Uncertainty Quantification In Large Computational Engineering Models

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Abstract

While a wealth of experience in the development of uncertainty quantification methods and software tools exists at present, a cohesive software package utilizing massively parallel computing resources does not. The thrust of the work to be discussed herein is the development of such a toolkit, which has leveraged existing software frameworks (*e.g.,* DAKOTA (Design Analysis Kit for OpTimizAtion)) where possible, and has undertaken additional development efforts when necessary. The contributions of this paper are two-fold. One, the design and structure of the toolkit from a software perspective will be discussed, detailing some of its distinguishing features. Second, the toolkit's capabilities will be demonstrated by applying a subset of its available uncertainty quantification techniques to an example problem involving multiple engineering disciplines, nonlinear solid mechanics and soil mechanics. This example problem will demonstrate the toolkit's suitability in quantifying uncertainty in engineering applications of interest modeled using very large computational system models.

Introduction

Several current Department of Energy (DOE) Defense Program (DP) mission responsibilities can only be accomplished through a significantly increased reliance on mathematical modeling and computational simulation of weapon systems, some of which can be described as possessing uncertainty both in their physical description and in their service environments. For such systems, it is well-known that results from classical deterministic analyses are not sufficient to describe response behavior in a meaningful way, thus motivating the need for approaches that account for these nondeterministic effects. Similar conclusions have been reached by researchers in the Department of Defense (DoD), NASA, industry, and academia. Further, the characterization of uncertainty present in such systems has been identified as a necessary step in the successful implementation of analytically-based processes for their design, and ultimately, their certification.

Sandia National Laboratories is in an ideal position to evolve this technology due, in large part, to its long history of research and development activities in computational engineering and science, coupled with significant experience in model validation through close relationships existing between analysts and experimentalists[1-2]. New computational capabilities provide a strong platform for continuing this process, as well as for exploring novel methods for addressing the issue of uncertainty quantification. In general, uncertainty quantification has to incorporate research and development efforts in three key, irreducible technical areas:

(1) Characterization of uncertainty in system parameters and the external environment;

(2) Propagation of this uncertainty through large computational engineering models; and

(3) Verification and validation of the computational models and incorporating the uncertainty of the models themselves into the global uncertainty assessment.

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Uncertainty Quantification:

The Big Picture

Before embarking on a description of the toolkit, its role in the context of the uncertainty quantification of large scale computational engineering systems needs to be discussed. As stated earlier, real physical systems display both systematic and random variations. These random variations might arise from a variety of sources including the geometry of the problem, material properties, boundary conditions, initial conditions, or excitations imposed on the system. As a result, depending on the source of these variations, the behavior of a system, or of a collection of nominally identical systems, will vary from one realization to another. While these realizations are individually deterministic, their effects in the collective are not; consequently, nondeterministic methods are needed to assess trends in the behavior of this collection of responses.

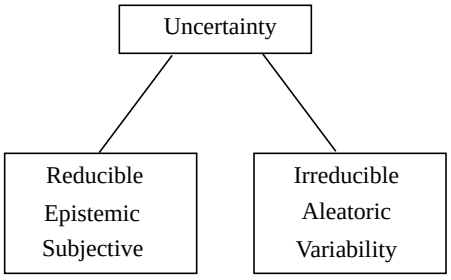


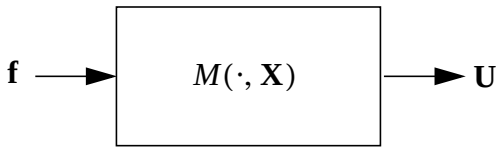
Figure 1. Simple Taxonomy of Uncertainty.

Uncertainty occurs in various forms; one simple taxonomy is displayed in Figure 1. There are two main classes of uncertainty. These are labeled by a variety of terms depending on the discipline(s) the problem involves. Although analysts might disagree on terminology, the delineation between the two types is generally agreed upon. The first is known as reducible or epistemic uncertainty; this uncertainty generally results from a lack of information about some aspect of the problem being considered. For instance, the form of the constitutive model of a joint connecting two members of a complex structural system is not known; this uncertainty results from a lack of information about the joint's behavior. Another example of epistemic uncertainty is the related situation where the constitutive model for the joint is known, but sufficient data to fully characterize the uncertainty in the models's parameters is not available.

The other branch of the taxonomy involves irreducible or aleatoric uncertainty; this type of uncertainty consists of fluctuations that are intrinsic to the problem being studied. For instance, turbulent fluctuations of a flow field around an airplane wing, or in a case related to the two just mentioned, sufficient data does exist to fully characterize a known joint model's parameters in a statistical manner. This is accomplished by specifying probability distributions for the parameters. This irreducible, parametric uncertainty is manifested in the uncertainty of the response of the complex structural system.

As mentioned previously, the first step in uncertainty quantification is the characterization of uncertainty in system parameters and the external environment. This characterization is not a trivial task and will involve the development of methods to model uncertainty of both epistemic and aleatoric type. Regardless of the type being considered, the characterization process will depend heavily on experimental researchers to provide the data and insight necessary to facilitate appropriate uncertainty models for the parameters. This fact reiterates the importance of experimental research and development efforts even as the engineering and scientific communities rely more heavily on computational prediction in their research.

The next step in the uncertainty quantification process is the propagation of uncertainty through, in this case, large computational engineering system models. While efforts investigating non-probabilistic approaches[3] to uncertainty quantification are being undertaken at Sandia, the only well-established methodology of propagating uncertainty through these models, at present, is the traditional probabilistic or statistical approach. Here, the uncertain parameters, $\mathbf{X}$, are assumed to be random variables or fields for the discrete and continuous cases, respectively. The model, M, maps a vector of given inputs, $\mathbf{f}$, which can be uncertain in nature, to a vector of outputs, $\mathbf{U}$. This input-output relationship is displayed in Figure 2.



$\mathbf{X}$: vector of uncertain parameters

M: a deterministic mapping

$\mathbf{U}$: output(s) of system

$\mathbf{f}$: input(s) to system

Figure 2. Input/Output Description of System.

The assumed uncertainty in $\mathbf{X}$ manifests itself as uncertainty in $\mathbf{U}$. To assess this, one seeks quantities such as $E[g(\mathbf{U})]$ where $g(\mathbf{U})$ is a prudently selected response metric and $E[\cdot]$ denotes the expectation operator. This form is very general in nature and captures many standard probabilistic metrics used in analysis and design, such as the mean and variance of the output, the cumulative distribution of the response metric, *etc*. It is important to note, however, what one generally is computing are actually conditional statistics for a particular form of the model, *e.g.*, $E[g(\mathbf{U})|M]$. While these quantities are an important step in the uncertainty quantification process, these conditional statistics need to be incorporated into the global uncertainty assessment.

This global assessment can be pictorially represented as shown in Figure 3, where the total uncertainty is composed of three parts. The first displayed in blue is due to random external loads imparted on the system such as those resulting from an earthquake on a building, or those due to slamming water waves on an offshore oil drilling platform, or those occurring from launch or separation events on a re-entry vehicle. The second piece, labeled in red, is that resulting from parametric uncertainties in the problem. These include intrinsic variabilities in geometric and/or material properties in the model and tolerances present in the system. Finally, the enveloping piece of the assessment is due to model uncertainty. For instance, the uncertainty of the form of the constitutive relationship of the jointed connection in the previously mentioned examples would be categorized as this type. By including all three sources of uncertainty in this nested fashion, one can compute the desired quantity, $E[g(\mathbf{U})]$.

This decomposition of uncertainty is equally valid regardless of the approach taken to quantify it. In the case of a non-probabilistic approach, the expectation operator would be replaced with an appropriate analogous quantity from the alternative theory. Further, the nested structure of the decomposition allows for flexibility in the selection of different uncertainty quantification techniques in each part of the uncertainty assessment.

DAKOTA/UQ

Although a large amount of effort has been expended in the development of uncertainty quantification methods[4-8] and software tools[9-16] over the last twenty years, a cohesive software package exploiting massively parallel computing resources does not exist. Consequently, a prime objective of the uncertainty quantification effort at Sandia is the development of a set of tools that manage the execution of the large number of necessary simulations required in an uncertainty assessment, aggregate the vast amount of information produced, and condense that information into a manageable set of meaningful metrics. The focus of this section is the development of such a toolkit.

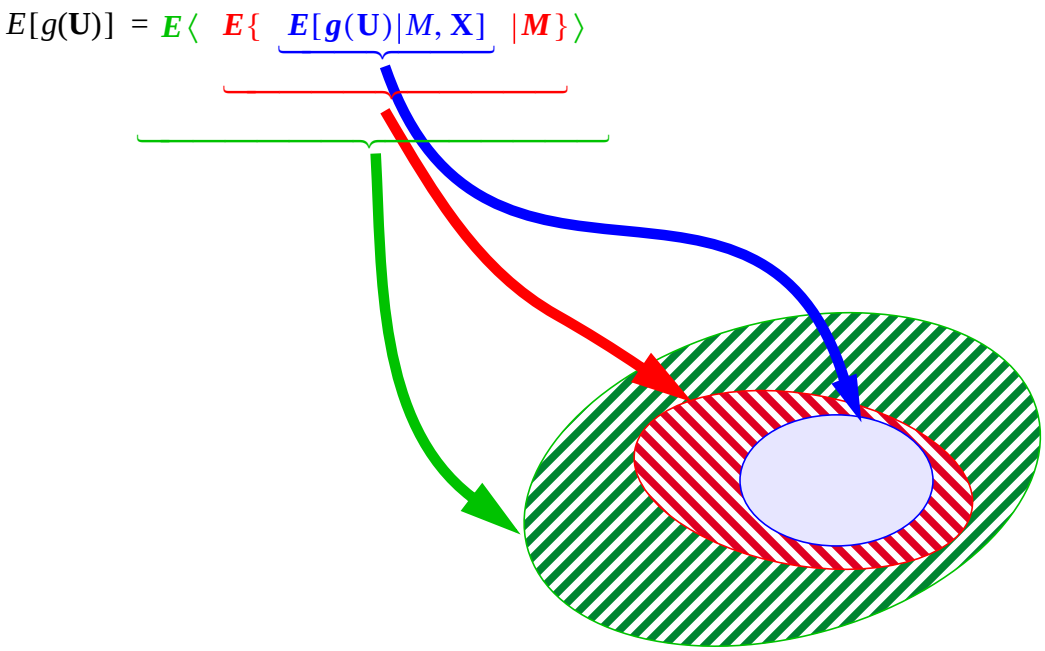


Figure 3 Anatomy of Global Uncertainty.

The DAKOTA (Design Analysis Kit for OpTimizAtion)[17-19] iterator toolkit is a flexible, extensible interface between simulation codes and iterative systems analysis methods. The toolkit implements optimization with a variety of gradient and non-gradient methods[20-23], uncertainty quantification with nondeterministic propagation methods, which will be discussed in greater detail shortly, parameter estimation with nonlinear least squares solution methods[23], and sensitivity/primary effects analysis[24] with general purpose parameter study capabilities and design of experiments capabilities, which include Latin hypercube sampling[25], orthogonal array sampling[26], Box-Behnken type design[27], and pure random sampling. By employing object-oriented design to implement abstractions of the key concepts involved in iterative system analyses, the DAKOTA toolkit provides a problem solving environment which uses point solutions from simulation codes to answer fundamental engineering questions, such as "what is the best design?", "how safe is my design?", or "how robust is my optimal design to parameter variations?".

In addition to these iterative systems analysis capabilities, advanced users can employ state of the art capabilities for (1) exploiting parallelism at multiple levels (coarse-grained and fine-grained)[19] and (2) building cascaded, nested, concurrent, and/or adaptive strategies which utilize multiple iterators and models to enact hybridization, sequential approximate optimization[28], mixed continuous-discrete optimization, or optimization under uncertainty.

While targeted for massively parallel computing platforms, *e.g.*, having thousands to tens of thousands of processors, DAKOTA can also be utilized on a single workstation or a network of workstations (NOW). It has been successfully ported to most common UNIX-based workstations including Sun, SGI, DEC, IBM, and LINUX-based PCs.

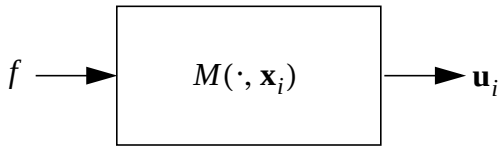
A synopsis of the capabilities of DAKOTA along with a schematic of the architecture of the toolkit is shown in Figure 4. The focus of the next section is a more detailed description of the nondeterministic analysis capabilities currently supported in DAKOTA/ UQ and those methodologies under consideration for future implementation.

Nondeterministic Analysis Capabilities

The available capabilities can be broadly divided into three categories: (1) sampling based methodologies, (2) analytically-based reliability techniques, and (3) robustness analysis. These methods can be applied to either the original computational system model, or alternatively, to a surrogate model, *e.g.*, response surface approximation, built using one of the available techniques within DAKOTA.

Sampling-Based Techniques

Here, sets of samples, $\mathbf{x}_i$, of the uncertain variables are generated according to a user-prescribed specification and subsequently propagated through the model, *M*, yielding a set of samples of output(s), $\mathbf{u}_i$ as displayed in Figure 5 for a given deterministic input, f.



$\mathbf{x}_i$: i^{th} sample vector of uncertain parameters
M**:** a deterministic mapping
$\mathbf{u}_i$: i^{th} sample of output(s) of system
f : input to system

Figure 5. Sampling Approach to UQ.

Relevant statistics and probabilities can be estimated from the sample values of the outputs of the model using standard statistical techniques. For instance, an estimate of the mean of the first component of the output vector is given by the unbiased estimator

$$E[U_1] \approx \frac{1}{N_S} \sum_{i=1}^{N_S} u_{1_i}, \qquad (1)$$

where N_s is the number of samples.

Currently, Monte Carlo (MC) and Latin hypercube Sampling (LHS) are supported by DAKOTA/UQ. In Monte Carlo sampling, the samples are selected randomly according to their user-specified probability distributions. Whereas, in Latin hypercube sampling, a stratified sampling technique, the range of each input variable, X_i, is divided into N_s segments of equal probability. One sample is selected randomly from each of the segments for X_1; the process is repeated for X_2 and so forth, until a set of N_s sample vectors has been formed. Latin hypercube sampling ensures full coverage of the range of the input variables, often a problem with Monte Carlo sampling when the number of samples is small. For further information on the method and its relationship to other sampling techniques, one is referred to the works by McKay, *et al.*,[25], Iman and Shortencarier[29], and Helton and Davis[30].

Figure 4. Overview of DAKOTA framework.

Advantages of sampling-based methods include their relative simple implementation, allowing them to be easily wrapped around existing deterministic analysis capabilities, and their robustness to factors such as the scientific disciplines involved in the analysis and the size of the computational system model being considered. The main drawback of sampling-based techniques is the large number of function evaluations required render such an analysis computationally very expensive, if not intractable, for a large computational model. In practice, Latin hypercube sampling often displays similar accuracy to Monte Carlo sampling with an order of magnitude fewer samples, thus partially addressing this problem; however, more work is needed to fully address this issue. In that vein, efforts are underway to implement more advanced sampling techniques in DAKOTA/UQ including bootstrap sampling (BS)[31], importance sampling (IS)[32], quasi-Monte Carlo simulation (qMC)[33], and Markov chain Monte Carlo simulation (McMC)[34].

Analytically-Based Reliability Techniques

A class of methods known as analytically-based reliability methods is also included in DAKOTA/UQ. These methods all answer the fundamental question, "Given that some subset of the design variables are uncertain (random variables), $\mathbf{X}$, and a response metric,

$$Z = g(\mathbf{U}) = g(M(f, \mathbf{X})), \tag{2}$$

as a function of the outputs, $\mathbf{U}$, what is the probability that the response metric is below a certain level?" Formally this can be written as

$$P[g(\mathbf{U}) < z_0] = F_Z(z_0), \tag{3}$$

where $F_Z(z_0)$ is the cumulative distribution function of Z.

These methods all involve the transformation of the user-specified input random variables, $\mathbf{X}$, which can be non-normal and correlated, to a space of unit variance independent Gaussian random variables. The Nataf transformation[35], which is identical to the Rosenblatt transformation[36] in the case of independent random variables, is used in DAKOTA/UQ to accomplish this mapping. Next, the most probable point (MPP) of failure is determined. Note, however, the methodology is equally applicable when $g(\mathbf{U})$ is a generic function of the outputs, $\mathbf{U}$, and not simply a failure criterion; this nomenclature is due to the methods' origin in structural safety and reliability.

The determination of the MPP can be posed as a constrained minimization problem, where the objective function is the minimum distance from the origin to a surface in the unit-normal space. This surface constitutes the constraint of the minimization problem and depends on the method being used in the analysis. Currently, the mean-value method (MV), the advanced mean-value methods (AMV/AMV+)[9,37], the first order reliability method (FORM) and the second order reliability method (SORM)[8,9] are implemented in DAKOTA/UQ. The MV and AMV/AMV+ methods are based in the original random variable space, while FORM/SORM are transformed-space-based methods. A more thorough discussion of the methods can be found in the recent text by Haldar and Mahadevan[8].

Robustness Analysis

The third type of available analysis technique, robustness analysis, is one possible approach to analyzing problems where insufficient information is available about the uncertain parameters to justify their characterization using probability distributions. In these cases, however, one can often specify bounds on the parameter values and formulate the problem statement, "Given the bounds on the input parameters, what range of response is possible?" This is a classical interval analysis problem[38].

However, most of that methodology is not germane to the problems of interest since the models are black boxes operating on vectors of real numbers via a function evaluation. That is, interval data on elements of the input is an allowable input quantity for very few engineering codes in their present form.

While most interval techniques are not applicable due to this intrusiveness to the analysis code, those posed as global optimization problems can be used in this context. That is, given that the uncertain parameters in the model lie in a hyper-rectangle, the maximum and minimum of the response metric are sought, *i.e.*,

$$g_{upper} = \max_{\mathbf{x}} g(M(f, \mathbf{x})) \tag{4}$$

and

$$g_{lower} = \min_{\mathbf{x}} g(M(f, \mathbf{x})) \tag{5}$$

such that

$$(x_i)_L \le x_i \le (x_i)_U \quad \forall \; i = 1 \ldots N \tag{6}$$

where N is the number of uncertain, input variables and $\mathbf{x}_L$ and $\mathbf{x}_U$ denote the lower and upper bounds, respectively, of the input parameter vector, $\mathbf{x}$.

The global extrema of these two optimization problems yield bounds on the response metric which can be expressed as

$$g(\mathbf{u}) \in [g_{lower}, g_{upper}]^{\nabla}. \tag{7}$$

It should be noted that these bounds simply envelope the response metric and aren't meant to imply that the response can take on any value in this interval, hence the nabla on the interval of the response metric.

Future capabilities

In addition to the methodologies just discussed, additional development efforts are ongoing at Sandia. These include polynomial chaos expansions[39], stochastic finite element techniques[40,41], and methods to account for epistemic uncertainty using both probabilistic and non-probabilistic[3] approaches.

The uncertainty quantification tools are evolving as additional analysis needs are identified. It is anticipated that as these efforts progress, the most promising methodologies will be implemented within the DAKOTA framework thereby augmenting its current uncertainty quantification capabilities.

Validation of Computational Models

As defined in the DOE Defense Programs (DOE/DP) ASCI Program Plan[42], validation is the process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model applications.

The final part of the uncertainty quantification process is the use of the tools previously discussed and those yet to be developed to perform distributional predictions of the output quantities of interest. These distributional predictions, produced by the UQ analysis, along with experimental data or other known information will be used to compute validation metrics. These metrics will be used to assess the predictive capability of the computer model(s) of interest.

The development of such metrics is a formidable task itself and is well beyond the scope of this document. However, one should note that regardless of the form of the metric(s) developed; uncertainty quantification and model validation are intimately linked as the former provides the machinery to perform the assessment of the latter.

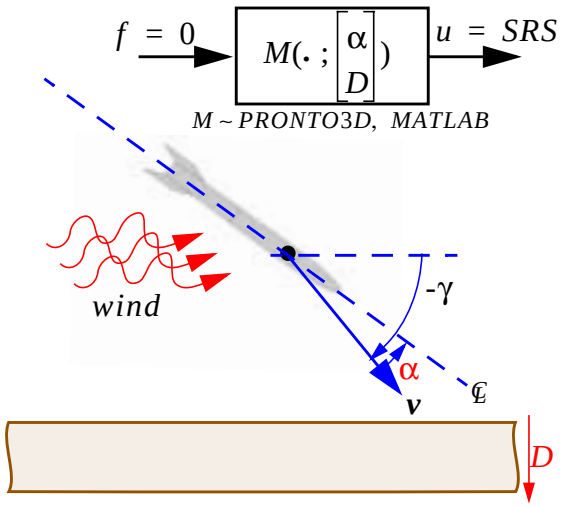


Figure 6. Schematic of the penetration system.

Example Problem

The penetration of a vehicle into a soil medium is a problem of engineering interest[43]. The question to be answered is whether or not the internal components of the vehicle will survive the shock environment induced by the penetration event. The response metric used to assess survival of a component, in this case, is known as the shock response spectrum (SRS)[44].

A schematic of this system as it impacts a target is shown in Figure 6, where $\boldsymbol{v}$ and γ are the velocity vector and impact angle of the system, respectively, taken to be deterministic. A considerable amount of uncertainty exists, however, in the knowledge of a particular soil depth parameter, D. In addition, the angle-of-attack α is nondeterministic due to uncertainty in the knowledge of the wind conditions. Hence, α and D were modeled as independent random variables, with normal and lognormal distributions, respectively. These two parameters constitute the $\mathbf{X}$ vector in the general uncertainty framework of Figure 2.

PRONTO3D[45], an in-house nonlinear, transient solid dynamics finite element code, is coupled to a spherical cavity expansion model[46], which accounts for the soil-structure interaction, to predict the internal component response during the penetration event. MATLAB[47] routines were used to filter the output from that analysis and compute the shock response spectrum (SRS). Therefore, in the general framework, the model, M, is composed of the cascaded system of PRONTO3D, the cavity expansion model, and the filtering processes effected in MATLAB.

Also, the output vector is the shock response spectrum at a discrete number of frequencies in the general framework, *i.e.*,

$$u_i = SRS(f_i) \quad \forall\, i = 1 \ldots n_f, \tag{8}$$

where f_i denotes the i^{th} natural frequency of the computed shock response spectrum and n_f is the number of frequency lines in the discrete representation of the shock spectrum. An intermediate quantity, $\bar{u}$, was defined to be the minimum difference between the computed SRS and a prescribed, reference specification over all frequencies, *i.e.*,

$$\bar{u} = \min_i \left(SRS(f_i) - u_i\right). \tag{9}$$

In the stated uncertainty assessment framework of Figure 3, the response metric is defined to be

$$g(\mathbf{u}) = g(\bar{u}(\mathbf{u})) = I(\bar{u}) \tag{10}$$

where $I(\bar{u})$, the indicator function, is defined as

$$I(\bar{u}) = \begin{cases} 1, & \bar{u} \geq 0 \\ 0, & \bar{u} < 0 \end{cases} \tag{11}$$

The failure threshold of the component is defined to be $\bar{u} = 0$. The probability of failure is simply

$$P_f = P[\bar{U} < 0] \tag{12}$$

which can be rewritten as

$$P_f = 1 - P[\bar{U} \geq 0] = 1 - E[g(\mathbf{U})]. \tag{13}$$

Results

A 50,000 degree-of-freedom PRONTO3D finite element model of the system was used to perform the analysis. Each simulation took approximately thirty-three hours of CPU time on a Sun SPARC Ultra II workstation. As a result, it was decided to utilize surrogate models for the uncertainty quantification analysis thus greatly reducing the computational costs incurred.

A set of 49 simulations were performed at a series of input locations that were chosen as part of a parallel investigation of the problem using quadrature methods[48], and the response metric computed for each simulation. These simulations were done in parallel on a network of Sun SPARC Ultra II workstations.

From these simulations, a series of response surface approximations were constructed using a variety of techniques including kriging[49,50], splines[51], neural networks[53], and quadratic polynomials[52]. Both available sampling techniques were applied to these response surface approximations using 10,000, 1,000,000, and 5,000,000 samples, and an estimate of the probability of failure noted in each case. These estimates are summarized in Tables 1-3.

Table 1: Probability of Failure
($N_s = 10,000$)

Response Surface Approximation Method	*MC*	*LHS*
Kriging	0.02000	0.02000
Splines	0.06900	0.06720
Neural Net	0.05024	0.05500
Quadratic Polynomial	0.04960	0.05070

Table 2: Probability of Failure
($N_s = 1,000,000$)

Response Surface Approximation Method	*MC*	*LHS*
Kriging	0.02600	0.02500
Splines	0.06784	0.06769
Neural Net	0.05616	0.05572
Quadratic Polynomial	0.05107	0.05069

Table 3: Probability of Failure
($N_s = 5,000,000$)

Response Surface Approximation Method	*MC*	*LHS*
Kriging	0.02300	0.02400
Splines	0.06781	0.06767
Neural Net	0.05588	0.05581
Quadratic Polynomial	0.05077	0.05071

From these results, one observes the more rapid convergence of the Latin hypercube sampling results with increasing sample size. Also, for this particular example, the kriging result is the least conservative among the four. Unlike the case of optimization with surrogate models, an assessment of the accuracy of uncertainty quantification with surrogates cannot be obtained with a single function evaluation of a "truth model", *i.e.*, the full computational system model.

The stated goal of demonstration of the variety surrogate models available in DAKOTA/UQ was accomplished. However, if this study had been conducted to determine the safety of the system, one would have subsequently sampled the full computational system model a sufficient number of times, determined based upon the stringency of the safety requirement, to obtain an estimate of the failure probability. The response surface approximation results would then have been compared to that estimate.

Summary

DAKOTA/UQ, a software toolkit for performing uncertainty quantification on large scale computational engineering models exploiting massively parallel computers, has been outlined and its role in the global uncertainty quantification process discussed. Current capabilities include analytical reliability techniques, including AMV+ and FORM, sampling techniques, both Monte Carlo and Latin Hypercube Sampling, and robustness analysis. Planned methodologies include enhanced sampling methods such as bootstrap sampling, importance sampling, and quasi-Monte Carlo sampling, polynomial chaos expansions for both random variables and random fields, and stochastic finite element techniques.

The efficacy of the toolkit has been demonstrated on a large-scale engineering example problem namely, the penetration of a vehicle into a soil medium. A variety of response surfaces of the system were built using DAKOTA's approximation building capabilities, which include the method of neural nets, splines, kriging, and global quadratic polynomials, to minimize computational expense. Sampling was performed on these response surfaces to obtain estimates of the probability of failure of a component inside the vehicle. These results agree well with those previously published[39,43,48].

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