Quantifying Total Uncertainty Using Different Mathematical Theories in a Validation Assessment

T. J. Ross, F.ASCE
University of New Mexico, Albuquerque, NM 87131
ross@unm.edu

J. M. Booker, F. M. Hemez, M. C. Anderson, B. J. Reardon, C. A. Joslyn
Los Alamos National Laboratory, Los Alamos, NM 87545
jane@lanl.gov, hemez@lanl.gov, mcanderson@lanl.gov, breardon@lanl.gov, joslyn@lanl.gov

ABSTRACT: This paper summarizes an on-going development of a metric to quantify total uncertainty in the validation of a computer code that might be used, for example, to assess the reliability of a structural system. The total uncertainty is expressed as an aggregation of various forms of uncertainty. Such an aggregation is based on a group of methods collectively called *generalized information theories*. Among these theories are evidence theory, possibility theory, fuzzy set theory and, of course, probability theory. A simple case study is used to illustrate how the validation of a computational prediction can be assessed by the representation and quantification of uncertainties that influence the difference between the prediction and the experimental results.

INTRODUCTION

Inherent in most constructed systems built for the public (e.g., buildings, bridges, dams) there is some margin of safety defined as the amount by which the system exceeds the limits of its nominal design requirements. Often, original design knowledge is not adequately documented, making later uncertainty quantification and safety margin estimation difficult. Constructed systems suffer degradation as they age. Design intent and its relationship with the structure's current condition are not easily determined. When we assess a structural system in terms of its reliability or safety, we are interested in how the system responds to external disturbances like wind or earthquake loading. But, what if the system changes with time, due to aging or other effects? Most structural designs are based on today's knowledge of environmental loads and today's material properties. However, how robust will that design be with different, potentially greater loads, and aging materials and undetermined workmanship? In other words, how robust is today's optimum design to the uncertainties in various design or environmental conditions? More importantly, if we want to ensure that our computational capabilities can assess these changes, we need a way to quantify the many uncertainties involved in making these predictions. Of particular concern in making predictions about structural response is the systems capacity to remain safe as time evolves and external conditions change. We are developing metrics to assess the quality of numerical predictions when compared to experimental evidence, in terms of the *total uncertainty* in the predictions.

This paper summarizes our on-going development of the *total uncertainty*, based on a group of methods collectively called *generalized information theories*, to represent the various uncertainties that impact validation assessments. Among these theories are evidence theory, possibility theory, fuzzy set theory and, of course, probability theory. A simple case study is used to illustrate how the validation of a computational prediction can be assessed by the representation and quantification of uncertainties that influence the difference between the prediction and the experimental results.

VALIDATION ASSESSMENTS

Validation is the process of evaluating a model's predictive capability and its ability to represent reality. It involves the act of quantifying how well and under what conditions a model or code matches real systems and thus can be trusted in a predictive capacity. Validation is also a process of determining the degree to which a computer simulation is an accurate representation of the real world, from the perspective of the intended uses of the model. Some have suggested that validation is easier to understand; e.g., that it is simply solving the appropriate governing equations. Within the context of model validation the ultimate goal of uncertainty quantification is to construct an uncertainty model for every component of the simulation, which taken all together summarize how well the predictions agree with the available test results (Shinn, et. al, 2003).

Inherent in validation activities is the understanding, characterization and propagation of different kinds of uncertainties, arising from sources such as model uncertainties, numerical errors, parameter uncertainties, and lack of knowledge. Some of these different kinds of uncertainties are discussed in the sections below.

QUANTIFYING UNCERTAINTY

Types of Uncertainty

The quality of any validation of computer predictions is inextricably linked to uncertainties. The better we can do to represent and quantify the uncertainties in both models and supporting data, the more useful these quantities are for making validation assessments. In representing *uncertainty* we distinguish between two general types. The first is the natural variability of things due to manufacturing processes–called *variability*. Variability cannot be reduced, but only quantified. The sizes of grains of sand or the specific shapes of a maple leaf are things that exhibit natural variability. If we want to predict either of these quantities we can only do so in an average sense for the population of grains or leaves. Another type of uncertainty is due to a lack of specific information, which we could call, generally, *complexity*, to distinguish it from *variability*. Complexity can be reduced–with the acquisition of more information. Complexity can result from ignorance, from scarce data, from misleading or conflicting information, from lack of knowledge, and from unknown biases. Collectively these various forms of non-randomness contain forms of imprecision, ambiguity, non-distinctiveness, vagueness or fuzziness. The *total uncertainty (TU)* in a problem is a combination of these two general forms: *variability* plus *complexity*.

Representation of Uncertainty

While there are several useful theories to represent the various types of uncertainties (see Klir and Wierman, 1999) we shall focus only on two of the more prevalent ones–*probability* theory and *possibility* theory. The fundamental difference between these two theories of quantifying uncertainty is that in *probabilistic* bodies of evidence all the evidence is concentrated on the singletons of a universe of information, whereas in *possibilistic* bodies the evidence is located on collections of nested sets within the universe of information. Both formalisms are uniquely represented by distribution functions, but their normalization requirements are different. The collection of values in a *probability* distribution are required to add (or integrate) to unity, while for *possibility* distributions the largest values are required to be unity (a condition called normality). These differences in mathematical properties of the two theories make each theory suitable for modeling various types of uncertainty and less suitable for modeling other types. For example, probability theory is an ideal tool for formalizing uncertainty in situations where event frequencies are known or where evidence is based on outcomes of a large number of independent and repeatable trials. Possibility theory, by contrast, is ideal for formalizing incomplete information expressed in terms of vague or ambiguous terms, or where evidence supports conflicting events.

Features of Total Uncertainty

This paper summarizes a new procedure to assess the total uncertainty in the process of validation assessment (Ross, et al., 2003). It is based on the hypothesis that *total uncertainty* should scale between two extreme conditions on uncertainty, i.e., between the case of *no-uncertainty* and the case of *maximum uncertainty*. If we make a prediction on the response of some structural system and the level of uncertainty that we express in that prediction is *close* to the extreme of *no-uncertainty* we can say that we are "highly confident" in that prediction; on the other hand, if we are *closer* to the other extreme, the case of *maximum uncertainty*, then we can say that we are not very confident in the prediction. Of more importance, however, is the fact that we can develop a "metric of confidence" that will scale linearly with our quantified level of uncertainty and, in a mathematical sense, measure the degree of *closeness*.

Calculation of Total Uncertainty

Suppose we are predicting the value of a variable of interest in a mechanics calculation, say the maximum stress in a bar. We then define the case of *no uncertainty* as one in which all information and evidence supports only one value of the variable of interest (stress) and there is no evidence on all other potential values of that variable, and in which any probability is associated with a value equal to unity on one value of the variable (stress) and zero probability on all other potential values of that variable. The other extreme of *maximum uncertainty* is then defined as the case where all potential values of stress are completely possible (i.e., certain) and all potential values of the variable are equi-probable (the case of a uniform probability distribution). In the literature, the forms of uncertainty associated with a possibility distribution are those called *non-specificity* and *discord*. By non-specificity we mean a kind of imprecision which is connected with sizes of relevant sets of alternatives. By discord we mean that there is conflict among the various sets of alternatives. The form of uncertainty associated with a probability distribution is a kind of strife, where again there is conflict among the various specific values of alternatives. *Probabilistic* strife (conflict) is most often term entropy, and it is different from *possibilistic* discord in that in the former all evidence is nested on single values of the variable of interest, whereas the latter supports evidence that is nested on collections, or sets, of various values of the variable of interest. Hence, *total uncertainty* as used in the context presented here is defined as the combination of possibilistic *non-specificity* with the probabilistic entropy, or *conflict*. We present here a new procedure to combine these uncertainties; other combination procedures in the literature first reduce the various uncertainties to the bit-level ($\log_2$)

before a combination is performed, or the various uncertainties are used to formulate a data-tuple (see Klir and Wierman, 1999).

We begin the development of the total uncertainty by first defining an uncertainty matrix, which contains the *possibilistic* uncertainty vector in its first column and the *probabilistic* uncertainty vector in its second column; we shall term this matrix A. For a variety of compelling and intuitive reasons (Ross, et al., 2003) a procedure known as singular value decomposition (SVD) was chosen as a means to calculate *total uncertainty*. Many of these reasons have to do with an analogy of this approach to the extraction of modal frequencies from a model of a structure undergoing dynamic motion. In this process we perform a modal extraction of frequencies using an eigenvalue analysis of the structure. The frequencies from the eigenvalue analysis represent the *total energy* of the structure during vibration in its normal modes (eigenvectors). In our analogy for the characterization of uncertainty, the singular values of our SVD analysis represent the *total energy of the uncertainty* in the matrix A, or more simply the *total uncertainty*.

To begin this development we start first with our decomposition,

$$\mathrm{A} = \begin{bmatrix} \pi_1 & p_1 \\ \pi_2 & p_2 \\ \pi_i & p_i \\ \pi_{i+1} & p_{i+1} \\ \pi_m & p_m \end{bmatrix} \text{ and } A = U\Sigma V^T \qquad (1)$$

where A is an m x 2 matrix of columns expressing the two types of uncertainty, U is an orthonormal m x m matrix whose columns are the left singular vectors of A, Σ is an m x 2 matrix containing the singular values of A, and V is an 2 x 2 orthonormal matrix whose columns are the right singular vectors of A. Parameter m is the length of the two uncertainty vectors.

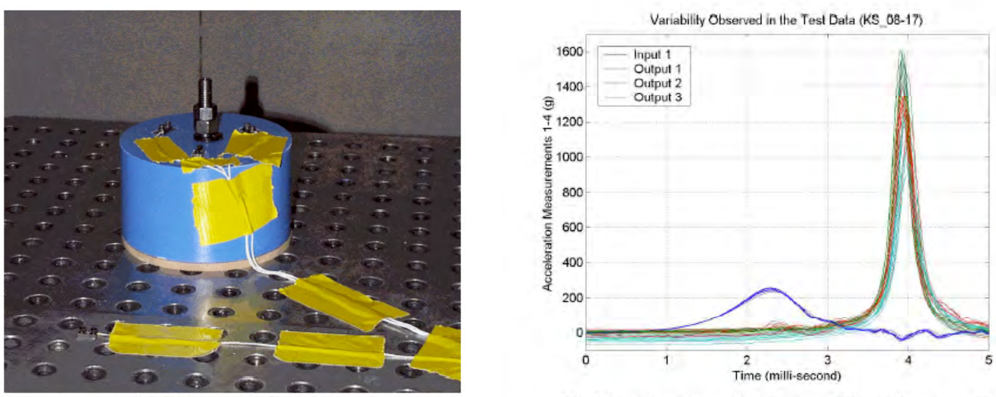
What is of particular interest is the fact that the singular values in the matrix Σ contain the "energy" or the *total uncertainty* of the quantifies expressed in A. The expression for *Total Uncertainty (TU)* is then given by:

$$TU = 2\left(\left(\sigma_{\max}\sum_{i=1}^{m}\sigma^2{}_i\right)-1\right), \text{ for i = 1, 2,...,m} \qquad (2)$$

where, $\sigma_{\max} = \left[\pi_{\max}^2 + p_{\max}^2\right]^{-1}$, where σ_i is the ith singular value in Σ, where, $\pi_{\max}$ is the largest possibility value in the first column of A, and where $p_{\max}$ is the largest probability value in the second column of A. Finally, the extreme cases for *no-uncertainty* and *maximum uncertainty* are given by the expressions, TU = 0, and TU= 2(m-1) (see Ross, et al., 2003).

CASE STUDY

The methods described in Eqns. 1-2 were organized and implemented for a case study involving the crushing of a hyperelastic foam from a simple impact loading. Of interest was the computational prediction of the peak acceleration within the foam. Although experiments were performed on this example (see Figure 1.b), only the uncertainties involved in a computational prediction of the peak accelerations were considered. A finite element code was used to model the system. Two types of analyses were performed on the uncertainties. First, *probability theory* was used to assess the uncertainties of the test results for the peak acceleration (PAC). Second, *possibility theory* was applied to various model configurations, whose parameters included such variables as friction coefficient, amount of preload applied, and impact angles of the drop table (see Figure 1.a). For example, uncertainties from previous test results on similar foam, simple first principle calculations, choices of material models, equation solvers, and boundary conditions were represented by possibility distributions. Table 1 contains the interval values of PAC from the various models and sources of information. These six intervals are formulated into a □-df (*possibility* distribution function) using a method developed in a dissertation by Donald (2003). That □-df and the corresponding *probability* density function (pdf) of the test results for PAC are plotted in Figure 2.



(a) Experimental set-up.

(b) Signals measured during 10 replicate tests.

Figure 1. Shock wave through hyper-elastic foam. (a) the experimental set-up and (b) the input and output signals for 10 tests.

Table 1. Intervals from Different Model / Information Sources.

Model	**Lower Value of PAC**	**Upper Value of PAC**
SDOF, Material Models [2 cubics]	0.2480	0.2850
SDOF, Material Models [cubic, bilinear]	0.8570	0.1250
SDOF, HKS/“ABAQUS”	0.2850	1.6435
Preload in Bolt [min, max]	1.1943	2.4771
Hand calculation on I-mv [.01s, .001s]	0.3000	3.0000
Old test data range from 3 gages	1.2170	1.5940

In Eqns. 1-2 we used m=30 as the length of the probability and possibility distributions. Using these equations we establish that the total uncertainty expressed by the combination of probabilistic and possibilistic types is equal to a value of TU = 17.44, which is 30% of the *maximum uncertainty* that the problem could contain (i.e., we get TU_{max} = 58). What this means is that the problem does contain a level of uncertainty that is closer to the case of *no-uncertainty* than it is to the case of *maximum uncertainty*. More important, if additional analyses on this problem were to be performed, and the value for TU decreased below 17.44, this would equate to a situation where the confidence in the prediction of peak accelerations would be higher.

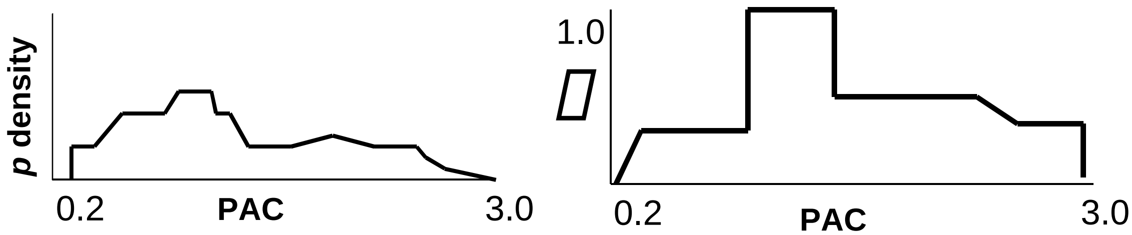


Figure 2. pdf for the tests and □-df for the models (PAC is in 10^3 g's).

SUMMARY

In this paper we have discussed the importance of validating our numerical predictive capability to assess various issues associated with a structures response to external disturbances. Such issues as a structure's reliability, its safety margin and its structural behavior as it ages are all conditions that are currently predicted by numerical codes. Implicit in the code predictions are the uncertainties that are inherent in the systems configuration, in the external disturbances, and in the knowledge we have about any confirmatory experimental or real world response data. We have proposed a new method to assess the *total uncertainty* in a physical system; such an assessment is necessary to fully exploit the process of validation. This new method is still under development, but significant promise has shown that the new method agrees with assessments of the total uncertainty in well-established canonical cases published previously (Klir, 2003). One of our current investigations is to segregate the TU information in Eqn. 2 into proportions that relate to the amount of *non-specificity* and to the amount of *conflict* which together combine to form the total uncertainty.

REFERENCES

Donald, S. (2003) "Development of Empirical Possibility Distributions in Risk Analysis," Ph.D. dissertation, University of New Mexico, Albuquerque, NM.

Klir, G. (2003), "Uncertainty-based Information", in Teodorescu and Melo (eds), Systemic Organization of Information in Fuzzy Systems, IOS Press, Amsterdam, pp. 21-52.

Klir, G. and Wierman, M. (1999) Uncertainty-based Information: Elements of Generalized Information Theory, Physica-Verlag/Springer-Verlag, Heidelberg and New York.

Ross, T., Booker, J., Hemez, B. Reardon, F., Anderson, M. and Joslyn, C. (2003) "Use of Total Uncertainty in Understanding Safety Margin and Model Validation in Structural Mechanics", in preparation.

Shinn R., Hemez F., and Doebling, S. (2003), "Estimating the Error in Simulation Prediction over the Design Space", Proc. 44th AIAA/ASME/ASCE/AHS Structures, Structural Dynamics, and Materials Conference, Norfolk, Virginia, April 7-10.