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The Method of Manufactured Universes for validating uncertainty quantification methods

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ABSTRACT

The Method of Manufactured Universes is presented as a validation framework for uncertainty quantification (UQ) methodologies and as a tool for exploring the effects of statistical and modeling assumptions embedded in these methods. The framework calls for a manufactured reality from which "experimental" data are created (possibly with experimental error), an imperfect model (with uncertain inputs) from which simulation results are created (possibly with numerical error), the application of a system for quantifying uncertainties in model predictions, and an assessment of how accurately those uncertainties are quantified. The application presented in this paper manufactures a particle-transport "universe", models it using diffusion theory with uncertain material parameters, and applies both Gaussian process and Bayesian MARS algorithms to make quantitative predictions about new "experiments" within the manufactured reality. The results of this preliminary study indicate that, even in a simple problem, the improper application of a specific UQ method or unrealized effects of a modeling assumption may produce inaccurate predictions. We conclude that the validation framework presented in this paper is a powerful and flexible tool for the investigation and understanding of UQ methodologies.

1. Introduction

The past decade has seen rapid advancement in complex computational projects and increasing dependence on these projects to support high-consequence decisions. An immediate result of this trend is the need for improved uncertainty quantification (UQ) methods to accompany the scientific simulations such that they deliver not only the best estimate of some quantity of interest, but also a measure of uncertainty in that estimate. One important example of UQ methods development is the quantification of margins and uncertainties (QMU) framework employed by the National Nuclear Security Administration's (NNSA) laboratories for assessment of the nation's nuclear weapon stockpile. This framework is a collection of methodologies designed to fuse decision inputs, such as experimental results, simulation results, theoretical understandings, and expert judgment, and their associated uncertainties in support of stockpile decisions.

Since its inception, the QMU framework has become an increasingly important link between scientific activities and stockpile stewardship priorities. Also of increasing importance, however, is the requirement that decision-support frameworks, like QMU, are themselves subjected to rigorous verification and validation assessments. In 2006, Congress issued a mandate for the National Academies to review the QMU framework and the consistency of its implementation at the national security laboratories [1]. Simply put, the review committee was tasked with deciding whether the combination of advanced simulation techniques, existing testing data, expert judgment, and the QMU framework appropriately support assessment and certification decisions in the absence of underground testing.

This QMU initiative is an example of the fundamental challenge to the predictive science and engineering community: How can we predict the behavior of complex systems using simulation *and* how can we assess our predictive capabilities? In recent years, the community released a number of predictive tools that attempt to infer the relationship between simulation and reality and use that inference to forecast uncertainty in predictions of new simulations or experiments. Validation of these predictive tools, however, is often hindered by little and/or uncertain experimental data or overwhelming complexities associated with real-world problems of interest. Nonetheless, validation is a fundamental requirement that provides confidence in predictive models and allows for an unbiased, knowledgeable evaluator to determine the credibility of that confidence.

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With this motivation in mind, we present the Method of Manufactured Universes (MMU) as a framework that facilitates a comprehensive validation study of a given UQ method, perhaps as implemented in a given software system. To apply MMU, one defines the laws that govern a system, uses these laws to construct "experimental" results, simulates the "experiments" using some computational model, and then tests the ability of the given UQ method to quantify the difference between simulation and "reality". This paper presents preliminary results from a computationally simple yet rich "universe" in which two UQ methodologies are examined: first, a Gaussian process code [2–4] from Los Alamos National Laboratory (LANL) and second, a Bayesian Multivariate Adaptive Regression Spline [5] (BMARS) technique combined with a filtering/weighting method. The conclusion drawn from these results is that MMU is a powerful technique that can help identify problems in UQ software, help computational scientists and engineers understand the subtleties, strengths, and weaknesses of various UQ methodologies, and help decision-makers to evaluate the credibility of predictive statements.

In Section 2 we define MMU in more detail, and in Section 3 we describe the manufactured universe that serves as the example in this paper. We also define the approximate mathematical model of the manufactured reality. In Section 4 we describe the two UQ methodologies that we use as examples in this paper. Sections 5 and 6 contain results from these methodologies, and Section 7 contains conclusions.

2. Introduction of the Method of Manufactured Universes

The motivation for this framework is the need to understand the assumptions embedded in UQ methods and the manner in which the effects of these assumptions propagate to the method's output. For example, a common practice for describing an unknown distribution (prior distribution or output uncertainty, for example) is to assume a Gaussian distribution with some estimated mean and standard deviation. The underlying function, however, may have only finite support and may be asymmetric; this information could be lost, excluded, or misrepresented by the assumed normal distribution. In some applications, this may be an acceptable approximation. It can easily be imagined, however, that a certain problem or set of physics might not be accurately represented in this manner.

We emphasize that it is not the purpose of this paper to expose every flaw or invalid assumption of every UQ method. Assumptions and limitations in statistical processes are often well known and documented. Instead, our purpose is to propose and illustrate a framework that others may use to determine the applicability of a given method to their specific problems. We champion the idea of "glass box" approaches to uncertainty quantification, and we believe that the simple study presented in this paper is a strong example of the value added in understanding the mechanics of the predictive software.

2.1. The MMU framework

The following list presents the basic steps of the MMU framework.

1. Define laws that govern the manufactured universe. This means creating mathematical models that define the laws that govern system behavior and the physical constants that serve as inputs to the models. As discussed below, these laws should reflect some key characteristics of modeler's real problem of interest.
2. Create "experiments" by defining physical problems and use the manufactured laws to create exact output quantities of interest (QOIs). Then, optionally, create "measured" data by perturbing these output QOIs using an error model.
3. Define an approximate model on which the UQ methodology is to be tested. This will include the choices of input parameters to the simulation and estimates their uncertainties (these estimates, themselves, could be uncertain).
4. Apply the given UQ methodology to the set of {approximate model, uncertain input constants, measured data}.
5. Define a new set of experiments and predict new values of the QOIs, with uncertainties, using what was learned from the UQ methodology. Generate "real" experimental results using the manufactured laws, and assess how well the UQ method quantified the uncertainties in the predictions.

Of course, this method can be repeated with variations on the approximate models, measurement-error models, data uncertainties, UQ methodology parameters, and universal laws.

2.2. Designing the "universe" given a real problem of interest

To maximize the utility of an MMU study, the modeler should try to manufacture a universe (that is, the physical laws, "experiments", approximate model, and the relationship between them) that properly reflects the physics, computational models, and uncertainties of the real-world predictive science or engineering problem. Further, the universe must also allow the modeler to explore, isolate, and further understand the characteristics of the UQ methodology. We identify two important factors that the modeler should consider when manufacturing the universe:

1. The manufactured universe should contain the same *types* and *sources* of uncertainty as the real-world problem.

   Unless care is taken with this, there is a risk that the lessons learned from using MMU may not apply to the real problem of interest. Some characteristics of the real problem that one might seek to mimic in the manufactured universe include the mix of epistemic and aleatory uncertainties, the nature of prior distributions of uncertain parameters, and the origin and path of propagation of the most important uncertainties.
2. The simplifications that lead from the manufactured laws to the MMU approximate model should be closely related to and simplifications of the real-world physics that lead to the real-world mathematical model of interest.

   As we emphasized before and will show by example, a complete treatment of uncertainty – which includes uncertainty due to model error – must be informed by the physics of the problem. Therefore, the model error in the MMU analysis should closely mimic the model error in the real problem to maximize the real-world value of the insight gained through the MMU analysis.

2.3. Example: a particle-transport universe

The examples in this paper will present results from a neutral particle transport "universe". The universe is relevant to our real-world problems in which transport calculations play key roles in the analysis of complex systems such as nuclear reactors or high energy-density laboratory experiments. Uncertainties in these real problems are often driven by material properties (such as interaction cross-sections), and we are often interested in the model fidelity and accuracy of material properties that are required to produce quantities of interest such as material