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Novel criteria for determination of material model parameters

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ABSTRACT

Parameter identification problems have emerged due to the increasing demanding of precision in the numerical results obtained by finite element method (FEM) software. High result precision can only be obtained with confident input data and robust numerical techniques. The determination of parameters should always be performed confronting numerical and experimental results leading to the minimum difference between them. However, the success of this task is dependent of the specification of the cost/objective function, defined as the difference between the experimental and the numerical results. Recently, various objective functions have been formulated to assess the errors between the experimental and computed data (Lin et al., 2002 [36]; Cao and Lin, 2008 [14]; among others). The objective functions should be able to efficiently lead the optimisation process. An ideal objective function should have the following properties: (i) all the experimental data points on the curve and all experimental curves should have equal opportunity to be optimised; and (ii) different units and/or the number of curves in each sub-objective should not affect the overall performance of the fitting. These two criteria should be achieved without manually choosing the weighting factors. However, for some non-analytical specific problems, this is very difficult in practice. Null values of experimental or numerical models also turn the task difficult. In this work, a set of novel objective functions for constitutive model parameter identification are presented. One is a generalization of the work of Cao and Lin and it is suitable for all kinds of constitutive models and mechanical tests, including cyclic and Baushinger tests with null values.

1. Introduction

Nowadays, the quest for secure input data for simulations and more specifically for finite element method (FEM) codes is increasing due to higher demands of industry in obtaining more reliable numerical results. One of the most important input data for FEM solvers is the material behaviour, mathematically described by the constitutive model equations. Due to the large amount of phenomena required to be described by the FEM codes, the constitutive material models became complex and generally include a large number of parameters to be identified for each specific material.

In the previous decades, inverse methodologies have been applied in order to improve the reliability of finite element analysis [1], including metal forming simulations. Even though the nonlinear parameter estimation was already a subject studied in the seventies [2,3], the need of determining parameters for nonlinear constitutive models became an important topic in the early nineties [4–9]. Furthermore, some works already presented and discussed the interaction between optimisation and finite element codes [7,10–12]. In recent times, other works have contributed to this kind of problems presenting new objective functions (e.g. [13,14]), using different optimisation methods (e.g. [15,16]), statistical approaches (e.g. [17]) and the influence of types of measurements used for the identification process including global (inverse analysis) and local (nonlinear regression) measurement [18]. Currently, the identification of constitutive model parameters represents a common problem in both scientific and industrial communities.

Parameter identification for constitutive material models can be accomplished by inverse analysis or/and by nonlinear regression. The first one generally uses global measurements and finite element analysis for computing the numerical values while the second approach can use local or global (average) measurements and analytical models for the estimation of the corresponding computed values. This latter approach is also called single-point analysis. Considering that both finite element method and the analytical nonlinear constitutive models are governed by partial differential equations, the main difference between the two approaches are the time and space integration methods used in each one. This fact influences the obtained results in the evaluation of the objective function and afterwards the optimisation process.

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For the nonlinear regression analyses, the numerical methods generally used to integrate the analytical equations in time are Runge–Kutta explicit methods with adaptive step and error control. Although this approach is computationally very inexpensive, it cannot be used to account for complex experimental tests and phenomena such as specimen necking or springback.

The finite element analysis using an implicit technique [19] generally uses Newton's method as a numerical technique for solving the nonlinear equilibrium equations. For each time increment, the implicit methods need to converge leading to a large computation time when compared with the explicit methods. However, the explicit methods can iteratively accumulate errors. For more details on the influence of using both approaches see, for example, [18]. Within the inverse methods for parameter identification, the comparison of the quantities measured in the mechanical test can be made either on the force measured during the test or including also the displacement field at the surface of the specimen. Full-field [20,21] methods or, more specifically, virtual field methods [22,23] are examples of these approaches.

The general methodology for parameter determination of material constitutive models, as an inverse problem, consists in the minimization of a function $\mathcal{L}$ that represents the difference of the experimentally observed material behaviour and the mathematical model chosen to reproduce it,

$$\begin{aligned} &\min \quad f=\mathcal{L}(\mathbf{A},\mathbf{Z}^c,\mathbf{Z}^e)\\ &\text{s.t.} \quad g(\mathbf{A},\mathbf{Z}^c,\mathbf{Z}^e)\le 0\\ &\qquad \mathbf{A}_{\min}\le \mathbf{A}\le \mathbf{A}_{\max}, \end{aligned} \tag{1}$$

where $\mathbf{A}$ represents the array of parameters that needed to be determined and $\mathbf{Z}$ stands for the set of measured properties, such as the stress, strain, etc. The superscripts c and e stand for computed and experimental values, respectively. The function g defines the set of functions used in the constraints of the optimisation process and $A_{\min}$ and $A_{\max}$ are the material parameter bounds. The minimization is achieved with the assistance of optimisation algorithms, whether they are gradient-based, direct search, metaheuristics or artificial intelligence-based algorithms. However, all those algorithms and their efficiency directly depend on the quality of the information given by the objective function (also called optimisation criterion), defined as $\mathcal{L}$ in Eq. (1).

1.1. Optimisation methodology

In order to determine the best parameters set (the ones that characterizes better the material) optimisation methods are applied. The choice of the technique of resolution of the optimisation problem is crucial because this technique controls the efficiency of the identification method. The three main families of optimisation algorithms are the gradient-based methods, the nature-inspired algorithms and artificial intelligence algorithms. The two last families belong to the class of direct and exploratory methods. The nonlinear optimisation methods based on the gradient function can find local minima through iterative processes guided by the Jacobian (first-order partial derivatives of the objective function vector) and the Hessian. However, commonly these are not the absolute minimum values and the final solution is much dependent of the initial parameters set. These methods are extensively used due to their efficiency and CPU low cost. The disadvantage of reaching a local minimum instead of the global one is not critical in engineering, where larger importance can be given to the time of reaching admissible errors and to improve the overall process. The direct search and nature-inspired optimisation techniques have large probability of finding the global minimum. However, this is reached at the expense of a lot more time to reach admissible error levels. Therefore, the gradient-based method is computationally less expensive. Both optimisation method types, the gradient-based and the direct search, are fully capable of successfully determining material parameter sets for mechanical constitutive models. However, the parameters obtained can be distinct. This problem can be diminished with the increase of experimental data and numerical constraints that enforce physical requirements on the material parameters. The increase of experimental data in order to reduce the problem of non-uniqueness of the material parameters should be done with different loading modes tests. Other approach to increase the robustness of the optimisation methods can be using optimisation strategies (in sequential, parallel or hybrid strategies depending specifically on the cost of the objective function evaluation) [18].

Although the results can be affected by the optimisation algorithm, the choice of the objective function should be independent of the optimisation algorithm to use. Nonetheless, the objective function should be smooth and continuous considering that gradient-based methods cannot be used with a non-continuous objective function.

1.2. Objective functions for parameter identification

Working as a guide, the objective function (OF) should efficiently find the best fit to the experimental data, always subjected to some specific constraints. In order to obtain reliable information about the difference between the experimental and numerical values the objective function should fulfill some criteria [14]

Criterion 1: the errors of the experimental data should not be accounted during the parameter identification process. This could be achieved by eliminating the experimental data points considered of doubtful quality.
Criterion 2: for each curve, all the experimental points should be taken in account and should have equal opportunity to be optimised.
Criterion 3: when using multiple curves, all experimental curves should also have equal opportunity to be optimised, independently of the number of points of each curve.
Criterion 4: if sub-objectives are required, the objective function should be able to deal with the inclusion of these sub-objectives and their account should be done giving equal opportunity to the sub-objective to be optimised.
Criterion 5: different units or scales should not affect the overall performance of the process.
Criterion 6: continuity must be achieved allowing to progressively evaluate the quality of the fitting. Therefore, integer and discrete functions should be avoided in the formulation of the objective function.
Criterion 7: the process should not be dependent of the user. Therefore, the weighting coefficients, useful for achieving some of the above criteria, should be found automatically.

The above criteria are difficult to satisfy in an automatic manner. Generally, these are accomplished manually choosing the weighting coefficients and based on the user empirical experience.

When two curves are intended to be correlated, the r-square function (r^2) is often used. The r-square function is based on the correlation coefficient by Pearson and it reflects an extension of a linear relation between two data set. The r-square function can be written for a correlation between the computed and experimental curve discretized in N points as

$$f=r^2=1-\frac{\sum_{i=1}^{N}(Z_i^c(\mathbf{A})-Z_i^e)^2}{\sum_{i=1}^{N}Z_i^e-\frac{1}{N}(\sum_{i=1}^{N}Z^e)^2}. \tag{2}$$

The r-square function ($-1\le r^2\le 1$) tends to the unity when the quality of the correlation increases. This information can be used