Identification of material parameters of inelastic constitutive laws from displacement fields

M. Springmann & M. Kuna
Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany

Abstract

In this work a non-linear optimization method is presented to identify material parameters of the Gurson–Tvergaard–Needleman damage model from inhomogeneous displacement fields. The ductile damage model is implemented into the finite element code SPC-PMHP for parallel computers. The material parameters are identified by comparison of the measured and calculated displacement fields. For determining the material parameters, the solution of the direct problem is embedded in a gradient based method. Deterministic optimization procedures are used to determine parameters by means of a least-squares functional. A semi-analytical sensitivity analysis is applied to calculate the gradient of the objective function. Numerical experiments with synthetically generated displacement fields were carried out to test the applicability and the efficiency of the optimization algorithm.

Keywords: damage mechanics, parameter identification, non-linear optimization, sensitivity analysis.

1 Introduction

The development and application of material models for inelastic material behaviour usually consists of the formulation of a mathematical model based on physical phenomena and of the identification of the material constants [1, 2]. To identify the material parameters, in many cases experiments with homogeneous stress and strain distributions are sufficient. However, for more complex inelastic deformation and damage laws we are faced with two problems:
• large deformations occur in the specimens (e.g. necking), which causes inhomogeneous stress and strain fields,
• the large number of unknown material parameters requires more comprehensive information from the experiment than a simple force–displacement curve.

To overcome this problem, complete deformation fields have to be exploited in combination with proper large strain finite element analysis. In [2, 3, 4] a method is deduced to determine the parameters with non-linear optimization procedures, which was applied especially to the GTN–model [5] as well as to the ROUSSELIER model [6, 7].

In this paper the parameters of the GURSON–TVERGAARD–NEEDLEMAN model (GTN–model) are investigated from inhomogeneous displacement fields. In the first part the basic equations of the GTN–model are resumed. The second part deals with the solution of the inverse problem for the parameter identification. Furthermore, several numerical experiments are performed in order to check the efficiency of the identification algorithm.

2 Gurson model

Failure of ductile metals is the result of various micro-mechanical mechanisms, characterized by nucleation, growth and coalescence of micro-voids. The GURSON–TVERGAARD–NEEDLEMAN model [8, 9] describes these effects in the frame of a porous plasticity by a flow potential with the parameters \((q_1, q_2, q_3)\) and with a modified damage variable \(f^*\):

\[
Y = \frac{-3II^D}{\sigma_{YM}^2} + 2q_1f^* \cosh \left( \frac{1}{2} \frac{q_2}{\sigma_{YM}} I_T \right) - \left(1 + q_3f^{*2} \right) = 0. \tag{1}
\]

\(T\) denotes the 2. PIOLA–KIRCHHOFF stress tensor and the superscript \(D\) signifies the deviatoric part. The material equations and the following relations of the parameter identification are considered in the LAGRANGE description for large deformation analysis. The damage variable \(f^*\) is a function of the void volume fraction \(f\):

\[
f^*(f) = \begin{cases} f & \forall f \leq f_c \\ f_c + \frac{q_1^{-1} - f_c}{f_F - f_c} (f - f_c) & \forall f > f_c \end{cases}. \tag{2}
\]

The parameter \(f_c\) characterizes the beginning of void nucleation and \(f_F\) denotes the final failure. The hardening of the matrix material depends on the equivalent plastic strain \(\varepsilon_{pM}^p\) and is given by a power law including three material parameters (initial yield stress \(\sigma_0\), hardening parameters \(\varepsilon_0\) and \(n\)):

\[
\sigma_{YM}(\varepsilon_{pM}^p) = \sigma_0 \left( \frac{\varepsilon_{pM}^p}{\varepsilon_0} + 1 \right)^n. \tag{3}
\]
Using plastic work equivalence one receives an evolution equation for the internal hardening variable ($\dot{\lambda}$ is the plastic multiplier):

$$\dot{\varepsilon}^p_{vM} = \dot{\lambda} \frac{1}{\sigma_{YM}(1 - f)} T : \frac{\partial Y}{\partial T}. \quad (4)$$

The damage evolution in a ductile metal arises from growth and nucleation of voids. Consequently, the evolution equation reads:

$$\dot{f} = \dot{f}_{growth} + \dot{f}_{nucleation}. \quad (5)$$

With the assumption of plastic incompressibility of the matrix material the void growth is given by:

$$\dot{f}_{growth} = \dot{\lambda}(1 - f) I \frac{\partial Y}{\partial T}. \quad (6)$$

The nucleation of voids is a very complex physical process depending on the microstructure of the material. CHU and NEEDLEMAN complemented the GURSON model by a statistical approach [10]:

$$\dot{f}_{nucleation} = \frac{f_N}{s_N \sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{\varepsilon^p_{vM} - \varepsilon_N}{s_N}\right)^2\right] \dot{\varepsilon}^p_{vM}. \quad (7)$$

In the represented form the GURSON model contains 12 material parameters:

$$p = (\sigma_0, \varepsilon_0, n, q_1, q_2, q_3, f_0, f_c, f_F, f_N, \varepsilon_N, s_N) \, T. \quad (8)$$

The described damage model is implemented in the finite element system SPC-PMHP, which was developed for numerical simulations of hyperelastic-plastic large deformation problems within the framework of the DFG-project “Scientific Parallel Computing” [11, 12]. The constitutive law is a system of differential and algebraic equations:

$$\frac{dC^p}{dt} - 2\dot{\lambda} \frac{\partial Y}{\partial T} = 0 \quad (9)$$

$$\frac{d\varepsilon^p_{vM}}{dt} - \varepsilon^p_{vM} = 0 \quad (10)$$

$$\frac{df}{dt} - \dot{f} = 0 \quad (11)$$

$$\dot{\lambda} Y = 0. \quad (12)$$

For the discretization in time a multi-step time integration method is used [6, 12] and the discretized initial value problem for local integration of the constitutive law can be written in a compact non-linear algebraic form:

$$G(z) = 0 \quad \text{with} \quad z = \left(C^p, \varepsilon^p_{vM}, f, \dot{\lambda}\right) \, T. \quad (13)$$

$C^p$ denotes the plastic part of the right CAUCHY–GREEN deformation tensor.
3 Parameter identification

The parameter identification is mathematically an inverse problem [1]:

\[ A^{-1} \cdot u = p. \]  \hspace{1cm} (14)

The operator \( A \) represents the solution of the direct boundary value problem and specifies the relation between the material parameters \( p \) and the displacements \( u \). Generally, the inversion of \( A \) is not possible explicitly. In this paper non-linear optimization procedures are used to identify material parameters by means of minimization of the least-squares functional:

\[ \Phi(p) = \frac{1}{2} \sum (u(p) - \bar{u})^2 \rightarrow \text{min}. \]  \hspace{1cm} (15)

The measured displacements \( \bar{u} \) and the calculated displacements \( u(p) \) will be compared and the material parameters must be improved until the least-squares function achieves the global minimum. The minimum is found by a non-linear iterative optimization procedure. Starting from the previous solution \( p_l \), an improved parameter set is found by:

\[ p_{l+1} = p_l + w s_l, \]  \hspace{1cm} (16)

where \( w \) is the step length and \( s \) is the search direction. To calculate the search direction the method of LEVENBERG and MARQUARDT is used [4, 13]:

\[ s_l = - \left( \nabla^2 \Phi_l + \mu E \right)^{-1} \cdot \nabla \Phi_l, \]  \hspace{1cm} (17)

whereby \( \mu \) decreases in the course of the iteration process and \( E \) denotes the identity matrix. The determination of the search direction (17) needs the knowledge of the first:

\[ \nabla \Phi = \Phi_{,m} = \sum_{i=1}^{n_L} \sum_{j=1}^{n_M} \sum_{k=1}^{n_D} \left( \{ u_k(p) \}_{ij} - \{ \bar{u}_k \}_{ij} \right) \frac{d \{ u_k \}_{ij}}{dp_m}, \]  \hspace{1cm} (18)

and second derivative of the objective function (15) with respect to the material parameters:

\[ \nabla^2 \Phi = \Phi_{,mn} = \sum_{i=1}^{n_L} \sum_{j=1}^{n_M} \sum_{k=1}^{n_D} \left[ \frac{d \{ u_k \}_{ij}}{dp_m} \frac{d \{ u_k \}_{ij}}{dp_n} + \left( \{ u_k(p) \}_{ij} - \{ \bar{u}_k \}_{ij} \right) \frac{d^2 \{ u_k \}_{ij}}{dp_m dp_n} \right]. \]  \hspace{1cm} (19)

In the following the second term in eqn (19) will be neglected.
4 Sensitivity analysis

The gradient of the least-squares functional needs the derivatives of the displacements with respect to the material parameters. An analytical calculation is not possible, because no explicit relation exists between the material parameters and the displacements. In the following the semi-analytical sensitivity analysis is used, which includes the implicit differentiation of the global equilibrium conditions for a finite element solution [1, 2]:

\[
\frac{d}{dp}( Ku = F ).
\]  \hspace{1cm} (20)

\( K \) is the global stiffness matrix and the vector \( F \) contains the external nodal forces. In eqn (20) the material law is included and in this context the derivatives of the stresses with respect to the material parameters must be realized. The stresses \( T \) depend on the material parameters both explicitly and implicitly [1, 2]:

\[
\frac{d}{dp}[T(C(p),p)] = \frac{dT}{dC} : \frac{dC}{dp} + \frac{dT}{dp}.
\]  \hspace{1cm} (21)

After some mathematical manipulations one receives [4, 5]:

\[
K_T \frac{du}{dp} = P_p
\]  \hspace{1cm} (22)

with the tangent stiffness matrix \( K_T \) known from the solution of the direct problem. For each element \( el \) we can write the right side of eqn (22):

\[
P_{p}^{el} = \int_{V_0^{el}} B^T \cdot \left( \frac{dT}{dp} \right) dV_0^{el}.
\]  \hspace{1cm} (23)

This equation contains the \( B \)–matrix relating strains to nodal displacements in a finite element formulation. The integration is done over the element volume \( V_0^{el} \) in the reference configuration. To obtain the first derivatives of the stress tensor with respect to the material parameters we consider the discretized constitutive law for the current load step [6]:

\[
G(z_{n-n_S}(p), \ldots, z_{n-j}(p), \ldots, z_{n-1}(p), z_n(p), p) = 0.
\]  \hspace{1cm} (24)

The constitutive law depends on the previous \( z_{n-1}, \ldots, z_{n-n_S} \) state vectors as well as on the current state vector \( z_n \) and both explicitly and implicitly on the
material parameters $p$. $n_S$ denotes the number of the maximal considered previous load steps. The total derivative of eqn (24) leads to:

$$\frac{dG}{dp} = \sum_{j=1}^{n_S} \frac{\partial G}{\partial z_{n-j}} : \frac{dz_{n-j}}{dp} + \frac{\partial G}{\partial z_n} : \frac{dz_n}{dp} + \frac{\partial G}{\partial p} = 0. \quad (25)$$

The partial derivatives $\partial G / \partial z$ and $\partial G / \partial p$ can be determined analytically, whereas the total derivative $dz / dp$ is obtained on the basis of a numerical computation:

$$\frac{\partial G}{\partial z_n} : \frac{dz_n}{dp} = -\sum_{j=1}^{n_S} \frac{\partial G}{\partial z_{n-j}} : \frac{dz_{n-j}}{dp} - \frac{\partial G}{\partial p}. \quad (26)$$

The iterated JACOBIAN matrix $\partial G / \partial z_n$ of the current load step follows from the solution of the direct problem. The total derivatives of $z_{n-1}, \ldots, z_{n-n_S}$ are known from the previous load steps. With the relation:

$$\frac{dT}{dp} = \frac{\partial T}{\partial C^p} : \frac{dC^p}{dp} \quad (27)$$

it is possible to calculate the derivatives of the stress tensor $T$ with respect to the material parameters $p$. The formulation of $\partial T / \partial C^p$ is given in [6] for three hyperelastic materials.

### 5 Numerical tests

To verify and to test the efficiency of the presented optimization method, a synthetic displacement field is generated by a forward finite element calculation with presumed parameters. These parameters should be re-identified by the method. To this end a quarter of a notched flat bar tension specimen is discretized (see fig.
1). This finite element mesh has the external dimensions of $4.5 \times 7.0$ mm$^2$, the notch has a radius of 4.0 mm and the width at the notch amounts to 1.5 mm. 2D isoparametric 8-node elements with 9 integration points assuming plane strain conditions are used for numerical simulation. The loading is displacement controlled and applied in 100 steps. The direct problem was calculated with the material parameters from table 1 and the displacements were written out for all nodes at every load step.

Table 1: Material parameters, GTN–model.

<table>
<thead>
<tr>
<th>$E$ [MPa]</th>
<th>$\sigma_0$ [MPa]</th>
<th>$\varepsilon_0$</th>
<th>$n$</th>
<th>$q_1$</th>
<th>$q_2$</th>
<th>$q_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>210000</td>
<td>690.0</td>
<td>0.03</td>
<td>0.2</td>
<td>1.5</td>
<td>1.0</td>
<td>2.25</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$f_0$</td>
<td>$f_c$</td>
<td>$\varepsilon_N$</td>
<td>$f_N$</td>
<td>$s_N$</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>0.001</td>
<td>0.01</td>
<td>0.15</td>
<td>0.01</td>
<td>0.3</td>
<td>0.1</td>
</tr>
</tbody>
</table>

In the first phase of investigation all parameters have been varied one by one with a start value of $p_i \pm 50\%$. If the solution of the direct problem did not converge at the first optimization step then the start values were chosen with $p_i \pm 30\%$. The maximum number of optimization steps was 20. In table 2 one can see that almost all parameters could be found with high accuracy, see column “Ident”. The parameter $q_3$ was not well identified, because the influence of this parameter on the displacements is very small in the given range.

In the following example the case is treated that three parameters are unknown. On the one hand the hardening parameters ($\sigma_0, \varepsilon_0, n$) and on the other hand three damage parameters ($f_0, f_c, f_N$) were varied with $p_i \pm 50\%$. In fig. 2 one can see, that all hardening parameters could be identified with two different sets of start values. So, it seems to be possible to find a unique set of hardening parameters, because these parameters are independent and the optimization algorithm found the global minimum. The damage parameters could not be re-identified. After a
Table 2: Relative errors of the identified material parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Start [%]</th>
<th>Ident [%]</th>
<th>Steps</th>
<th>Start [%]</th>
<th>Ident [%]</th>
<th>Steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_0$</td>
<td>+50</td>
<td>0.00</td>
<td>8</td>
<td>-50</td>
<td>0.00</td>
<td>7</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>+50</td>
<td>0.87</td>
<td>20</td>
<td>-50</td>
<td>0.87</td>
<td>20</td>
</tr>
<tr>
<td>$n$</td>
<td>+50</td>
<td>0.04</td>
<td>20</td>
<td>-50</td>
<td>0.01</td>
<td>20</td>
</tr>
<tr>
<td>$q_1$</td>
<td>+50</td>
<td>0.01</td>
<td>20</td>
<td>-50</td>
<td>0.00</td>
<td>14</td>
</tr>
<tr>
<td>$q_2$</td>
<td>+50</td>
<td>0.00</td>
<td>17</td>
<td>-50</td>
<td>0.00</td>
<td>14</td>
</tr>
<tr>
<td>$q_3$</td>
<td>+50</td>
<td>2.16</td>
<td>15</td>
<td>-50</td>
<td>10.1</td>
<td>20</td>
</tr>
<tr>
<td>$f_0$</td>
<td>+50</td>
<td>0.00</td>
<td>19</td>
<td>-50</td>
<td>0.00</td>
<td>18</td>
</tr>
<tr>
<td>$f_c$</td>
<td>+50</td>
<td>0.00</td>
<td>16</td>
<td>-50</td>
<td>0.00</td>
<td>15</td>
</tr>
<tr>
<td>$f_F$</td>
<td>+50</td>
<td>0.00</td>
<td>15</td>
<td>-30</td>
<td>0.00</td>
<td>13</td>
</tr>
<tr>
<td>$f_N$</td>
<td>+50</td>
<td>0.01</td>
<td>20</td>
<td>-50</td>
<td>0.01</td>
<td>20</td>
</tr>
<tr>
<td>$\varepsilon_N$</td>
<td>+50</td>
<td>0.00</td>
<td>13</td>
<td>-50</td>
<td>0.00</td>
<td>16</td>
</tr>
<tr>
<td>$s_N$</td>
<td>+30</td>
<td>0.12</td>
<td>20</td>
<td>-30</td>
<td>0.05</td>
<td>20</td>
</tr>
</tbody>
</table>

Few optimization steps the algorithm found a local minimum (see table 3), because the surface of the objective function is not convex. To receive the global minimum one can vary the start values and compare the values of the objective function $\Phi$.

Table 3: Identified damage material parameters.

<table>
<thead>
<tr>
<th></th>
<th>$f_0$</th>
<th>$f_c$</th>
<th>$f_N$</th>
<th>Steps</th>
<th>$\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start [%]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>+50</td>
<td>0.00120</td>
<td>0.0228</td>
<td>0.0168</td>
<td>5</td>
<td>3.3E-3</td>
</tr>
<tr>
<td>-50</td>
<td>0.00068</td>
<td>0.0052</td>
<td>0.0065</td>
<td>7</td>
<td>6.1E-4</td>
</tr>
</tbody>
</table>

In the next example three hardening and two damage parameters were optimized together with a start value $p_i \pm 20\%$. The maximum number of optimization steps was 30. In table 4 one can see, that on the one hand the parameters could be re-identified and on the other hand only a local minimum was found. In this case it is possible to find the global minimum using various sets of start parameters.

In the last example experiments with scatter (noise) in the displacements were accomplished. For this reason to each displacement a stochastic error in the range of $-5\%$ to $+5\%$ is added. In table 5 the identified material parameters are listed with two different sets of start values.
Table 4: Identified material parameters.

<table>
<thead>
<tr>
<th>Start [%]</th>
<th>$\sigma_0$</th>
<th>$\varepsilon_0$</th>
<th>$n$</th>
<th>$f_0$</th>
<th>$f_c$</th>
<th>Steps</th>
<th>$\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+20</td>
<td>691.8</td>
<td>0.0306</td>
<td>0.201</td>
<td>0.00094</td>
<td>0.0097</td>
<td>30</td>
<td>1.1E-5</td>
</tr>
<tr>
<td>−20</td>
<td>669.6</td>
<td>0.0232</td>
<td>0.185</td>
<td>0.00149</td>
<td>0.0288</td>
<td>26</td>
<td>8.3E-3</td>
</tr>
</tbody>
</table>

Table 5: Identified material parameters (±5% error in the displacements).

<table>
<thead>
<tr>
<th>Start [%]</th>
<th>$\sigma_0$</th>
<th>$\varepsilon_0$</th>
<th>$n$</th>
<th>$f_0$</th>
<th>$f_c$</th>
<th>Steps</th>
<th>$\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+20</td>
<td>675.1</td>
<td>0.0257</td>
<td>0.192</td>
<td>0.00093</td>
<td>0.0279</td>
<td>5</td>
<td>2.8E-1</td>
</tr>
<tr>
<td>−20</td>
<td>673.0</td>
<td>0.0246</td>
<td>0.189</td>
<td>0.00175</td>
<td>0.0929</td>
<td>16</td>
<td>2.7E-1</td>
</tr>
</tbody>
</table>

In this case it cannot be assumed that a global minimum was reached. Considering the errors in the displacement field, the hardening parameters could be well identified. The damage parameters could not be well identified, because the influence of these parameters is significant only in the last 15% of the loading. In fig. 3 one can see that the decrease of the force–displacement curve could not be reproduced.

6 Summary

In this contribution an approach is presented for parameter identification of the GTN–model using non-linear optimization procedures. The inelastic material behaviour is modelled in the framework of large strain finite element method, whereby the identification routines are implemented in the FE–code SPC-PMHP. The solution of the inverse problem is based on the minimization of a least-squares functional. The gradient of the objective function has been calculated by a semi-
analytical sensitivity analysis. For this purpose the derivatives of the discretized constitutive law with respect to the GTN material parameters have been determined. The optimization algorithm was verified by a self-consistent test, whereby prescribed material parameters were re-identified. The identification of only one parameter was in general trouble free. Experiments with three or more unknown parameters showed that not in every case the global minimum was found, particularly for the identification of damage parameters. Future work will be concerned with experiments on flat bar tension test specimen using the grating method to receive a three-dimensional displacement field.

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References


