A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing

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1 INTRODUCTION

Uncertainty quantification has been applied in various fields to acquire approximate outcomes to use in real-world applications. It helps in the optimization and decision-making process. A predictive uncertainty framework is designed in a way to treat both epistemic and aleatory uncertainties by propagating both uncertainties through a model to System response quantities. This paper starts by explaining the types of uncertainties and subsequently the various sources of uncertainties. Then the predictive framework is explained to treat all those sources of uncertainties. There are six phases in this framework, the First phase is to identify all sources of uncertainty, the second phase is to characterize the model uncertainties, the third phase is to eliminate or estimate the code and solution verification errors, and the fourth phase is to propagate the uncertainties through the model, the fifth phase is to quantify the model form uncertainty, and the sixth phase is to estimate the model form uncertainty. In the end, for decision-makers, there are various methods for verdict the total predictive uncertainty. For the purpose of illustration, they used a hyper-sonic wind tunnel in computational fluid dynamics.

2 CLASSIFICATION OF UNCERTAINTIES

The uncertainty is classified as aleatory and epistemic uncertainty[2]. The aleatory uncertainty is a representative of randomness that differ for each iteration of the same experiment. It is also known as irreducible uncertainty and it is Characterized either by probability density function or cumulative distribution function. Epistemic uncertainty occurs due to a lack of knowledge during the phase of analysis. It is also known as reducible uncertainty and it is characterized by intervals. As it is mentioned, this uncertainty could be reduced through conducting various experiments, also through improved numerical approximation, and even suggestions from experts' opinions.

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3 SOURCES OF UNCERTAINTIES

The sources of uncertainties are broadly classified as aleatory, epistemic, or mixed uncertainties. If in case, there is any fixed value uncertainty then it is treated as deterministic. All possible sources of uncertainty must be identified and characterized. These uncertainties occur in model inputs, numerical approximations, or model form. This figure 1 represents the various other sources of uncertainties.

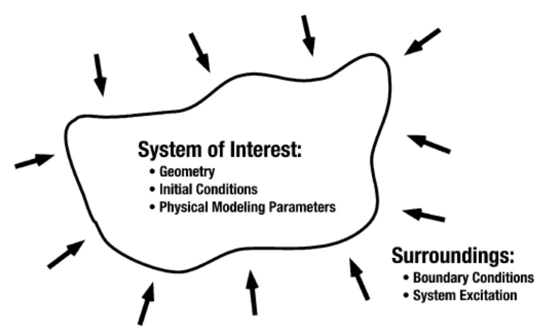

Figure 1: Model input uncertainty sources(from[4])

3.1 Model Input

The model Input uncertainties can be characterized as aleatory, epistemic, or mixed uncertainty which includes parameters both from the model as well as the data from surroundings (i.e boundary conditions, system excitation, initial conditions, or expert opinion).

3.2 Numerical approximation

The numerical approximation errors include discretization error, iterative convergence error, roundoff error, and also errors due to programming bugs. Discretization error is the largest of all numerical errors and it is hard to evaluate for real-world issues. To obtain a steady-state solution we use relaxation techniques that results in Iterative convergence errors. The effects on the numerical solution in coding mistakes are hard to estimate. A single solution is not sufficient for a mathematical model of nondeterministic methods; thus ensemble simulations are preferred. For accuracy, the mapping depends on four key factors (1) the nonlinearity of the partial differential equations, (2) the dependency structure between the uncertain input quantities, and (3) the type of the uncertainties, i.e., whether they are aleatory, epistemic, or mixed uncertainties, and (4) the numerical methods for computing the mapping mentioned in the below figure 2.. To propagate input uncertainties into the model, various techniques like Monte Carlo and Latin hypercube sampling are used. The most common technique is Monte Carlo sampling [1].

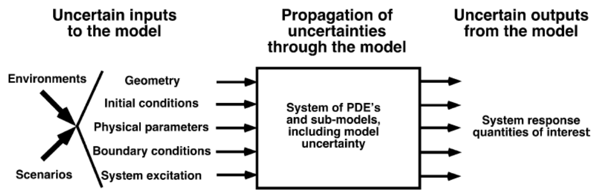

Figure 2: Propagation of I/O uncertainties (from[4])

3.3 Model form

The source of model form are from all conceptualizations, assumptions, abstractions, approximations, and mathematical formulations on which the model relies [3]. The model form is characterized as validation in a way of comparing outcomes with the experimental data for model accuracy purposes. The validation process is carried out as a standard procedure but in addition to it, there are a few steps to proceed further. Initially, the disagreement between the simulation and experimental results is statistically quantified, then it extrapolates the structure of uncertainty where is no availability of experimental data.

4 UNCERTAINTY FRAMEWORK

The main objective of the framework is to be able to estimate the uncertainty in an SRQ where no experimental data is available. The mathematical model which we are going to use includes numerical approximation uncertainties and extrapolation to predict the uncertain SRQ. The process of identifying the sources of uncertainty is explained in the next paragraph.

4.1 Identify all sources of uncertainty

The potential sources of uncertainty are identified on the basis of what is considered fixed(deterministic) and uncertain (minimal uncertainty in all SRQs in the interest of all analysis). So now we can categorize the sources as model inputs, numerical approximations, and mathematical models. In the case of models where it is difficult to identify the uncertainty assumptions are made to deal with it. Some of them are

- Assumptions about what type of environment (normal, abnormal, hostile) the system is in.
- Assumptions about the scenarios the operating system is working under (can be a misuse of the system).
- Assumptions about the situations where no experimental data is available in the relevant systems to predict the sources of uncertainty.

4.2 Characterize uncertainties

To characterize the uncertainties, we have to define the mathematical structure of all the sources of uncertainties. The mathematical structures are made based on whether it is a purely aleatory uncertainty or purely epistemic uncertainty, or a mixture of the two uncertainties. For purely aleatory uncertainties, it is characterized as a precise distribution. For purely epistemic uncertainties, such as numerical approximations and model form, the uncertainty is characterized as an interval. For an uncertainty which is a mixture of aleatory and epistemic uncertainty, it is characterized as an imprecise distribution.

Additionally, characterizing input uncertainties is derived from a) experimentally measured data from the system, b) data generated from separate models which support the current system, and c) opinions expressed by experts who are familiar with the system.

4.3 Estimate uncertainty due to numerical approximations

Estimating numerical errors includes discretization error, iterative error, round-off error, and coding mistakes. In the case of discretization error, it can be categorized as higher-order estimators (Type I) or residual-based estimators (Type II). The Type I methods includes post-processing of the solution(s) and Richardson extrapolation, order extrapolation, and recovery methods from finite elements. The Type II methods include discretization error transport equations, defect correction methods, and implicit/explicit residual methods in finite elements. Round-off errors are small but can be reduced by increasing the number of significant figures used in floating-point computations. Errors due to unknown coding mistakes or algorithm inconsistencies should be minimized by deploying good software engineering practices and scientific computing software such as order of accuracy verification and the method of manufactured solutions. To overcome the difficulties in getting accurate estimates in numerical approximation errors they should be represented as epistemic uncertainties. The methodology for converting error estimates to uncertainties is to use the magnitude of error estimate and apply uncertainty bands above and below the simulation prediction along with the factor of safety.

4.4 Propagate input uncertainties through the model

Propagation of input uncertainties can be done by aleatory and epistemic uncertainties in order to determine the effect on all SRQs. Let us consider a sampling-based approach for propagating combined aleatory and epistemic uncertainty. Sampling an aleatory uncertainty means the sample is taken from a random variable and that each sample is related to probability. But, sampling an epistemic uncertainty means the sample is taken from a range of possible values. So it is referred to as probability bounds analysis and is a fundamental concept of the proposed uncertainty framework.

4.4.1 Aleatory uncertainty. In aleatory uncertainty, propagation is done through the samp[ling procedure.Even though sampling methods are simple, large numbers of samples are needed in order to accurately characterize low-probability events which are necessary for SRQs.Some of the advanced approaches include polynomial chaos, stochastic collocation, and response surface approximation methods. If the sample has larger numbers of uncertain variables or statistical correlations exist between input quantities, traditional sampling methods have better performance.

4.4.2 Combined aleatory and epistemic uncertainty. In the scenario where both aleatory and epistemic uncertainties occurred in the input quantities, the propagation of each type is separated. For example, each of the samples obtained from an aleatory uncertainty is associated with a probability of occurrence. But when a sample is taken from an epistemic uncertainty, there is no probability associated with the sample. In that case, it is simply a possible realization over the interval-valued range of the input quantity. For each sample of all of the epistemic uncertainties, the aleatory uncertainties are propagated through the model to produce a single CDF of the SRQ. This type of combined sampling between aleatory and epistemic uncertainties is usually referred to as double-loop or nested sampling. The p-box (probability box) is a special type of CDF that contains both aleatory and epistemic uncertainties (see Fig.3). A p-box expresses both epistemic and aleatory uncertainty in a way where it gives interval-valued probability rather than precise probability.

4.5 Estimate model from uncertainty

Model form uncertainty is estimated by the process of model validation. Firstly, we quantitatively estimate the model form uncertainty where experimental data are available using a mathematical operator referred to as a validation metric. Secondly, we extrapolate the uncertainty structure expressed by the validation metric to the required conditions. The extrapolated model form uncertainty is used in the prediction of the model as an epistemic uncertainty. The below sections discuss these steps.

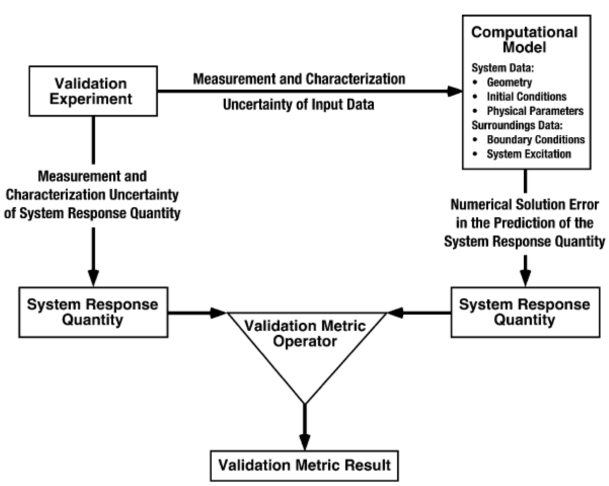

Figure 3: Steps to compute validation metric (from[4])

4.5.1 Validation metrics. A validation metric is a mathematical operator that has two inputs a) the experimental measurements of the SRQ b) the prediction of the SRQ used in the experimental measurements.A flowchart for computing a validation metric is given in Fig. 4.The flowchart explains that the experimental processes of nature on the left side are expected to reproduce by the mathematical model on the right side. Figure 3 provides the overall steps to compute the validation metric.

4.6 Determine total uncertainty in the SRQ

To determine the total uncertainty, firstly we use the p-box that was generated by propagating the aleatory and epistemic uncertainties in the model input parameters through the model. This approach provides valuable information to decision makers using the results from the simulation. The width of the original p-box gives information on the effects of epistemic uncertainties in the model inputs on the predicted SRQ. The range of the two bounding CDFs of the p-box provides data on the effects of aleatory uncertainties in the model inputs. The validation metric d informs the decision maker of the estimated magnitude of the uncertainty which is due to model form uncertainty. and U_NUM due to numerical approximations. From the graph below one can see that the epistemic uncertainty in the SRQ has increased due to model form uncertainty because of the area validation metric that is appended to the sides of the p-box. If extrapolation of the model from uncertainty is required, then extrapolated d values of the p-box are used.

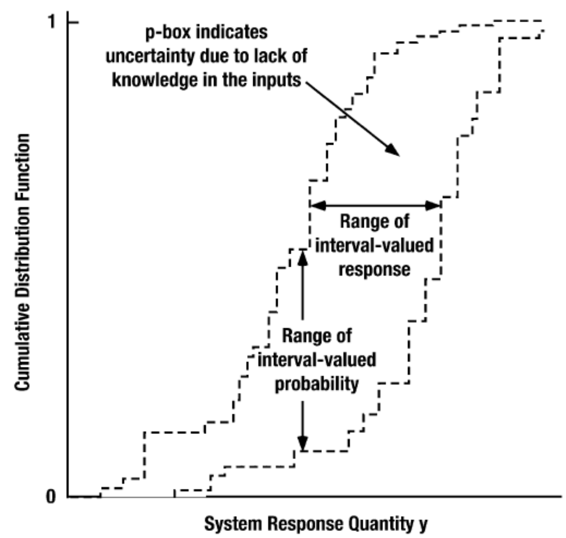

Figure 4: Increase in predictive uncertainty of model form(from[4])

5 ILLUSTRATION: HYPERSONIC WIND TUNNEL

The predictive uncertainty framework VVUQ framework is illustrated with the simulation of hypersonic nozzle flow which uses a quasi one-dimensional Euler equation to get cross-sectional area variations in the nozzle. This wind tunnel replicates the air movement over aircraft, vehicles, and other objects. Engineers use this simulation technique for further improvement in design, stability, cost-effectiveness, etc. In the given example, the wind tunnel radius of the test section could vary based on the tunnel wall layer (i.e laminar, transitional, or turbulent. Given that the nominal value of effective radius would be r=0.14m. From the previous experimental data, it is known that if the static temperature in the tunnel section falls below 80K there exists the formation of condensation. This condensation damages the aircraft when there is a simulation test is performed. During the simulation test there exist a high pressure in the air to test the stability and the performance of the aircraft if in case there occurs condensation, that high pressure it could lead to critical damage to the aircraft. Thus the analysis is carried out at 95% confidence that the test section temperature should be greater than or equal to 80K.

5.1 Identify all sources of uncertainty

The primary sources of uncertainty include wind tunnel stagnation temperature and the area downstream of the tunnel. The other sources of uncertainty inputs are stagnation pressure, the ratio of specific heats, specific gas constant, and tunnel throat radius which has fixed values from the experimental data and is so-called deterministic in nature.

5.2 Characterize uncertainties

The Wind tunnel stagnation temperature is an aleatory uncertainty. Through run-to-run experiments, variations are normally distributed with a mean stagnation temperature of 1200k with a 3.33% coefficient of variation and 40k of standard deviation. The Wind tunnel stagnation temperature is an aleatory uncertainty. Through run-to-run experiments, variations are normally distributed with a mean stagnation temperature of 1200k with a 3.33% coefficient of variation and 40k of standard deviation. In the area downstream of the tunnel throat the wind tunnel side-wall boundary layer is not measured. The state of the boundary layer (laminar, transitional, or turbulent)is not known. Separate boundary layer simulations are performed(i.e fully laminar and turbulent) to find the effective radius of tunnel. From experimental the effective radius is found to beLaminar boundary layer - 0.13m and forTurbulent boundary layer - 0.14m. In the figure 5, the effective area versus static temperature is plotted.

5.3 Estimate uncertainty due to numerical approximations

As an initial step the Code Verification is done. It is done by removing the coding mistakes in the code. All of these coding mistakes or also known as bugs are found by comparing them to the exact solution. By comparing it to the exact solution, the unknown error are found and solved. The roundoff error and iterative error are treated with simulations. These simulations are advanced by means to achieve a steady state. To achieve steady state significant floating point values are used in the results. All these are done by inserting the current solution of the discrete equations and evaluating the non-zero remainder. Iterative residuals are converged 2 orders of magnitude from their initial levels to eliminate at ease level. The Discretization error was Estimated by running simulations on three systematically-refined meshes the 128, 256, and 512 cells, the

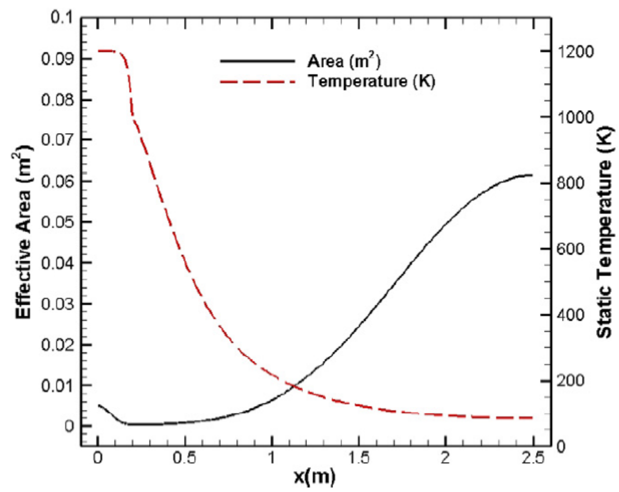

Figure 5: Effective area Vs static temperature(from[4])

test section static temperature was found to be 85.307, 85.824, and 85.954 K, respectively. They used order of convergence followed by Richardson extrapolation which uses two fines grids to obtain an estimate of the value. Then Roache's grid convergence index is used to estimate uncertainty due to discretization on the coarse mesh of 128 cells.

5.4 Propagate input uncertainties through the model

As discussed above, the aleatoric uncertainty is characterized either by probability density function or through cumulative distribution function. Here we use Monte Carlo sampling, wherein we used a set of random sample inputs from which we computed the system response of interest (i.e response 'y' value). Once computed each SRQ value of interest are plotted together as a cumulative distribution function where in we could find the range of both the input and response parameters. For epistemic uncertainties, the input would be a range of interval. In this case a rane of interval which is splitted into 10 subinterval is took to determine the value. From each subinterval a random sample is chosed, this random sample will then generate a system response using monte carlo sampling technique(Figure 6). Thus each random sample thus produces a CDF which then combined to form a massive system response which is technically known to be ensemble CDF. The process of combining the entire CDF as a single output is known be a ensemble technique. This ensemble technique helps for more accurate predcitions.

5.5 Estimate model from uncertainty

To explain the model form uncertainty estimation, Consider an example, for stagnation pressure of 20 MPa, the area validation metric is unknown. Provided three random validation experiment outcomes as sample for stagnation pressure 7MPa,10MPa, and 12MPa. The ten synthetic measurements of the SRQ (test section static temperature) are chosen to be: SRQEXP = [78.5, 80.2, 81.6,81.8,

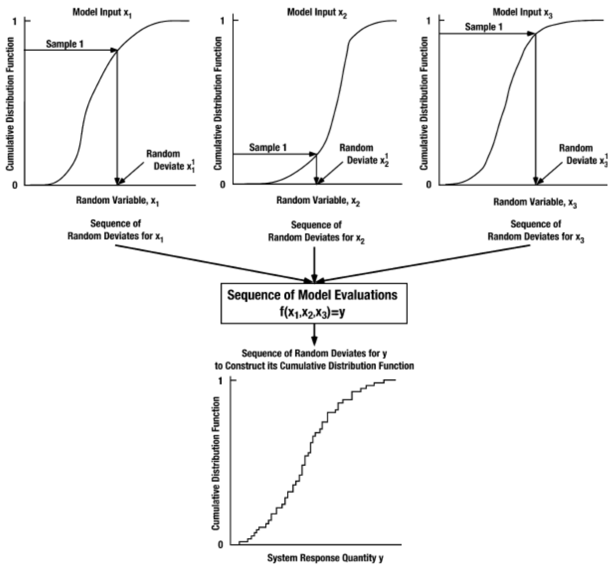

Figure 6: Monte carlo sampling technique(from[4])

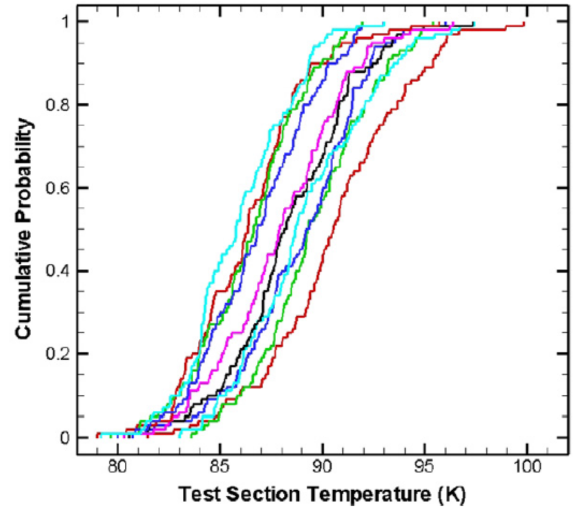

Figure 7: Ensembled CDF (from[4])

81.9,82.5, 82.7,83.6, 84.7,86.4] K. Then Propagating the input uncertainty (aleatory and epistemic) through the model to form CDF. This generated CDF is then compared with the experimental result CDF from the observation. The area between these two CDFs is known to be the area validation metric d=2.89K. Similarly, for other input stagnation pressure, the values are found as 7Mpa as 3.1k,10Mpa as 2.89k, and 12MPa as 2.8k are computed. Then compute the Simple Linear Regression from the obtained value considering the stagnation temperature as an independent variable, and area validation metric as the dependent variable y≙ 3.518 - 0.0608xk. Finally, the predicted interval is computed with a 95 percent of confidence interval at an area validation metric at p=20Mpa is d=3.27k. The below figure represents the ensembled CDF.

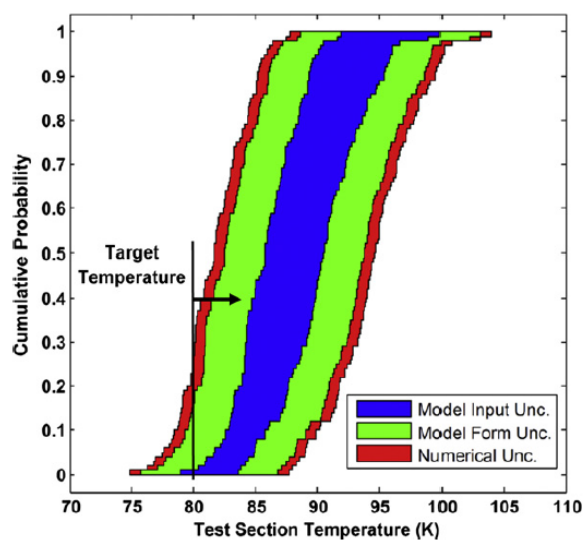

Figure 8: Total predictive uncertainity(from[4])

5.6 Determine total uncertainty in the SRQ

The p-box is determined by propagating aleatory and epistemic uncertainties model inputs through the model in condition (p = 20 MPa). Then append the area validation metric, i.e., d = 3.27 K, to the left and right sides of the p-box. Uncertainty due to numerical approximation UNUM = 0.86 K is appended to the left and right sides of the p-box. There is a 25% chance that the test static temperature would fall below 80k at 95% CI.This figure clearly describes the p-box plot with definite labels.

6 CONCLUSION

This predicted uncertainty is precisely shown to the decision-makers to avoid putting customers or environments at risk from uncertainties. It separates the aleatory and epistermic uncertainty and focus on numerical solution error and model form uncertainty directly. This framework could be used when the decision-makers find the observations or system response quantities to be inaccurate such as predictions of high consequences of the system (human lives, national security, safety measures).

7 DISCUSSIONSIONS

This framework focused on both aleatoric and epistemic uncertainty either by resolving or by providing an alternate way to quantify uncertainties. The conversion of numerical approximation errors into epistemic uncertainties through the verification technique is discussed briefly. Similarly, quantification of model form uncertainty, by adding additional steps on top of the standard validation technique for no experimental data was described in detail. The six phases of the framework are discussed in aspect with definite examples for a better understanding of the techniques used. The specific advantage of this paper is, that they well discussed how to quantify pure aleatoric and pure epistemic as well as the combination of both. In certain cases, as in numerical approximation errors, they stated all possible sources of error occurrence and provided definite research work on it for further improvement in it. The author of this paper already presented a book on the topic of "Verification and validation in scientific computing" [?] wherein he described a systematic development of the foundational concepts for the procedure of verification and validation of models and simulations. The methods in the book are described by partial differential and integral equations. For further in-depth understanding especially in the stages of verification and validation, this book's content and methodologies contribute a lot. In the validation techniques instead of traditional methodologies, he introduced even more concepts to get more accurate predictions when comparing the simulation outcomes with experimental data. A detailed description of the steps in computing a validation metric is explained followed by extrapolation of the validation metric is used due to the point that there are no experimental data available for the conditions of interest. The level of confidence is determined in a way to find the predicted interval with available data and conditions. Thus this comprehensive framework provided a

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