Goal-oriented model calibration using the adjoint framework

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Abstract. *We define and analyze a goal-oriented procedure for model calibration in Computational Mechanics. In this procedure, priority is given in the updating to parameters which are the most influent to predict a given quantity of interest. The strategy uses the constitutive relation error framework as well as duality and adjoint techniques. The objective is thus to perform a partial model validation that enables to obtain the value of the quantity of interest with sufficient accuracy and minimal modeling effort.*

Keywords: Model calibration; Goal-oriented methods; Adjoint problem; Constitutive relation error.

Mathematical models are fundamental in science and engineering activities, particularly due to the fact that they are the basic ingredient of numerical simulations that enable to reproduce physical phenomena and make predictions. However, a major concern is the capability of these models to represent a faithful abstraction of the real world. To address this issue and control the error between physical and mathematical models, model validation methods have been used for a long time [1, 2, 3]. In such methods, model parameters are identified or updated in order to minimize the discrepancy between numerical predictions and experimental measurements. The process leads to inverse problems [4] which are usually ill-posed and require special care and specific techniques, such as regularization techniques proposed in [5], in order to ensure solvability. Getting missing information of the model from measurements is a procedure that is now commonly used in many scientific fields such as geophysics where soil characteristics (density, permeability) are studied, non-destructive control to identify defects [6], or imaging where we can obtain images from a noised version using deconvolution [7] or detect damaged tissus using tomography [8, 9].
We focus here on Computational Mechanics models, in which a major component is the constitutive equation that describes the local behavior of the material. It is characterized by a set of material parameters whose values may highly influence results given by numerical simulations. In order to reduce modeling errors, it is thus important to address the issue of constitutive models calibration. For complex models, it is difficult to design experiments where observed model responses depend explicitly on model parameters. We rather use in practice experimental data that depend implicitly on these parameters, and the calibration is then viewed as an optimization problem in which parameter values are searched such that optimal agreement between experimental and simulated responses is achieved [10].

When a large number of experimental data is available, as it is the case with full-field kinematic measurements performed by means of imaging techniques (DIC for instance), many calibrations methods can be applied for inverse analysis and identification of material properties [11]. Among all of them, we can mention the Equilibrium Gap Method (EGM) which is based on the discretization of equilibrium equations and minimization of the equilibrium gap, the FEMU method (balance method FEMU-F or displacement method FEMU-U) which is an intuitive approach that consists in performing iteratively finite element computations to find constitutive parameters that achieve the best match between computed and actual measurements, or the Constitutive Equation Gap Method (CEGM) which was initially developed for updating finite element models from vibrational data and assessing quality of finite element meshes.
We consider in this paper the case where only few localized measurements are available. Again, several procedures

exist in this framework to identify parameters, such as minimization of cost functions associated with regularization techniques [4], or the Bayesian inference approach that formulates parameter identification in a stochastic setting [12, 13]. Using the concept of Constitutive Relation Error (CRE) defines another model validation method on which we focus here. First introduced in [14, 15] for dynamics models, this method was latter successfully used in many validation applications with uncertain measurements and behaviors [16, 17], or corrupted measurements [18, 19]. Recent applications of the method dealt with the updating of models used in bolted assemblies [20], or association with PGD reduced models to deal with real-time calibration of machining models [21]. The use of the CRE presents interesting advantages; it has excellent capacities to localize structural defects spatially, it is very robust with respect to noisy measurements, and it has good convexity properties.

If the determination of the values of unknown model parameters is the primary goal of the validation process, the problem is called *parameter identification problem*. Here, we rather tackle *model calibration problems* as we are only interested in the computation of given quantities of interest which are outputs of the model depending implicitly on the unknown parameters. Therefore, if a quantity of interest is not very sensitive with respect to some parameters, there is probably no need to estimate this parameter with high accuracy. This goal-oriented model validation approach is motivated by the fact that the objective of numerical simulations is usually not the global response of the model, but only specific features which are relevant for design (such as local stress, maximal displacement or temperature, etc.). It aims at performing a partial calibration of the model so as to ensure the quality of predicted quantities of interest with a minimal validation effort.
Several works have already addressed this scientific issue. In [22, 23], an optimization problem coupled with a dual method was introduced to assess, in a goal quantity, the sensitivity with respect to the observed data (uncertainty or noise), as well as discretization error affecting the computed value of parameters. The a posteriori discretization error estimator was also used in an adaptive algorithm to construct economic meshes. In [24], the goal-oriented a posteriori error estimation for identification problems was extended to accommodate the combined identification and subsequent simulation problems which may be governed by different state equations (and only coupled via model parameters). For a given tolerance in a quantity of interest, depending on the solution of the simulation problem, three sources of errors were controlled: modeling error, discretization error polluting the identification problem, and discretization error in the simulation.

Here, we wish to extend this setting to validation methods performed using the CRE. We assume that the discretization error is negligible compared to the modeling error, and focus on the sensitivity of the considered quantity of interest with respect to parameters and measurements. This enables to define a convenient goal-oriented validation process, and gives information to define optimal experiments and measurements (sensor location, type of measure) with respect to the output of interest to predict. The procedure leans on the definition of a new cost function to minimize, which is dedicated to the quantity of interest under study. Together with the (modified) constitutive relation error framework, its lead to a convenient strategy that selects a relevant parameter set to be updated and also provides for useful information in order to define optimal experiments. Performances of the approach are analyzed on several validation examples with linear models.

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