Omega_0 = \int_{\Omega_0} (C_u - p_k) q_u \mathrm{d}\Omega_0 \quad \forall q_u \in Q \text{ fulfilling (40)} .$$

A solution $(\Delta U, \Delta p, \xi, \xi_l, \xi_u)$ of (34) under the above modifications denotes the SQP update for (25) with Lagrange multipliers ξ_l and ξ_u enforcing the bounds of the box constraints.

As a last modification of (34) we assume, that multiple measured displacement fields U^i_{data} are available. Then the Lagrange functional is defined according to J_{SQP} in (25) as

$$L_{mult}(U; \xi|p) := \frac{1}{2} \sum_{i=1}^{n_{data}} \left[\omega^i \|\mathcal{P}^i U^i - U^i_{data}\|^2_{L^2(\Omega_0)} + a(U^i; \xi^i|p) - f(\xi^i) \right]$$

with $2n_{data} + 1$ variables $U = (U^1, \ldots, U^{n_{data}})$, $\xi = (\xi^1, \ldots, \xi^{n_{data}})$, and p ($i = 1, \ldots, n_{data}$). For simplicity we omit the force measurements $\vec{h}^i_{data}$, which can be handled analogously.

Under the above assumptions, the adaption of the system (34) for L_{mult} is calculated as

$$\alpha_k b_p(\Delta p, q) + \sum_{i=1}^{n_{data}} \left[a_1(U^i_k; \xi^i_k|p_k; \Delta p, q) + a_1(U^i_k; \Delta U^i, \xi^i_k|p_k; q) + a_0(U^i_k; \xi^i|p_k; q) \right]$$
$$= \alpha_k b_p(q, p^*_k)$$
$$\forall q \in Q \tag{41}$$

$$a_1(U_k^i;\xi_k^i,V^i|p_k,\Delta p)+\omega_i\, b_U(\Delta U^i,V^i)+a_1(U_k^i;\Delta U^i,\xi_k^i,V^i|p_k)+a_0(U_k^i;\xi^i,V^i|p_k)$$
$$=\omega_i\langle U^i_{data}-\mathcal{P}^iU_k^i,\mathcal{P}^iV^i\rangle_{L^2(\Omega_0)}$$
$$\forall V^i\in Z,\ i=1,\dots,n_{data} \tag{42}$$

$$a_0(U_k^i;W^i|p_k;\Delta p)+a_0(U_k^i;\Delta U^i,W^i|p_k)=f(W^i)-a(U_k^i;W^i|p_k)$$
$$\forall W^i\in Z,\ i=1,\dots,n_{data}\quad , \tag{43}$$

which is a linear system of the dimension $(2n_{data}+1)\times(2n_{data}+1)$.

Concluding this section, we want to give a general scheme for the introduced algorithm of solving [IP] via SQP methods.
Algorithm 3.1 (SQP identification algorithm for [IP])**.** The SQP iteration holds the following scheme:

START		set $k:=0$ choose initial guess U_0,p_0 set the Lagrange multiplier $\xi_0=0$ choose regularization parameter α_0
REPEAT		
SQP ITERATION		
	a)	calculate a solution $\Delta U,\Delta p,\xi$ of (34)
	b)	update $U_{k+1}:=U_k+\Delta U$, $p_{k+1}:=p_k+\Delta p$, $\xi_{k+1}:=\xi$
	c)	$k:=k+1$
UNTIL		stopping rule fulfilled

In this context we discuss the choice of initial guesses and stopping rules for the SQP iteration. The initial displacement field has to fulfill the given Dirichlet boundary conditions. In particular, if the Dirichlet boundary conditions are inhomogeneous, the initial value U_0 has to be set appropriately. Thus it follows, that all displacement updates ΔU can be restricted to homogenous Dirichlet boundary, i. e. $\Delta U\in Z$. Therefore all the equations derived in this section hold for inhomogeneous Dirichlet boundary, too. An adequate choice for U_0 is given by calculating $U_0:=U(p_0)$ as a solution of the forward problem (2) for an initial material parameter p_0.

The initial parameter p_0 should be chosen as close as possible to the exact solution $p^\dagger$. As shown in [2], under some conditions the SQP iteration converges locally in a ball $\mathcal{B}_{\rho_U}(U^\dagger)\times\mathcal{B}_{\rho_p}(p^\dagger)$ around the exact solution $(U^\dagger,p^\dagger)$ with ρ_U,ρ_p being small enough. We refer to [2] also for the question, which conditions have to be fulfilled for the choice of the regularization parameter α_k, such that well posedness of each iteration step and convergence of the iteration is guaranteed.

Another important question is, how to find a stopping index K_0, such that the SQP iteration can be terminated after the K_0th iteration with adequate results.

Common and natural stopping rules are e.g.

- terminate, if the residual norm is smaller than a given tolerance:

$$K_0 : \quad \|\mathcal{P}U_{K_0} - U_{data}\| \leq tol_{res}$$

- terminate, if the norm of the updates in the K_0th iteration is smaller than given tolerances:

$$K_0 : \quad \|\Delta U\| \leq tol_U, \|\Delta p\| \leq tol_p$$

- terminate, if an a priori defined maximum number of iterations is reached:

$$K_0 := K_{max}.$$

These stopping rules work quite well for well posed problems or noiseless data. In the case of ill posed problems with noisy data, the stopping index has to be defined appropriately with respect to the noise level δ. This denotes an iterative regularization method, which is discussed in detail in [2]. Under the assumption, that the given data is corrupted by noise with a noise level δ, i. e.

$$\|U^{\delta}_{data} - \mathcal{P}U(p^{\dagger})\| \leq \delta \ ,$$

a suitable choice for the stopping index K_0 is given by the generalized discrepancy principle

$$\|\mathcal{P}U_{K_0} - U^{\delta}_{data}\| \leq \tau\delta < \|\mathcal{P}U_k - U^{\delta}_{data}\| \quad \forall k < K_0 \tag{44}$$

with an appropriately chosen $\tau > 1$. See [2] for details.

3.4 Parameter identification for linear elastic material

Now we to apply the identification algorithm presented above for the linear elastic material law (10). According to (11), the 2nd Piola-Kirchhoff stress tensor holds

$$\overset{2}{T} = \mathbb{C} : E(U)$$

with a symmetrical material tensor $\mathbb{C} = \mathcal{C}(p) = \mathcal{C}(\lambda, \mu)$. Note, that $\mathbb{C}$ is depending linearly on the parameter $p = (\lambda, \mu)$. Consequently, the semilinearform $a(U; V|p)$ is defined as

$$a(U; V|p) = \int\limits_{\Omega_0} E(U) : \mathbb{C}(p) : E(U; V) \mathrm{d}\Omega_0 \ .$$

We calculate linearizations of $a(U;V|p)$. As deduced in [11], the first order linearization with respect to U is given by

$$a_0(U;W,V|p) := \int\limits_{\Omega_0} \left[E(U;W) : \mathbb{C}(p) : E(U;V) + \left(\overset{2}{T}(U) \cdot \mathrm{Grad}W \right) : \mathrm{Grad}V \right] \mathrm{d}\Omega_0 \ .$$

The linearization of $a_0(U;W,V|p)$ with respect to U reads as

$$\begin{aligned} a_0(U+\Delta U;W,V|p) &= \int\limits_{\Omega_0} \Big[E(U+\Delta U;W) : \mathbb{C} : E(U+\Delta U;V) \\ &\qquad + \big((E(U+\Delta U) : \mathbb{C}) \cdot \mathrm{Grad}W \big) : \mathrm{Grad}V \Big] \mathrm{d}\Omega_0 \end{aligned}$$

with

$$E(U+\Delta U) = E(U) + E(U;\Delta U) + \mathcal{O}(\|\Delta U\|^2)$$

and

$$E(U+\Delta U;V) = E(U;V) + \frac{1}{2} \big((\mathrm{Grad}\, \Delta U) \cdot (\mathrm{Grad}\ V)^T + (\mathrm{Grad}\ V) \cdot (\mathrm{Grad}\, \Delta U)^T \big) \ .$$

Hence it follows

$$\begin{aligned} & a_0(U+\Delta U;W,V|p) = a_0(U;W,V|p) \\ &+ \int\limits_{\Omega_0} \left[E(U;W) : \mathbb{C} : \frac{1}{2} \big((\mathrm{Grad}\, \Delta U) \cdot (\mathrm{Grad}\ V)^T + (\mathrm{Grad}\ V) \cdot (\mathrm{Grad}\, \Delta U)^T \big) \right] \mathrm{d}\Omega_0 \\ &+ \int\limits_{\Omega_0} \left[\frac{1}{2} \big((\mathrm{Grad}\, \Delta U) \cdot (\mathrm{Grad}\ W)^T + (\mathrm{Grad}\ W) \cdot (\mathrm{Grad}\, \Delta U)^T \big) : \mathbb{C} : E(U;V) \right] \mathrm{d}\Omega_0 \\ &+ \int\limits_{\Omega_0} \Big[\big((E(U;\Delta U) : \mathbb{C}) \cdot \mathrm{Grad}W \big) : \mathrm{Grad}V \Big] \mathrm{d}\Omega_0 \\ &+ \mathcal{O}(\|\Delta U\|^2) \end{aligned}$$

and consequently

$$\begin{aligned} a_1(U;\Delta U;W,V|p) &:= \int\limits_{\Omega_0} \Big[\big((E(U;\Delta U) : \mathbb{C}) \cdot \mathrm{Grad}W \big) : \mathrm{Grad}V \\ &\qquad + \big((E(U;W) : \mathbb{C}) \cdot \mathrm{Grad}V \big) : \mathrm{Grad}\Delta U \\ &\qquad + \big((E(U;V) : \mathbb{C}) \cdot \mathrm{Grad}\Delta U \big) : \mathrm{Grad}W \Big] \mathrm{d}\Omega_0 \ . \end{aligned}$$

Referring to remark 3.2 the linearizations with respect to p are defined as

$$\begin{aligned} a_0(U; V|p; q) &:= a(U; V|q) \\ a_1(U; V|p; q, \Delta p) &:= 0 \\ a_1(U; W, V|p; q) &:= a_0(U; W, V|q) \end{aligned}$$

and therewith the system (34) is completely defined for linear elasticity.

4 Future work, ideas and problems

A couple of questions concerning the solution of [IP] is still open:

- The convergence analysis in [2] includes a large number of conditions (e. g restriction of nonlinearity, choice of τ for (44), and a lot of others) that have to be fulfilled in order to guarantee convergence of the SQP iteration. In this paper we omitted a discussion of such conditions, and if they coincide with our framework.
- We also ignored the question, whether [IP] has a unique solution or not. In the paper [15] the unique identifiability of material parameters for linear elasticity with small deformations is shown, if the Dirichlet-to-Neumann map is known. Up to now (see e. g. [1] and [5]) it is not clear, if this result can be adapted for large deformations. But as a consequence, stepwise applying of loads with measuring of multiple displacement fields may improve the results of the identification problem compared to single measurements.
- A convergence analysis for the Newton iteration in algorithm 2.1 may answer questions on how to define Δt (or $\Delta U, \Delta p$ if the update of $a(U; V|p)$ via (35) is used) small enough.
- The identification algorithm was only applied for the linear material law (10). For an application of nonlinear materials, the corresponding linearizations have to be introduced.

A numerical study referring to the contents of this paper will be presented in [13].

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