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HYBRID METHODS FOR MATERIAL CHARACTERISATION

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Abstract: Material parameters are adjustable coefficients in constitutive equations of the mechanical behaviour. Their identification requires a combined experimental and numerical approach, which results in a generally ill-posed inverse problem. Methods commonly applied in computational mechanics like optimisation and neural networks are addressed, and problems like sensitivity, uniqueness and stability are discussed.

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1. Material or Model Parameters?

The notion of what material parameters are has changed in the history together with the expansion of theory and mathematics into strength of materials, which allowed for reducing different phenomena to just different boundary value problems (BVP) governed by the same basic equations, namely deformation kinematics, Cauchy's stress principle, Cauchy's equation of motion and material-specific constitutive equations. Material parameters are only meaningful in the context of models of the mechanical behaviour. If a model is simple and the stress state is uniaxial, the respective BVP can be solved analytically and the respective material parameters directly evaluated from a mechanical test.

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Material behaviour is manifold, however, and so is the number of models proposed in the literature. The more complex the observed phenomena are, the more sophisticated the models have to be and the more parameters appear in the models. No analytical solutions can be obtained any more, and the tests and their evaluation become more and more complicated. This is the background of hybrid methods, which actually indicate the synergy between experimental and numerical methods for material characterisation [2], [8], [1].

We shall understand material parameters as model parameters, which may depend on other state variables not explicitly included in the particular model, e.g. temperature, strain rate etc., but which are supposed to be independent of the basic mechanical quantities, stresses and strains. This definition gives up the universal claim of characterising inherent features of a material for the benefit of a more manageable and pragmatic meaning.

2. The Identification Problem

The response of a structure to applied mechanical or thermal actions can be described by a functional,

$$\mathbf{R}(\mathbf{x},t) = \mathcal{F}_{\tau=0}^{t}\left\{\mathfrak{G},\mathbf{c},\mathbf{F}(\mathbf{x},\tau)\right\}, \tag{1}$$

in dependence on the geometry, $\mathfrak{G}$, the material parameters, $\mathbf{c}$, and the external actions or loading history, $\mathbf{F}(\mathbf{x},t)$. The functional $\mathcal{F}$ can be given by an experiment or by an analytical or numerical solution of a BVP, and the respective response will be denoted as $\mathbf{R}_{test}$ and $\mathbf{R}_{sim}$, respectively. Here, this solution is obtained by a finite element (FE) model of the structure, which is a test specimen that is particularly designed for parameter identification. Equation (1) is addressed as direct problem, where $\mathfrak{G}$, $\mathbf{c}$, and $\mathbf{F}$ are the input and $\mathbf{R}(\mathbf{x},t)$ is the output or response in terms of a displacement, strain or stress field, $\mathbf{x}$ and t being the coordinates and the time, respectively, which is recorded in a finite number of geometrical points, $\mathbf{x}_i$, and time steps, t_j.

In the inverse problem, the values of input quantities, namely the material geometry, $\mathfrak{G}$, and the loading history, $\mathbf{F}$, are determinate, a solution of the direct problem, equation (1), and a procedure for finding it exist, the functional $\mathcal{F}$ reduces to a mapping,

$$\mathbb{R}_c \overset{\mathfrak{G},F}{\longmapsto} \mathbb{R}_R: \quad \mathbf{R} = \mathcal{R}(\mathbf{c}), \tag{2}$$

with $\mathbf{c} \in \mathbb{R}_c$ and $\mathbf{c} \in \mathbb{R}_R$, $\mathbb{R}_c$ and $\mathbb{R}_R$ being the spaces of physically meaningful material parameters and response data, respectively. The corresponding in-

verse problem consists of finding the parameters, $\mathbf{c}$, for a given experimentally measured response, $\mathbf{R}_{test}$,

$$\mathbb{R}_R \overset{\mathfrak{G},F}{\longmapsto} \mathbb{R}_c : \quad \mathbf{c} = \mathcal{R}^{-1}\left(\mathbf{R}_{test}\right)\big|_{\mathfrak{G},\mathbf{F}(\mathbf{x}_i,t_j)} . \tag{3}$$

Mathematically, this implies that the given information allows for a unique solution, i.e. $\mathcal{R}^{-1}$ is unique and $\mathbf{R}$ is complete. In order that the parameters, $\mathbf{c}$, may be called material parameters, $\mathcal{R}^{-1}$ is supposed to be independent of $\mathfrak{G}$ and $\mathbf{F}$. It is assumed, that the numerical calculation yields correct results, i.e. the implementation of the material model is correct, the chosen boundary conditions represent the test conditions and an adequate solution strategy including a reasonable meshing of the structure has been chosen. Numerous uncertainties interfere with the need for a unique solution [1], however, which cannot be detailed here due to space restrictions.

3. Methods for Parameter Identification

Common methods for solving the inverse problem, equation (3), are numerical optimisation and neural networks.

Optimisation techniques minimise the deviation between simulated and experimental results with respect to some "target" or "quality function":

$$q(\mathbf{c}) = \|\mathbf{r}(\mathbf{c})\| = \|\mathbf{R}_{sim}(\mathbf{c}) - \mathbf{R}_{test}\| \rightarrow \min_{\mathbf{c}\in\mathbb{R}_c} . \tag{4}$$

Deterministic methods calculate variations of the parameter vector by a unique algorithm, so that the path in the design space is always the same for identical starting vectors, leaving no room for randomness. The advantage is a fast convergence for continuous functions. If there is more than one minimum of the target function, the method will find the local minimum next to the starting vector only. Stochastic methods determine variations of the parameter vector by a random generator. They are comparably slow in convergence but better suited for finding the global minimum independent of the starting vector.

Using deterministic optimisation methods to minimize equation (4), the optimal vector, $\mathbf{c}^*$, is determined from the necessary condition

$$\nabla q(\mathbf{c}^*) = \mathbf{J}^T(\mathbf{c}^*)\,\mathbf{r}(\mathbf{c}^*) = \mathbf{0}, \tag{5}$$

with $\mathbf{J}$ being the Jacobian, to be calculated by finite differences. A sequence of parameter vectors $\mathbf{c}_{k+1} = \mathbf{c}_k + \Delta\mathbf{c}_k = \mathbf{c}_k + \alpha_k\mathbf{d}_k$ with $\|\mathbf{r}_{k+1}\| < \|\mathbf{r}_k\|$ is generated, where $\mathbf{d}_k$ is the search direction and α_k is the step length. The search direction can be assumed along the direction of steepest decent, for

instance. The search for a minimum point $\mathbf{c}^*$ of equation (4) is thus reduced to a sequence of one-dimensional optimisation problems [4].

The objective function may exhibit multiple local minima, so that the result of the minimisation process will depend on the starting vector. In these cases, evolutionary algorithms provide a way out. They include stochasticity combined with search models mimicking natural phenomena, namely genetic inheritance and Darwinian strife for survival. Individuals, whose properties are better coordinated with the environment, have an advantage over others. Badly adapted individuals lose the competition and are rejected.

An evolutionary algorithm uses stochastic processes, but the result is non-random. Due to mutation and recombination, the procedure is non-deterministic and follows a non-unique "convergence path". This feature allows for finding a global extremum of the target function independent of the choice of the starting point. Among the various evolutionary algorithms, the evolution strategy became the most prominent representative, which is commonly referred to be the best, i.e. fastest and most efficient, for optimisation tasks [9], [5].

The concept of neural networks is derived from observations on flow of information between biological neurons. Mathematically, a neural network is an operator $\mathcal{N}$, mapping an input vector, $\mathbf{x}$, to an output vector, $\mathbf{y}$, of different dimensions. Here, this operator is applied to solve the inverse problem, equation (3), in order to determine the material parameters from the mechanical response of a test specimen [10], [6], [7]. A neural network is arranged in N layers, where the output of one layer, $\mathbf{y}^{(n-1)}$, becomes the input of the subsequent layer, $\mathbf{x}^{(n)}$. The synaptic weights have to be adapted to the specific problem. This is done by training of the neural network using the results of numerical simulations for given parameter sets, $\mathbf{c}$, as input.

4. Example

Applications for various constitutive models with numerous parameters can be found in the literature [2], [8], [1], [6], [7], potentially suffering from all problems of non-uniqueness, interdependencies between parameters etc. addressed above, but difficult to discover due to the complexity of the models. To keep the problem handy, a simpler example with just two material parameters is presented here, namely the modelling of ductile tearing of metals by the cohesive model [3]. Cohesive models describe various kinds of decohesion processes by a relation between surface tractions, σ, and material separation, δ. Interface

elements are introduced at the boundaries of solid elements along a pre-defined crack path, which obey a cohesive law, $\sigma(\delta)$, with commonly two parameters, the cohesive strength, σ_c, and the critical separation, δ_c. An evolution strategy

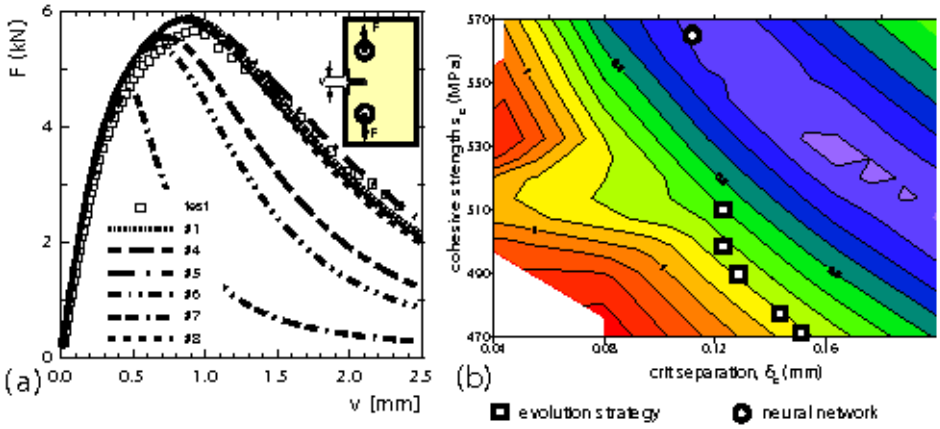

Figure 1: Force vs. displacement of a Kahn specimen; comparison of test and simulation results (left); Iso-contours of the error in the plane of the cohesive parameters, σ_c and δ_c (right)

has been applied for determining both parameters from Kahn test data of an aluminium sheet. Figure 1a shows the test results in terms of the applied force, F, versus the resulting displacement, v, compared to the eight simulation results of the 41-st generation [3]. The specimen starts tearing shortly before the maximum force and a crack initiates and grows with increasing displacement.

A cumulative error has been defined as

$$\varepsilon(v_m) = \frac{1}{v_m} \int_0^{v_m} \left[\frac{F_{sim}(v)}{F_{test}(v)} - 1 \right]^2 dv. \tag{6}$$

Little differences between the simulation and the test results exist for the parameter sets #1, #2, #3, #5, #8 with an error of $0.60\% \leq \varepsilon \leq 0.91\%$ though the respective parameter values differ quite significantly: 477 MPa $\leq \sigma_c \leq$ 510 MPa,0.123 mm $\leq \delta_c \leq$ 0.152 mm. This indicates a rather shallow minimum of the target function. The neural network yielded $\sigma_c = 566$ MPa, $\delta_c = 0.112$ mm. Figure 1b shows iso-contours of the error in the plane of the cohesive parameters, σ_c and δ_c, revealing a canyon-like structure of the error surface. This unfavourable property of the minimisation problem inhibits a more accurate identification of the parameters. It is not clear, however, whether it is due to the cohesive model in general, the specific material properties, the geometrical

configuration of the Kahn specimen or the kind of response data chosen for the evaluation.

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