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TWO-SCALE PARAMETER IDENTIFICATION FOR HETEROGENEOUS ELASTOPLASTIC MATERIALS

U. SCHMIDT*, J. MERGHEIM AND P. STEINMANN

*Chair for Applied Mechanics
University of Erlangen-Nuremberg
Egerlandstr. 5, 91058 Erlangen, Germany
e-mail: ulrike.schmidt@ltm.uni-erlangen.de
www.ltm.uni-erlangen.de

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Abstract. The aim of this paper is to describe a method for identifying micro material parameters using only macroscopic experimental data. The FE^2 method is used to model the behavior of the complex materials with heterogeneous micro-structure. The resulting least squares problem, with the difference of the simulated and the measured macroscopic data in the objective function, is minimized using gradient-based optimization algorithms with respect to the microscopic material parameters. The gradient information is derived analytically within the discretized scheme.

1 INTRODUCTION

Advanced materials are characterized by their heterogeneity and diverse functionality at multiple scales. In order to use and employ these new materials and exploit their whole potential a good understanding of the functioning and mechanism is necessary. Mechanical modeling of heterogeneous materials is an essential part of this, but still presents a challenge for computational mechanics. Computational homogenization is designed to handle heterogeneity at different scales.

The concept of (computational) homogenization requires separated scales, that means macro phenomena appear on a much larger length scale than the micro scale and its phenomena. Thus the material behavior of each macroscopic point is determined by an underlying microscopic domain. It is assumed that there exists a subdomain of finite volume on the micro scale, which is representative for the mechanical behavior of the entire microscopic domain, thus often called representative volume element (RVE). In contrast to the macro scale, the material behavior on the micro scale is determined directly by a constitutive law and the micro material parameters. The mechanical equilibrium equations at macro and micro scale are further complemented by a scale linking condition,

often called macro homogeneity condition. An appropriate choice of the boundary condition on the microscopic scale leads to the formulation for the macroscopic stresses and strains as the volumetric means (or more general, some adequate boundary integrals) of their microscopic counterparts.

Since the micro material parameters are an important ingredient for this two-scale simulation, knowledge of the parameters and its acquisition is quite an important topic. Classical parameter identification and its macroscopic experiments are well established and one might want to utilize this experience, when given the task to identify microscopic material parameters. Ultimately, the task at hand is to identify microscopic material parameters using only macroscopic experiments.

The identification of micro parameters in a two-scale homogenization problem is also investigated in [1, 2, 3], using numerical sensitivities or gradient-free optimization techniques together with miscellaneous homogenization techniques. This paper couples classical parameter identification [4] and computational homogenization, more precisely the FE^2 method [5]. Gradient-based optimization is used to solve the resulting two-scale parameter identification problem.

In a previous work [6] a two-scale parameter identification using analytical gradient-information was investigated for elasticity, which yields simplifications and less computational costs compared to the present extension to plasticity. The main focus of this work is on the derivation of the gradient information in a two-scale FE scheme.

The paper is structured as follows: In section 2 a short overview of the direct problem, the FE^2 method and a fix of notation is given. In section 3 the two-scale parameter identification problem is defined and the gradient information derived. An example in section 4 illustrates the functionality of the method. The paper is concluded in the last section with a discussion and an outlook on further investigation.

2 DIRECT PROBLEM

For the equilibrium at the macro domain $\bar{\Omega}$ we have a standard quasi-static problem (1) with body forces $\bar{\mathbf{b}}$ and stresses $\bar{\boldsymbol{\sigma}}$ and adequate boundary conditions. Herein macroscopic quantities are marked by an overbar. At the micro scale neglecting body forces leads to the equilibrium equation (2) in the micro domain $\Omega(\bar{\mathbf{X}})$ at the macroscopic point $\bar{\mathbf{X}}$. The continuous formulation is complemented by the macro homogeneity condition (4). The micro boundary condition on e.g. the displacements $\mathbf{u}$ (3) links the macro strain $\bar{\boldsymbol{\varepsilon}}$ to the microscopic scale. The up-scaling of the micro stresses leads to the definition of the macro stresses (5) as the boundary integral of the dyadic product of the reference point

and the tractions $\mathbf{t}$ at the micro scale. In summary:

$$\nabla \cdot \bar{\boldsymbol{\sigma}} = \bar{\mathbf{b}} \qquad \text{in } \bar{\Omega} \quad \text{with } \bar{\mathbf{u}}|_{\partial\bar{\Omega}_D} = \bar{\mathbf{u}}_p,\ (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{n}})|_{\partial\bar{\Omega}_N} = \bar{\mathbf{t}}_p \tag{1}$$

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \qquad \text{in } \Omega(\bar{\mathbf{X}}) \quad \text{with appropriate b.c., e.g.} \tag{2}$$

$$\mathbf{u} = \mathbf{X} \cdot \bar{\boldsymbol{\varepsilon}} \qquad \text{on } \partial\Omega(\bar{\mathbf{X}}) \quad \text{(down-scaling)} \tag{3}$$

$$(\delta\bar{\boldsymbol{\varepsilon}} : \bar{\boldsymbol{\sigma}})(\bar{\mathbf{X}}) = \int_{\Omega(\bar{\mathbf{X}})} \delta\boldsymbol{\varepsilon} : \boldsymbol{\sigma}\, \mathrm{d}V \tag{4}$$

$$\bar{\boldsymbol{\sigma}}(\bar{\mathbf{X}}) = \int_{\partial\Omega(\bar{\mathbf{X}})} \mathbf{X} \otimes \mathbf{t}\, \mathrm{d}A \qquad \text{(up-scaling)} \tag{5}$$

The material behavior on the micro scale is modeled by the common von Mises plasticity for small strains with linear isotropic hardening, whereas the material behavior on the macro scale is solely determined by the micro scale and has no constitutive law of its own. The micro material parameters are compression modulus K and shear modulus μ for the elastic part and yield stress σ_Y and hardening modulus h for the plastic part. For the convenience in the subsequent analysis the parameters are summarized in vector $\boldsymbol{\alpha} = (K, \mu, \sigma_Y, h)$.

Application of the standard FE^2 method [5] results in the vectorial residuals $\bar{\mathbf{R}}(\bar{\mathbf{u}}(\boldsymbol{\alpha}), \boldsymbol{\alpha})$ and $\mathbf{R}(\mathbf{u}(\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}), \boldsymbol{\alpha}), \boldsymbol{\alpha})$ on the macro and micro scale, respectively. The residuals vanish in equilibrium (6), (7). The discrete down-scaling (8) is now defined at each boundary node j of the RVE. The discrete macroscopic stresses can be computed as the sum over the boundary nodes of the discrete quantities (9).

After application of the FE^2 method, the following discrete equations for the direct problem are important for the parameter identification:

$$\bar{\mathbf{R}}(\bar{\mathbf{u}}(\boldsymbol{\alpha}), \boldsymbol{\alpha}) = \mathbf{0} \tag{6}$$

$$\mathbf{R}(\mathbf{u}(\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}), \boldsymbol{\alpha}), \boldsymbol{\alpha}) = \mathbf{0} \tag{7}$$

$$\mathbf{u}_j = \mathbf{X}_j \cdot \bar{\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}) \tag{8}$$

$$\bar{\boldsymbol{\sigma}} = \sum_j \mathbf{X}_j \otimes \mathbf{f}_j \tag{9}$$

A short remark on the microscopic boundary conditions: There are other appropriate choices besides the 'linear displacement' boundary condition given here. The 'periodic' (periodic fluctuations and anti-periodic tractions) boundary condition is often chosen. However, the resulting discretized problem can be transformed in such a way that the structure is the same as for the system resulting from the 'linear displacement' boundary condition. After the transformation of the system to contain only the independent nodes one has prescribed displacements $\mathbf{u}_J = \mathbf{X}_J \cdot \bar{\boldsymbol{\varepsilon}}$ at the nodes J spanning the RVE, while the forces on the remaining nodes vanish.

3 INVERSE PROBLEM

3.1 Problem formulation

The objective function measures the difference between simulated and measured displacements $\bar{\mathbf{u}}$ and forces $\bar{\mathbf{f}}$ of the macro scale. Both contributions have weighting factors, w_u and w_f, to compensate for dimension differences.

$$f = w_u \sum_i \|\bar{\mathbf{u}}_i(\boldsymbol{\alpha}) - \bar{\mathbf{u}}_i^{\text{measured}}\|^2 + w_f \sum_j \|\bar{\mathbf{f}}_j(\boldsymbol{\alpha}) - \bar{\mathbf{f}}_j^{\text{measured}}\|^2 \tag{10}$$

Displacements and forces can be measured at different points, which is indicated by the different indices i and j. The goal is to identify the microscopic material parameters, which minimize the difference for the given data. Then the task at hand can be described as a minimization problem under certain constraints, namely that the material parameters are feasible and the mechanical equilibria on micro and macro scale are satisfied.

$$\min f(\boldsymbol{\alpha}) \quad \text{s.t. } \boldsymbol{\alpha} \text{ is feasible and } \bar{\mathbf{u}}, \mathbf{u} \text{ in equilibrium} \tag{11}$$

The model with the identified parameters can be validated if the objective function is sufficiently small also for a separate data set of measured displacements and forces resulting from a different experiment.

3.2 Gradient information

In order to employ gradient-based optimization techniques to minimize the objective function, the gradient information is required. Due to better convergence behavior and lower computational costs the analytical derivation is preferred over a numerical calculation, e.g. using finite differences. The necessary gradient information is calculated as a total derivative of the objective function with respect to the parameter vector $\boldsymbol{\alpha}$, denoted by $\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}}$.

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\alpha}} = w_u \sum_i (\bar{\mathbf{u}}_i(\boldsymbol{\alpha}) - \bar{\mathbf{u}}_i^{\text{measured}}) \cdot \frac{\mathrm{d}\bar{\mathbf{u}}_i(\boldsymbol{\alpha})}{\mathrm{d}\boldsymbol{\alpha}} + w_f \sum_j (\bar{\mathbf{f}}_j(\boldsymbol{\alpha}) - \bar{\mathbf{f}}_j^{\text{measured}}) \cdot \frac{\mathrm{d}\bar{\mathbf{f}}_j(\boldsymbol{\alpha})}{\mathrm{d}\boldsymbol{\alpha}} \tag{12}$$

A look at the macroscopic residual $\bar{\mathbf{R}}(\bar{\mathbf{u}}(\boldsymbol{\alpha}), \boldsymbol{\alpha}) = \bar{\mathbf{R}}^{\text{int}}(\bar{\mathbf{u}}(\boldsymbol{\alpha}), \boldsymbol{\alpha}) - \bar{\mathbf{R}}^{\text{ext}}(\boldsymbol{\alpha}) = \mathbf{0}$, consisting of an internal part $\bar{\mathbf{R}}^{\text{int}}$ and an external part $\bar{\mathbf{R}}^{\text{ext}}$, is necessary in order to determine the derivatives of the simulated quantities. The force term $\mathbf{f}_j$ in the objective function incorporates the external forces contained in $\bar{\mathbf{R}}^{\text{ext}}$ in an way appropriate to the experiments and available measurements. The degrees of freedom (DOFs) of the macroscopic residual are partitioned into prescribed displacement DOFs (p) and remaining DOFs (r). Here the remaining DOFs contain DOFs at internal nodes, where the body forces are prescribed and DOFs at the boundary, where tractions are prescribed. The vectorial residual at the macro scale is differentiated w.r.t. the material parameters, the partial derivatives

are denoted as $\frac{\partial}{\partial \bar{\mathbf{u}}}$ and $\frac{\partial}{\partial \boldsymbol{\alpha}}$, respectively. The assumption, that the prescribed terms are independent of the material parameters, i.e. $\frac{\mathrm{d}\bar{\mathbf{u}}_p}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{0}$, $\frac{\mathrm{d}\bar{\mathbf{R}}_r^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{0}$, finally leads to

$$\mathbf{0} = \frac{\partial \bar{\mathbf{R}}_p^{\mathrm{int}}}{\partial \bar{\mathbf{u}}_r} \cdot \frac{\mathrm{d}\bar{\mathbf{u}}_r}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \bar{\mathbf{R}}_p^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} - \frac{\mathrm{d}\bar{\mathbf{R}}_p^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} \tag{13}$$

$$\mathbf{0} = \frac{\partial \bar{\mathbf{R}}_r^{\mathrm{int}}}{\partial \bar{\mathbf{u}}_r} \cdot \frac{\mathrm{d}\bar{\mathbf{u}}_r}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \bar{\mathbf{R}}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{14}$$

With the assumption that $\bar{\mathbf{K}}_{rr} := \frac{\partial \bar{\mathbf{R}}_r^{\mathrm{int}}}{\partial \bar{\mathbf{u}}_r}$, a part of the stiffness matrix of the direct problem, is regular, we can calculate the derivative of the displacements w.r.t. the material parameters:

$$\frac{\mathrm{d}\bar{\mathbf{u}}_p}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{0}, \quad \frac{\mathrm{d}\bar{\mathbf{u}}_r}{\mathrm{d}\boldsymbol{\alpha}} = -\bar{\mathbf{K}}_{rr}^{-1} \cdot \frac{\partial \bar{\mathbf{R}}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{15}$$

Furthermore, one can calculate the total derivative of the macroscopic external forces from (13) using $\bar{\mathbf{K}}_{pr} := \frac{\partial \bar{\mathbf{R}}_p^{\mathrm{int}}}{\partial \bar{\mathbf{u}}_r}$ and equation (15) as

$$\frac{\mathrm{d}\bar{\mathbf{R}}_r^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{0}, \quad \frac{\mathrm{d}\bar{\mathbf{R}}_p^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \bar{\mathbf{R}}_p^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} - \bar{\mathbf{K}}_{pr} \cdot \bar{\mathbf{K}}_{rr}^{-1} \cdot \frac{\partial \bar{\mathbf{R}}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{16}$$

Now it can be seen, that the determination of the derivatives is similar to solving the linearized direct problem with an artificial load $\frac{\partial \bar{\mathbf{R}}^{\mathrm{int}}}{\partial \boldsymbol{\alpha}}$. In order to construct this artificial load vector, the partial derivative of the macroscopic stresses w.r.t. microscopic parameters will be determined in the following. The element-wise contributions to the internal residual consist of the derivatives of the macro shape functions, summarized in the B-matrix $\bar{\mathbf{B}}_e^T$ (independent of material parameters) and the macro stresses $\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha})|_e$

$$\frac{\partial \bar{\mathbf{R}}^{\mathrm{int}}(\bar{\mathbf{u}}, \boldsymbol{\alpha})|_e}{\partial \boldsymbol{\alpha}} = \int_{\bar{\Omega}_e} \bar{\mathbf{B}}_e^T \cdot \frac{\partial \bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha})|_e}{\partial \boldsymbol{\alpha}} \mathrm{d}V \tag{17}$$

In the classical one scale parameter identification the derivative of the stresses can be obtained by differentiating the constitutive law. However, the use of a two-scale modeling scheme in the present work necessitates further calculations at this point. By definition (9) we calculate the macro stresses as the sum of dyadic products of the reference position and the reaction forces at boundary nodes and thus its derivative can be expressed as

$$\frac{\partial \bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} = \sum_j \mathbf{X}_j \otimes \frac{\partial \mathbf{f}_j(\bar{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \tag{18}$$

Clearly, it is necessary to calculate the derivatives at the micro scale. Starting once again with the vectorial residual, but now for the microscopic problem, and its total derivative w.r.t. the material parameters, we use the partitioning into prescribed displacement DOFs and prescribed force DOFs. An illustration is given in figure 1.

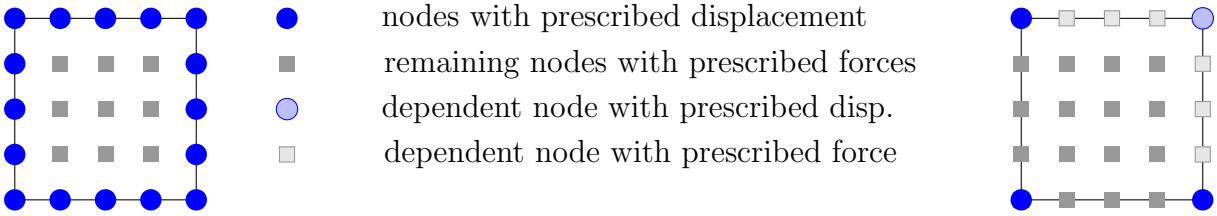

Figure 1: Schematic distribution of prescribed displacements/forces for 'linear displacement' (left) and 'periodic' (right) boundary conditions in 2D

On the micro scale the prescribed forces do not depend on the material parameters, but the prescribed displacements do. The prescribed displacements on the micro scale depend on the macro strain and therefore on the material parameters. Their derivative follows from equation (8) as

$$\frac{\mathrm{d}\mathbf{u}_p}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}}. \tag{19}$$

Therefore, the total derivative of the micro residual can be expressed as

$$\mathbf{0} = \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \mathbf{R}^{\mathrm{int}}}{\partial \mathbf{u}} \cdot \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} - \frac{\mathrm{d}\mathbf{R}^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} \tag{20}$$

$$= \begin{pmatrix} \mathbf{K}_{pp} & \mathbf{K}_{pr} \\ \mathbf{K}_{rp} & \mathbf{K}_{rr} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} \\ \frac{\mathrm{d}\mathbf{u}_r}{\mathrm{d}\boldsymbol{\alpha}} \end{pmatrix} + \begin{pmatrix} \frac{\partial}{\partial \boldsymbol{\alpha}} \mathbf{R}_p^{\mathrm{int}} \\ \frac{\partial}{\partial \boldsymbol{\alpha}} \mathbf{R}_r^{\mathrm{int}} \end{pmatrix} - \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}} \mathbf{R}_p^{\mathrm{ext}} \\ \mathbf{0} \end{pmatrix}. \tag{21}$$

The derivative of the internal residual w.r.t. the displacement $\frac{\partial \mathbf{R}^{\mathrm{int}}}{\partial \mathbf{u}}$ is the stiffness matrix $\mathbf{K}$ of the direct micro problem, containing the submatrices $\mathbf{K}_{pp}, \mathbf{K}_{pr}, \mathbf{K}_{rp}, \mathbf{K}_{rr}$ related to prescribed or remaining nodes, respectively. One can reformulate the second line associated with the prescribed force DOFs in (21) by using the assumption that $\mathbf{K}_{rr}$ is regular and arrive at an expression for the total derivative of the displacements.

$$\mathbf{0} = \mathbf{K}_{rp} \cdot \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} + \mathbf{K}_{rr} \cdot \frac{\mathrm{d}\mathbf{u}_r}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{22}$$

$$\Rightarrow \frac{\mathrm{d}\mathbf{u}_r}{\mathrm{d}\boldsymbol{\alpha}} = -\mathbf{K}_{rr}^{-1} \cdot \left(\mathbf{K}_{rp} \cdot \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \right) \tag{23}$$

Inserting this in the first line of (21) and reordering of the terms leads to

$$\frac{\mathrm{d}\mathbf{R}_p^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{K}_{pp} \cdot \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} - \mathbf{K}_{pr} \cdot \mathbf{K}_{rr}^{-1} \cdot \left(\mathbf{K}_{rp} \cdot \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \right) + \frac{\partial \mathbf{R}_p^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{24}$$

$$= \left(\mathbf{K}_{pp} - \mathbf{K}_{pr} \cdot \mathbf{K}_{rr}^{-1} \cdot \mathbf{K}_{rp} \right) \cdot \mathbf{X}_p \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} - \mathbf{K}_{pr} \cdot \mathbf{K}_{rr}^{-1} \cdot \frac{\partial \mathbf{R}_r^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} + \frac{\partial \mathbf{R}_p^{\mathrm{int}}}{\partial \boldsymbol{\alpha}} \tag{25}$$

When we express $\frac{\mathrm{d}\mathbf{R}_p^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}}$ by means of partial derivatives

$$\frac{\mathrm{d}\mathbf{R}_p^{\mathrm{ext}}}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \mathbf{R}_p^{\mathrm{ext}}}{\partial \bar{\boldsymbol{\varepsilon}}} \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}_p^{\mathrm{ext}}}{\partial \boldsymbol{\alpha}} \tag{26}$$

we can identify by comparison of coefficients the following terms

$$\frac{\partial \mathbf{R}_p^{\text{ext}}}{\partial \bar{\boldsymbol{\varepsilon}}} = \left(\mathbf{K}_{pp} - \mathbf{K}_{pr} \cdot \mathbf{K}_{rr}^{-1} \cdot \mathbf{K}_{rp}\right) \cdot \mathbf{X}_p \tag{27}$$

$$\frac{\partial \mathbf{R}_p^{\text{ext}}}{\partial \boldsymbol{\alpha}} = \frac{\partial \mathbf{R}_p^{\text{int}}}{\partial \boldsymbol{\alpha}} - \mathbf{K}_{pr} \cdot \mathbf{K}_{rr}^{-1} \cdot \frac{\partial \mathbf{R}_r^{\text{int}}}{\partial \boldsymbol{\alpha}}. \tag{28}$$

The sum to calculate the macro stress is constructed over the boundary nodes, where displacements are prescribed, i.e. $\frac{\partial \mathbf{f}_j}{\partial \boldsymbol{\alpha}} = \left(\frac{\partial \mathbf{R}_p^{\text{ext}}}{\partial \boldsymbol{\alpha}}\right)_j$. Therefore we only need (28) to construct the partial derivative of the macro stresses. It remains to calculate the partial derivative of the internal residual w.r.t. the material parameters. For this the internal variables like plastic strain, back stress and hardening evolution are summarized in the vector $\boldsymbol{\beta}$. The inelastic material model is dealt with by using a recursive strategy to differentiate w.r.t. the material parameters, described in detail in [4]. The key point of this strategy is to view the stress and internal variables $\boldsymbol{\beta}$ as dependent on the current and last load steps as well as the material parameters, i.e. $\boldsymbol{\sigma}^k = \boldsymbol{\sigma}^k(\boldsymbol{\varepsilon}^k, \boldsymbol{\varepsilon}^{k-1}, \boldsymbol{\beta}^k, \boldsymbol{\beta}^{k-1}, \alpha)$, and $\boldsymbol{\beta}^k = \boldsymbol{\beta}^k(\boldsymbol{\varepsilon}^k, \boldsymbol{\varepsilon}^{k-1}, \boldsymbol{\beta}^{k-1}, \alpha)$, and differentiate accordingly. The partial derivatives needed for parameter identification consider all dependencies but the strain of the current step, i.e. $\frac{\partial \boldsymbol{\sigma}^k(\boldsymbol{\varepsilon}^k, \alpha)}{\partial \boldsymbol{\alpha}}$ and $\frac{\partial \boldsymbol{\beta}^k(\boldsymbol{\varepsilon}^k, \alpha)}{\partial \boldsymbol{\alpha}}$. The total derivatives from the last step are a vital ingredient for this calculation and are constructed at the beginning of the current step using the results from the last step. The total derivative of the microscopic displacements w.r.t. the material parameters (23) can be constructed by means of the partial derivatives

$$\frac{\partial \mathbf{u}_r(\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}), \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} = -\mathbf{K}_{rr}^{-1} \cdot \frac{\partial \mathbf{R}_r^{\text{int}}}{\partial \boldsymbol{\alpha}}, \quad \frac{\partial \mathbf{u}_r(\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}), \boldsymbol{\alpha})}{\partial \bar{\boldsymbol{\varepsilon}}} = -\mathbf{K}_{rr}^{-1} \cdot \mathbf{K}_{rp} \cdot \mathbf{X}_p \tag{29}$$

as $\frac{\mathrm{d}\mathbf{u}_r}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \mathbf{u}_r}{\partial \bar{\boldsymbol{\varepsilon}}} \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\varepsilon}}$, once $\frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}{\mathrm{d}\boldsymbol{\alpha}}$ is known. Thus, we have a classical parameter identification step in the integration points. The special dependency of the prescribed micro displacements on the material parameters resulting from the two-scale homogenization scheme influences only the global microscopic equations (23) and (25).

3.3 Algorithm

The iteration procedure to calculate micro material parameter derivatives of displacements and forces at macroscopic scale and its steps are illustrated by the following scheme.

INIT ($k = 0$): Initialize the derivatives of the macro displacements $\frac{\mathrm{d}\bar{\mathbf{u}}^0}{\mathrm{d}\boldsymbol{\alpha}} = \mathbf{0}$. Furthermore, initialize the derivatives of the micro displacements $\frac{\partial \mathbf{u}^0}{\partial \boldsymbol{\alpha}} = \mathbf{0}$, $\frac{\partial \mathbf{u}^0}{\partial \bar{\boldsymbol{\varepsilon}}^0} = \mathbf{0}$, and of the micro internal variables $\frac{\partial \boldsymbol{\beta}^0}{\partial \boldsymbol{\alpha}} = \mathbf{0}$, $\frac{\partial \boldsymbol{\beta}^0}{\partial \boldsymbol{\varepsilon}^0} = \mathbf{0}$ on all micro domains.

ITERATION

I) set $k \to k+1$, known: $\frac{\mathrm{d}\bar{\mathbf{u}}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$

II) after macro equilibrium calculations, on each macro element for each integration point:

A) construct $\frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$ from $\frac{\mathrm{d}\bar{\mathbf{u}}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$

B) invoke subproblem on micro scale for each integration point

i) known: $\frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$, $\frac{\partial \mathbf{u}^{k-1}}{\partial \boldsymbol{\alpha}}$, $\frac{\partial \mathbf{u}^{k-1}}{\partial \bar{\boldsymbol{\varepsilon}}^{k-1}}$, $\frac{\partial \boldsymbol{\beta}^{k-1}}{\partial \boldsymbol{\alpha}}$, $\frac{\partial \boldsymbol{\beta}^{k-1}}{\partial \boldsymbol{\varepsilon}^{k-1}}$

ii) construct $\frac{\mathrm{d}\mathbf{u}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \mathbf{u}^{k-1}}{\partial \bar{\boldsymbol{\varepsilon}}^{k-1}} \cdot \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \mathbf{u}^{k-1}}{\partial \boldsymbol{\alpha}}$

iii) after micro equilibrium calculations, on each micro element for each integration point:

a) construct $\frac{\mathrm{d}\boldsymbol{\varepsilon}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$ from $\frac{\mathrm{d}\mathbf{u}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}}$

b) construct $\frac{\mathrm{d}\boldsymbol{\beta}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}} = \frac{\partial \boldsymbol{\beta}^{k-1}}{\partial \boldsymbol{\varepsilon}^{k-1}} \cdot \frac{\mathrm{d}\boldsymbol{\varepsilon}^{k-1}}{\mathrm{d}\boldsymbol{\alpha}} + \frac{\partial \boldsymbol{\beta}^{k-1}}{\partial \boldsymbol{\alpha}}$

c) calculate $\frac{\partial \boldsymbol{\sigma}^{k}}{\partial \boldsymbol{\alpha}}$, $\frac{\partial \boldsymbol{\beta}^{k}}{\partial \boldsymbol{\varepsilon}^{k}}$, $\frac{\partial \boldsymbol{\beta}^{k}}{\partial \boldsymbol{\alpha}}$ and save $\frac{\partial \boldsymbol{\beta}^{k}}{\partial \boldsymbol{\varepsilon}^{k}}$, $\frac{\partial \boldsymbol{\beta}^{k}}{\partial \boldsymbol{\alpha}}$ for next step

d) calculate $\frac{\partial \mathbf{R}^{\mathrm{int,k}|_e}}{\partial \boldsymbol{\alpha}}$

iv) assemble global artificial load vector $\frac{\partial \mathbf{R}^{\mathrm{int,k}}}{\partial \boldsymbol{\alpha}}$

v) determine $\frac{\partial \mathbf{u}^{k}}{\partial \boldsymbol{\alpha}}$, $\frac{\partial \mathbf{u}^{k}}{\partial \bar{\boldsymbol{\varepsilon}}^{k}}$ (29), $\frac{\partial \mathbf{f}^{k}}{\partial \boldsymbol{\alpha}}$ (28) and save $\frac{\partial \mathbf{u}^{k}}{\partial \boldsymbol{\alpha}}$, $\frac{\partial \mathbf{u}^{k}}{\partial \bar{\boldsymbol{\varepsilon}}^{k}}$ for next step

vi) calculate $\frac{\partial \bar{\boldsymbol{\sigma}}^{k}}{\partial \boldsymbol{\alpha}}$ (18) from $\frac{\partial \mathbf{f}^{k}}{\partial \boldsymbol{\alpha}}$ and give it back to macro scale

C) use $\frac{\partial \bar{\boldsymbol{\sigma}}^{k}}{\partial \boldsymbol{\alpha}}$ to calculate $\frac{\partial \bar{\mathbf{R}}^{\mathrm{int,k}|_e}}{\partial \boldsymbol{\alpha}}$ (17)

III) assemble global artificial load vector $\frac{\partial \bar{\mathbf{R}}^{\mathrm{int,k}}}{\partial \boldsymbol{\alpha}}$

IV) solve for $\frac{\mathrm{d}\bar{\mathbf{u}}^{k}}{\mathrm{d}\boldsymbol{\alpha}}$ (15), $\frac{\mathrm{d}\bar{\mathbf{f}}^{k}}{\mathrm{d}\boldsymbol{\alpha}}$ (16) and go to step I).

4 NUMERICAL EXAMPLE

In a first investigation on the functionality of the proposed multi-scale method for parameter identification, reidentification for numerical examples is considered. Therefore the numerical simulations are carried out for given material parameters on the micro scale. Then the optimization algorithm is employed to solve the problem for several starting points.

The example setting is illustrated in figure 2. The geometry at the macroscopic scale is a punched disk, which is elongated in five steps to a total of 1.5 % elongation. The hole has a radius of 1 mm and is centered at the quadratic disk with base length 4 mm and thickness 1 mm. The microscopic domain consists of a cube with an ellipsoidal void. The ellipsoid with radii $a = 4.8, b = 3.2, c = 4.0$ is placed at the center of a cube with base length 10. 'Linear displacement' boundary conditions were employed.

We assume a microscopic material law of von Mises plasticity with linear isotropic hardening. For the reference solution the material parameters at the micro scale are given as $K = 73.53, \mu = 28.20, \sigma_Y = 0.30, h = 15.00$ in GPa. The displacements at the

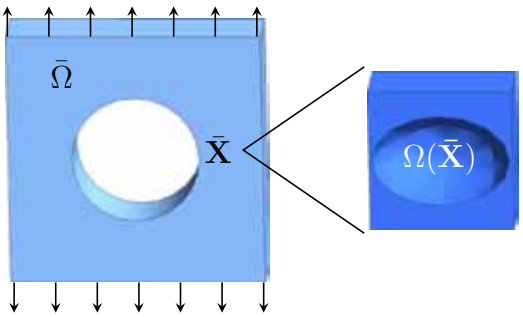

Figure 2: Example setting

front and back as well as the resultant force on top and bottom of the macro disk are the entries in the objective function. The optimization algorithm `lsqnonlin` from MATLAB's Optimization Toolbox is used to minimize the optimization problem. Four starting points are presented: 1 (80.47, 31.63, 0.27, 16.86), 2 (84.23, 34.07, 0.28, 18.50), 3 (69.26, 33.93, 0.23, 17.85), 4 (88.90, 30.61, 0.25, 15.94).

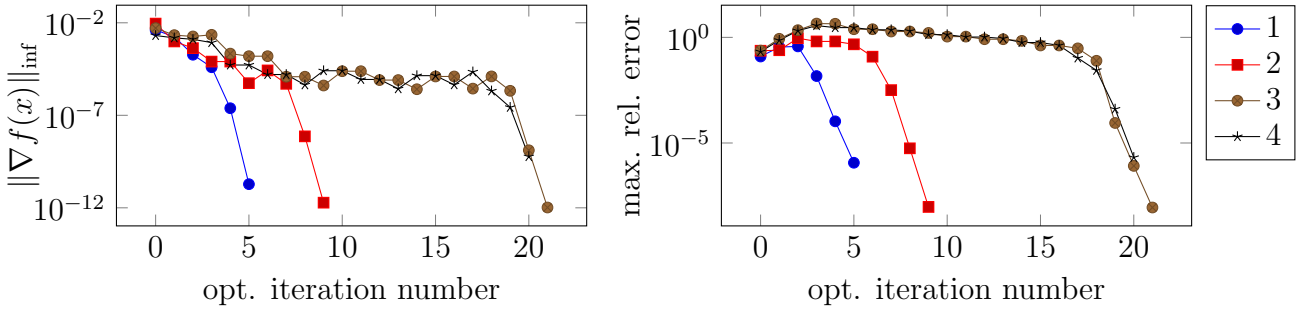

Figure 3: Optimization characteristics

Results for each stating point are shown in figure 3. The plot on the left depicts the infinity norm of the gradient of the objective function against the iterations of the optimization. The decrease indicates the convergence to a stationary point. The plot on the right depicts the maximal relative error of the identified material parameters with respect to the reference parameters, also against the iterations of the optimization. In both plots the y-axes use a logarithmic scale. As can be seen, the optimization convergences and the identified micro parameters indeed coincide with the reference parameters.

5 CONCLUSIONS

In this paper the coupling of classical parameter identification and the FE^2-method is described. The gradient information of the objective function is derived leading from macroscopic derivatives down to microscopic derivatives. A calculation scheme covering

the main steps within the recursive approach at the two scales is shown. The example illustrates that the correct material parameters of the micro scale, both elastic and plastic ones, can be identified using only the macroscopic data. The optimization converges successfully in a small to moderate number of steps. Thus we conclude that the two-scale parameter identification can be solved using the proposed scheme.

However, more research into the stability and robustness of the method is required. The method relies on observable nonlinear effects at the macro scale. If the plastic effects on the micro structure appear only very locally confined, the effects on the macro scale may become negligible small and therefore pose only insufficient data.

Furthermore, for improving the computational costs we will investigate the effects of separate identification of elastic and plastic materials as well as the effects of the coupling of 2-D macro to 3-D micro simulations.

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