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The Monte Carlo Method for evaluating measurement uncertainty: Application for determining the properties of materials

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ABSTRACT

Many statements about the quality of a numerical model can only be made by including the appropriate experiments (e.g. the quantification of the statistical uncertainties of model input parameters while calibrating the confidence level estimator model, which is heavily dependent on the definition of the experiment and the quality of its implementation). Focus is thus placed on developing methodology for quantitatively assessing the quality of the results of experiments and their exemplary implementation.

This paper presents a qualitative evaluation method for experimental results. The probabilistic approach in particular can provide substantial information during the evaluation. Therefore, methodology for predicting the uncertainty in the qualitative evaluation of experimental models. An appropriate way to propagate probability density functions through an experimental model is based on the Monte Carlo Method (MCM). The probability distributions are obtained by applying the MCM coupled with appropriate definitions for the total measurement uncertainty. This paper elaborates on the computational aspects of calculating measurement uncertainty of experimental models. The MCM has a higher conversion rate, generates narrower intervals, and produces more stable (evaluation) results. This method should reduce the analytical effort required for complicated or nonlinear models, especially because partial derivatives of the first or higher order (used in providing sensitivity coefficients for the law of propagation of uncertainty) are required. This method thus provides a mathematical and a computational tool for quantifying the uncertainty of models. Moreover, it can be used to improve measurements in order to promote quality and capacity with respect to decision-making.

1. Introduction

Experimental and numerical models are required to reliably assess the safety and usability of newly constructed and existing structures. The quality of numerical and experimental models must be evaluated in order to reliably predict structural behaviour and design. Many statements about the quality of a simulation model can only be made by including the appropriate experiments (e.g. the quantification of the statistical uncertainties of model input parameters during the calibration of the confidence level estimator model, which is heavily dependent on the definition of the experiment and the quality of its implementation). Metrological aspects should therefore be used in order to guarantee the equivalence of results between different laboratories and evaluate the measurement or simulation results. However, methodology for quantitatively assessing the implementation and results of experimental models is lacking. Furthermore, the quantitative assessment of the behaviour and performance of materials is essential for achieving reliable high-quality products. Experimental models have been to:

- validation of theoretical/numerical models,
- determination of required input parameters for these theoretical/numerical models,
- calibration of input parameters.

When validating models, experimental models are used to both quantitatively and qualitatively compare the results of simulations. The experimental results often only consider the aleatoric uncertainties as a target for the simulation. A consistent and quantitative evaluation of experimental error or the experimental model itself is often neglected.

Experimental models are composed of different partial models (PMs), such as specimen, boundary, and load conditions or sensor technology. Because these PMs are correlated quantification of the quality of all PMs is crucial for evaluation the quality of the global experimental model. An experimental model illustrates a reality

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bound by certain restrictions and definitions in the context of a scientifically manageable theory. In general, not all aspects of reality can be described with experimental models. Therefore, experimental modelling is often referred to as abstraction. In this context, a PM describes the partial aspects of a global experimental model.

Measurements always entail uncertainty. Measurement results can therefore not be used directly. The uncertainty analysis should take into consideration the measurement method, measurement devices, measurement process, human error, and mathematical analysis (e.g. data modelling, uncertainty analysis, parameter estimation, hypothesis test, precision evaluation) [1]. The applicability of the method for calculating uncertainty should therefore be reviewed and verified in order to evaluate the assessment of experimental models in the field of engineering.

At present, there is no scientifically-based methodology for quantitatively assessing the quality of an experimental model. Apart from a few specialised exceptions [2–6] the qualitative evaluation of experimental models in civil engineering solely been based on the practical phenomenological knowledge of the user. In experimental modelling, there are numerous experimental models with different complexities [7].

Experimental models are fundamental for guaranteeing the quality of scientific and industrial activities. The results of such measurements must be valid, comparable, and reproducible; their uncertainty is the quantitative measurement that expresses the quality of such results. Generally, when a parameter or value has to be compared with a limit or threshold, a simple mathematical comparison between two values should be avoided. In fact, the result of any measurement is affected by uncertainty. The analysis of conventional uncertainty via the Root Sum of Square (RSS) method is often difficult in complex systems and requires approximation at each stage of processing, thereby placing serious doubts on the validity of the results. In accordance with the ISO/IEC 17025:1999 [8] standard, all calibrations or testing laboratories must have and apply procedures to evaluate uncertainty in measurement as a guarantee of their technical competence. In order to perform this evaluation, the ISO 98:1995 guide, which is commonly known as the "Guide to the Expression of Uncertainty in Measurement" (GUM) [9], has been widely used and accepted by the metrological accreditation organization. Various supplements to the GUM are being developed. These will progressively come into effect. In the first of these supplements (GUM S1) [10], an alternative procedure for calculating uncertainties is described: the Monte Carlo Method (MCM). This include non-symmetric measurement uncertainty distributions, non-linearity within the measurement system, input dependency, and systematic bias. The main elements of the formalism were originally proposed by Weise et al. [11]. The procedure was then succinctly outlined by [12] and focused on its relation to MCM described by JCGM2008 [10]. Wübbeler et al. [4] explained similarities and differences between the GUM and GUM S1 approaches. Many groups have recently applied Bayesian updating to evaluate measurement uncertainty (e.g. [11,13–18]). Several books [19–21] also discuss issues relevant to this general evaluation method. The approach introduces a state of knowledge distribution about the quantity on interest and is derived from prior information about the quantity as well as other influencing quantities and measured data, using probabilistic inversion or inverse uncertainty evaluation.

The standard uncertainty of an experimental model decreases if available of data set increases. Conversely, the cumulative uncertainty of the data set increases as the amount of available data decreases. Hence, the final uncertainty of the measurement, which is the degree of standard uncertainty and systematic and random deviation, does not monotonically decrease. Consequently, for each data set, an optimal model complexity in which the complexity of the models is directly related to the number of variables used by the model must be determined [22]. In the field of experimentation, it is difficult to determine the optimal model [23–25].

Despite the need, there are no scientific studies about the qualitative evaluation of the global experimental model. Thus, the development of a new method is urgently needed, especially for the qualitative assessment of experimental models in the field of engineering. One of the reasons for this has to do with the specified requirements for the investigated models, which require deterministic and probabilistic analysis. Although there are many models that could be used to represent physical reality, they are not applicable because of the high experimental costs. Therefore, an experimental model of qualitative analysis based on reducing the uncertainty and cost of experiments and increasing the reliability and robustness of experimentation is developed.

2. Propagation of distribution by the Monte Carlo

For the detailed descriptions of GUM procedure refer to [3,8,9,17,19]. The MCM only defines those probability functions considered by JCGM2008 [10] that have a univariate Gaussian portability density. The MCM provides a general approach for numerical approximation to the distribution function $g_Y(\eta)$ for the output quantity:

$$Y = f(X) = f(X_1, X_2, \ldots, X_N). \tag{1}$$

The input quantities of the model are $X = (X_1, X_2, \ldots, X_N)^T$. The distribution function for output quantity Y obtained from Monte Carlo simulation is defined as [10,26]:

$$G_Y(\eta) = \int_{-\infty}^{\eta} g_Y(z)\, dz \tag{2}$$

and

$$\mu(y)^2 = \int_{-\infty}^{\infty} g_Y(\xi)(\xi - y)^2\, d\xi. \tag{3}$$

The probability density function is defined as:

$$g_Y(\eta) = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} g_{X_1 \ldots X_N}(\xi_1 \ldots \xi_N)\delta(\eta - (\xi))\, d\xi_1 \ldots d\xi_N \tag{4}$$

where δ is the Dirac function, $g_{X_i}(\xi_i)$, and $i = 1, \ldots, N$, are the probability density function of the input quantities X_i, $i = 1, \ldots, N$.

Measurement uncertainty matrix is given by:

$$g(\xi) = \frac{1}{((2\pi)^N \det V)^{1/2}} \exp\left\{-\frac{1}{2}(\xi - x)^T V^{-1}(\xi - x)\right\}. \tag{5}$$

This probability density function reduces to the product of N univariate Gaussian probability density functions when there are no covariance effects for the following equation. In that case,

$$U_x = \mathrm{diag}(\mu^2(x_1), \ldots, \mu^2(x_N)), \tag{6}$$

An uncertainty matrix U_x with vector estimate x and input quantities can be expressed by covariance matrix

$$U_x = \begin{bmatrix} \mu(x_1)^2 & \cdots & \mu(x_1 x_N) \\ \vdots & \ddots & \vdots \\ \mu(x_N x_1) & \cdots & \mu(x_N x_N) \end{bmatrix} \tag{7}$$

where $\mu(x_i)^2$ is the variance (squared standard uncertainty) associated with x_i and $\mu(x_i x_j)$ is the covariance associated with x_i and x_j. $\mu(x_i, x_j) = 0$ if elements are uncorrelated.

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