Application of a frequentist metric for the validation of computational mechanics models.

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Introduction

Simulations are an integral part of scientific analysis of phenomena in many different branches of engineering. The development of advanced computational mechanics models makes it possible to perform virtual experiments and obtain data that would otherwise be very difficult or impossible to collect. However, due to the nature of simulations, specifically being based on assumptions and involving uncertainties, the credibility of results is a big concern. Confidence in simulations and the quality of the outcomes relative to reality can be evaluated through performing verification and validation [1]. As verification precedes validation, in the current work it will be presumed that verification of the deployed algorithms have been completed by following accredited benchmarks [2] and thus the application of validation approaches can be investigated.

Discussions on validation have been ongoing for half a century and have led to the development of guides applicable across many engineering disciplines (see e.g. [1, 3, 4]). These clarify the definition of validation and provide an overview of important steps that should be performed, but have left a definitive methodology open to interpretation. Subsequently, research has concentrated on interpreting the guidance to develop a metric, i.e. a function to determine discrepancy between two sets of data [5], that would allow the implementation and achievement of the validation aim (see e.g. [6, 7]). Despite these efforts, there is no widely applied and recognised methodology to validate computational mechanics models. Also, validity statements often only state whether a model is valid or not, and has no indication of the degree of quality, as required by the definition from the ASME guide [1]. This gap has motivated the current research, which aims to develop an objective and quantitative validation metric based on various statistical approaches.

The objective of this work is to present and evaluate a recently developed validation metric, and its applicability to computational mechanics models that simulate surface displacement or strain (Fig. 1 b, c, d).

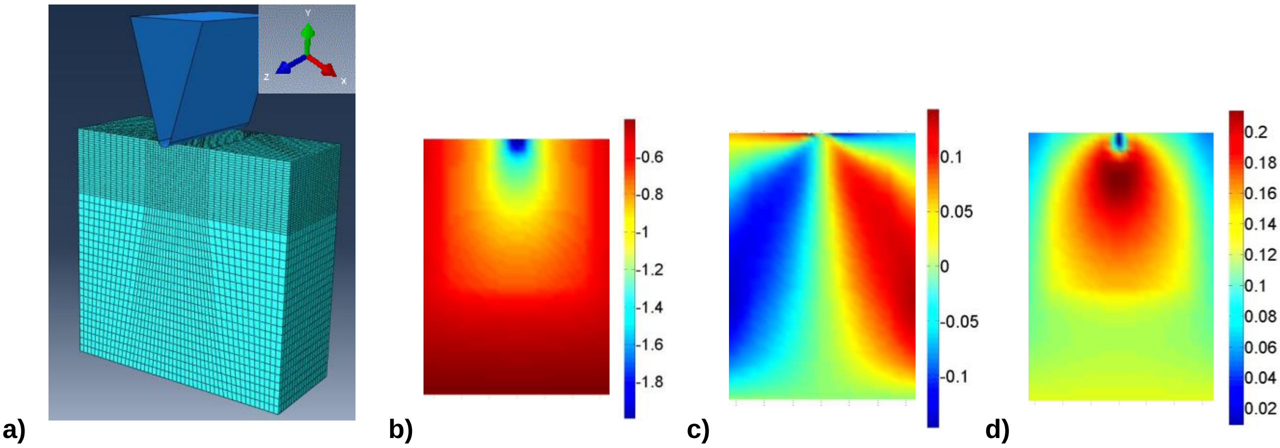

Figure 1: a) Finite element model of a rubber block (60mmx60mmx25mm) subject to a 2mm indentation by a rigid wedge and the corresponding displacement maps in b) X, c) Y and d) Z directions.

Methods

In the literature validation methodologies can be categorised in three distinct approaches: hypothesis testing, frequentist and Bayesian analyses. Our research was concentrated on frequentist approaches, which are based on mapping a discrepancy in the computational response relative to referent or, in the case of validation, relative to experimental data. Of particular interest to this work are simulations of deformation and the corresponding data in the spatial domain obtained from optical measurement techniques.

In this study, a new methodology is proposed that can be applied to data fields, e.g. displacement (Fig. 1b), and allows the quantification of the quality of the model in terms of a probability statement. The novel metric incorporates uncertainty quantification and is based on relative error analysis [8, 9], i.e.

$$\%\text{Relative Error} = \left|\frac{x_p - x_m}{x_m}\right| \times 100 \qquad (1)$$

where x_p refers to predicted data and x_m refers to measured data. Contrary to previously published methods, the new method is expected to be more robust for data sets with high variance and values close to zero. The robustness of the metric is evaluated by validating previously published results, i.e. deformation of a rubber block subject to indentation [10].

Application

Rubber components are frequently used in engineering structures for a variety of applications and usually undergo compression in service, nonetheless only a limited understanding of the material behaviour is currently available. In this study, a rubber block (60x60x25 mm) indented by 2mm with an aluminium wedge, as shown in Fig.1a, was considered. A finite element model was developed using Abaqus 6.11 software package and equivalent experimental data was acquired from a previously conducted study, which utilised Digital Image Correlation [10]. Predicted and measured data fields were treated as images, thus in the present work validation has involved employing image decomposition technique and then comparing corresponding vectors of shape descriptors using the novel metric. In the scope of the proposed metric, model's validity was obtained by computing relative error between two sets of vectors and evaluating the result against an accuracy requirement, which in this study was specified as an uncertainty in experimental results. This process led to a probability of computed relative errors being equal or less than the experimental uncertainty. From a validation perspective, we propose to interpret this outcome as the probability of a model being valid.

Conclusion and future work

Validation is necessary to build confidence in computational mechanics models. Due to the lack of definitive methodologies and the complexity of the process, very often validation outcome only states whether a model is valid or not. Such outcome is not in accordance with the ASME guidelines and thus research on more comprehensive validation metrics has to be performed. In this work, we have presented a new metric based on relative error analysis and uncertainty quantification. As an outcome, it is proposed to interpret validation in terms of probability, which we believe allows to quantify the quality of the model relative to reality and thus is a great advancement in this field of research. However, further research is necessary to improve understanding of the uncertainties associated with experimental and computational data, and to validate phenomena associated with a temporal domain.

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