AN APPROACH TO EXPERIMENTAL DESIGN FOR THE COMPUTER ANALYSIS OF COMPLEX PHENOMENON

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ABSTRACT

The ability to make credible system assessments, predictions and design decisions related to engineered systems and other complex phenomenon is key to a successful program for many large-scale investigations in government and industry. Recently, many of these large-scale analyses have turned to computational simulation to provide much of the required information. Addressing specific goals in the computer analysis of these complex phenomenon is often accomplished through the use of performance measures that are based on system response models. The response models are constructed using computer-generated responses together with physical test results where possible. They are often based on probabilistically defined inputs and generally require estimation of a set of response modeling parameters. As a consequence, the performance measures are themselves distributed quantities reflecting these variabilities and uncertainties. Uncertainty in the values of the performance measures leads to uncertainties in predicted performance and can cloud the decisions required of the analysis. A specific goal of this research has been to develop methodology that will reduce this uncertainty in an analysis environment where limited resources and system complexity together restrict the number of simulations that can be performed. An approach has been developed that is based on evaluation of the potential information provided for each "intelligently selected" candidate set of computer runs. Each candidate is evaluated by partitioning the performance measure uncertainty into two components – one component that could be explained through the additional computational simulation runs and a second that would remain uncertain. The portion explained is estimated using a probabilistic evaluation of likely results for the additional computational analyses based on what is currently known about the system. The set of runs indicating the largest potential reduction in uncertainty is then selected and the computational simulations are performed. Examples are provided to demonstrate this approach on small scale problems. These examples give encouraging results. Directions for further reasearch are indicated.

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I. INTRODUCTION

The ability to make credible system assessments, predictions and design decisions related to engineered systems and other complex phenomenon is key to a successful program for many large-scale investigations in government and industry. Recently, many of these large-scale analyses have turned to computational simulation to provide much of the required information. Addressing specific goals in the computer analysis of complex phenomena is often accomplished through the use of performance measures that are based on system response models. The response models are constructed using computer-generated responses together with physical test results where possible. They are often based on probabilistically defined inputs and generally require estimation of a set of response modeling parameters. As a consequence, the performance measures are themselves distributed quantities reflecting these variabilities and uncertainties. Uncertainty in the values of the performance measures leads to uncertainties in predicted performance and can cloud the decisions required of the analysis.

A specific goal of this research has been to develop methodology that can be used to select informative additional (computer) experiments to perform that will reduce this uncertainty in an analysis environment where limited resources and system complexity together restrict the number of simulations that can be performed. An approach, referred to as the response modeling approach throughout this report, has been developed that is based on evaluation of the potential information provided for each "intelligently selected" candidate set of computer runs. Each candidate is evaluated by partitioning the performance measure uncertainty into two components – one component that could be explained through the additional runs and a second that would remain. The portion explained is estimated using a probabilistic evaluation of likely results for the additional computational analyses based on what is currently known about the system. The set of runs indicating the largest reduction in uncertainty is then performed. While the primary focus of this research has been on design for computational experimentation, the approach has been used for physical experiment designs as well. Problems involving model validation, together with prediction, can involve both.

The purpose of this paper is to illustrate some of the applications of this "response modeling" experimental design approach.. Section II provides a brief review of other approaches to the problem together with an overview of the response modeling approach, highlighting the essential components. Sections III through V describe and illustrate applications. In section III, a simple uncertainty analysis, using an analytical function in place of the computer code, is used to illustrate the goals and procedures of the approach. Section IV illustrates how the approach can be used in engineering design. Here, the response modeling methodology is used to select further experiments in search of settings that yield stable (less variable) rolamite performance. Section V extends the approach to a more complicated response. Uncertainty related to a continuous output pulse is evaluated using the response modeling methodology combined with a capacitive discharge unit model. The report is concluded with a Summary and Conclusions Section. Included in this section are some directions for future research.

II. THE RESPONSE MODELING AND OTHER APPROACHS TO COMPUTER EXPERIMENTAL DESIGN

SAMPLING AND RESPONSE SURFACE APPROACHES

A number of approaches have been taken to experimental design for computer analyses. The designs specify input levels for computer simulation runs performed to satisfy specific analysis objectives. These approaches can be grouped roughly into one of two categories -- sampling approaches, and response surface approaches. Figures 1 and 2 are used to establish some terminology and to illustrate these approaches and their differences.

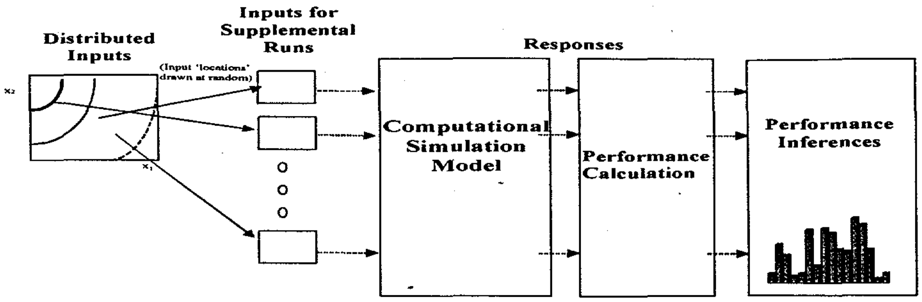

Figure 1. Flow Diagram for Sampling Approaches to Experimental Design (Input Selection) for Computer Analyses.

For an uncertainty or prediction analyses, it is often the case that some of the inputs will be defined probabilistically as indicated by the distributed input contours on the left of Figure 1. In these cases, sampling approaches (see Figure 1) will generally follow the steps: (a) the distributions associated with the inputs are sampled; (b) the computational simulation model is run using the sampled inputs; (c) the responses are obtained and (d) performance measures are computed. The probabilistic interpretation on the inputs carries over to the performance measures (i.e., the results are treated as a random sample of performance). As further simulations are carried out, the distribution of the performance measures still includes the variability resulting from uncertain inputs, but the sampling variability is reduced. One general problem with sampling approaches is that even when more efficient methods (relative to strict Monte Carlo sampling) are used, such as Latin Hypercube, [1] or importance sampling, see [2], for example these approaches require a large number of simulations for even moderate-sized problems.

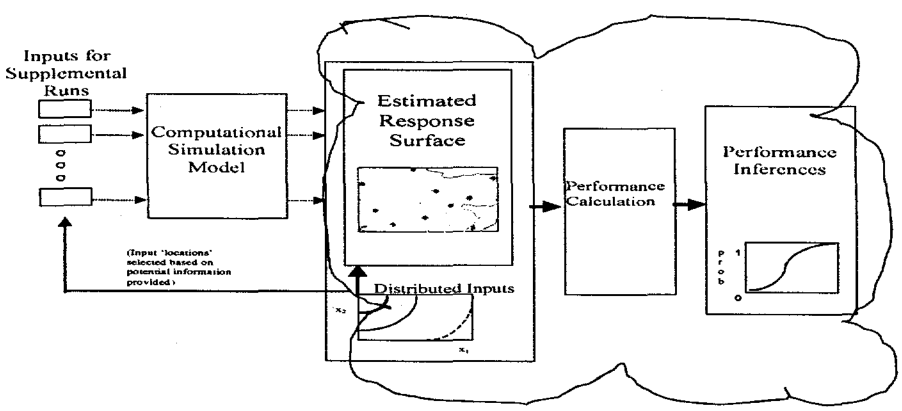

Figure 2. Flow Diagram for Response Surface Approaches to Experimental Design for Computer Analyses.

Response surface approaches were developed, in part, to try to reduce the number of computational experiments required. The additional modeling step of constructing a response surface or response model changes the process significantly, as illustrated in Figure 2. The input probabilities (where applicable) are now applied to a response estimate constructed based on previous analyses. This makes it possible to "direct" further experimentation (using prior information indicated by the cloud in Figure 2) to portions of the input space that produce the most information or reduce the response uncertainty or performance uncertainty most. One could loosely classify several approaches to experimental design for computer simulations into this category: classical response surface methods, see [3] for example; reliability or analytical methods, see [4] for example; and other response modeling approaches such as those used regularly in the geosciences for physical response regions, see [5] for example. These geoscience response-modeling approaches were introduced in the engineering literature in Sacks et al[6]. The response modeling approach discussed in this paper fits roughly into this category. The additional response-modeling step, however, is more involved for this approach.

RESPONSE MODELING APPROACH

The methodology used in this report was first proposed in Rutherford [7], for experimental design in computational experiments involving prediction uncertainty analysis. Briefly, this response modeling approach to experimental design follows the steps listed below. More detail is given in the paragraph that follows.

1) Construct a probabilistic representation of the response based on results of the prior experimentation. Use this "probability measure" to characterize the distribution of the performance measures of interest. This characterization will include uncertainty that is inherent to the problem through input uncertainty or variability and also uncertainty that results from modeling the response based on limited data. It is the goal of the experimental design to select a set of computational runs that will reduce this later component as efficiently as possible.

2) For a candidate design (sets of input specifications), evaluate the potential reduction in the uncertainty discussed above through inclusion of likely responses at the design locations where "likely" is evaluated using the probability measure in (1). The process of constructing the response ensemble and the performance measure distribution (as in (1)) is repeated here using, in addition, the hypothetical supplemental data at the design locations. No computational runs are performed at this stage.

3) Step (2) is repeated for different candidate designs selected using an evolutionary algorithm-based optimization routine. The candidate design that indicates the greatest potential reduction in performance uncertainty is then selected for computer experimentation.

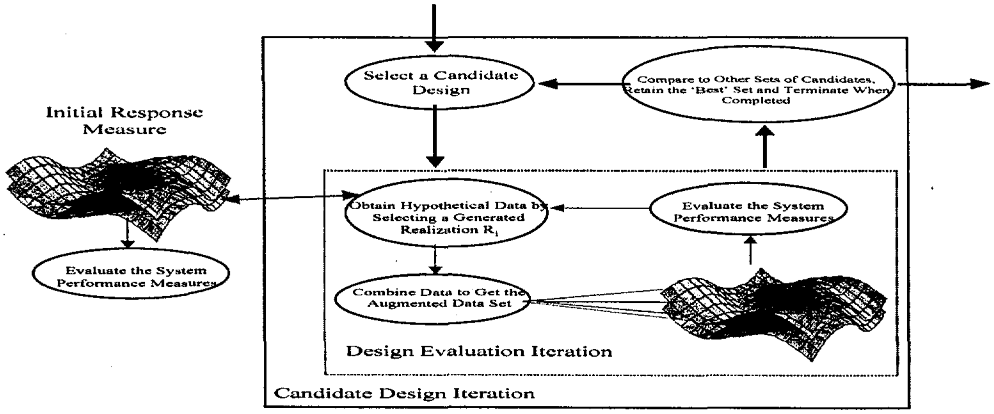

Figure 3. Flow Diagram Giving the Algorithm for the Response Modeling Approach to Experimental Design.

Figure 3 provides a flow diagram of the process. The discrete "ensemble of realizations" indicated on the left represents an approximation to the initial probability measure discussed in (1). The process currently used to construct this approximation is discussed in Deutsch[5] and references given there. Note that a candidate design applied to any specific realization will yield a set of values at the specific design locations. This additional data is used in the inner "design evaluation loop". The inner loop is traversed once for each realization in the initial ensemble for every candidate design considered. Each iteration of that loop conditions on a different set of values at the design locations. This process is used to evaluate the potential new information provided by the candidate design; it partitions the variability associated with the initial estimate of the performance distribution into components that are used to assess the candidate design (this is the process described in (2)). The outer loop in Figure 3 is repeated for each candidate design considered. Finally, as described in (3), the most informative design according to these criteria is selected and the computational simulation runs are performed.

III. A SIMPLE UNCERTAINTY ANALYSIS PROBLEM

A simple analytical example in two dimensions is provided here to demonstrate how this approach works. Figure 4 shows the true (usually unknown) response $r(x_1,x_2)$ and a plot of the average of twenty-five realizations used to approximate the probability measure. The analytical function replaces the computational simulation code for this simple example. The realizations are based on a "sample" taken from the true surface at ten input locations (see Figure 5).

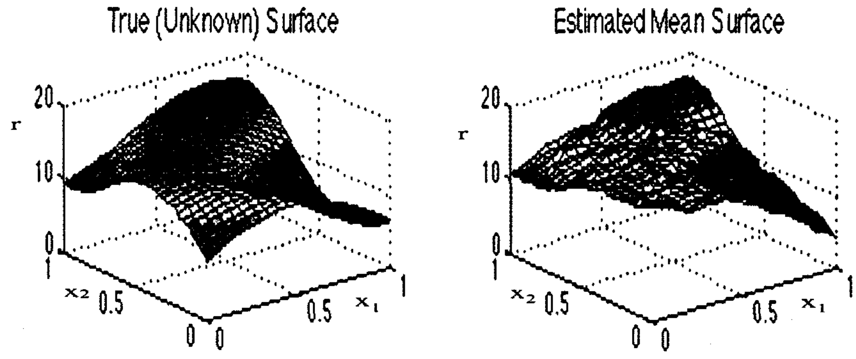

Figure 4. True Response Surface and Mean Response of the Realization Ensemble that Approximates the Response Probability Measure

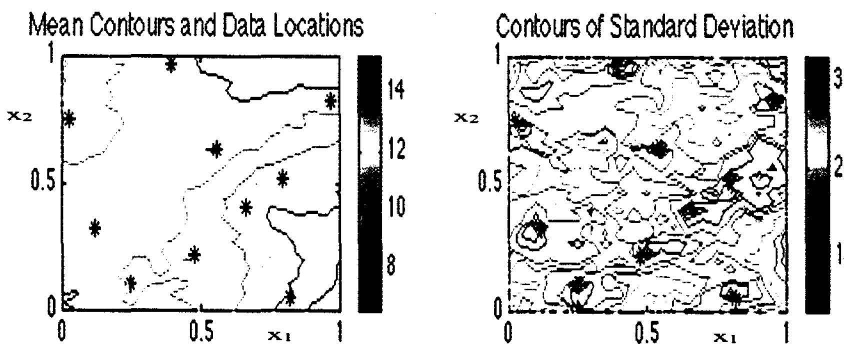

Figure 5. Mean and Standard Deviation Contours taken from the Ensemble of Realizations.

For any value of x_2, the performance measure for this example is computed as:

$$pm(x_2) = \int \mathbf{I}(\mathbf{r}(x_1,x_2),10)(\mathbf{r}(x_1,x_2) - 10)^2 dx_1$$

where the indicator I(a,b) equals 1 when a > b and 0 otherwise. The problem is essentially one-dimensional except that evaluating the system gives one response for a two-dimensional input (ie. one value on the response surface). The distribution function of the performance measure is computed assuming a uniform distribution for x_2 as:

$$F_{pm}(z) = \int \mathbf{I}(z, pm(x_2))dx_2 .$$

Prior to determining the experimental design, the initial ensemble is constructed and performance is evaluated. This process is illustrated next.

Figure 5 shows mean and standard deviation contours computed from the twenty-five (this number chosen somewhat arbitrarily) initial realizations. Six of these realizations (due to space limitations) are plotted in Figure 6.

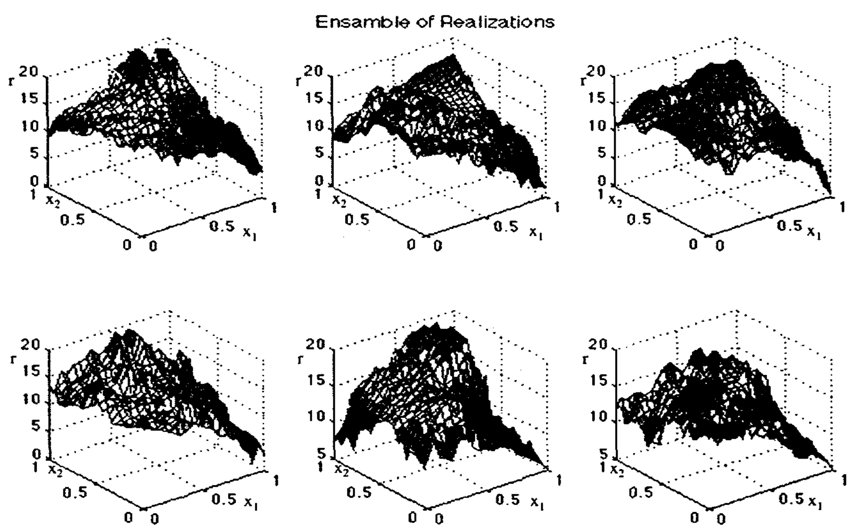

Figure 6. Six (of twenty-five) Realizations Used to Approximate the Response Probability Measure.

Figure 7 shows (some of) the performance measure cumulative distribution functions associated with the realizations together with the distribution function calculated for their equally-weighted mixture. This (darker) cumulative distribution function includes response-modeling uncertainty as well as uncertainty propagated through to the performance measure from the distributed input x_2. The goal of the experimental design process is to efficiently choose computational simulation runs that will focus in on which of the lighter curves (or some similar curve) is appropriate for describing performance. The input-based component to variability will remain.

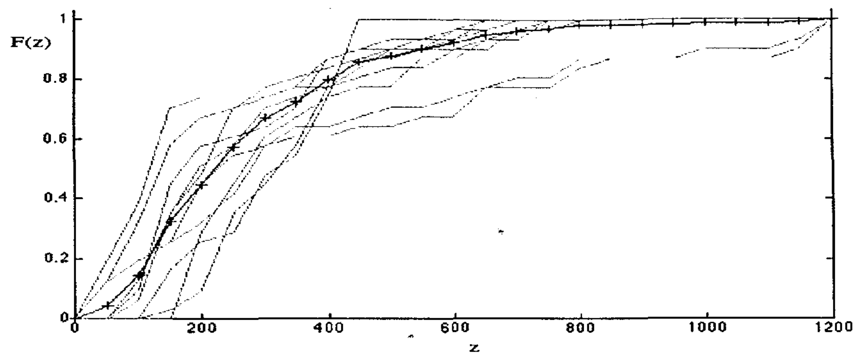

Figure 7. Performance Distribution Examples Computed by Applying the Performance Formulas above to Individual Realizations of the Ensemble.

The response modeling design algorithm described above was run to select a 3-location experimental design. Figure 8 illustrates the resulting design on the contour maps of mean and standard deviations together with data from the initial runs. Note that this selection tends to support criterion for a good experimental design. The design points are at input locations that are of relatively high values of the response which are important in computing the performance measure (this is indicated in the left contour map) and they are located in regions of relatively high model uncertainty (as indicated in the right contour map). Further detail on criterion for a good computer experimental design are provided in Rutherford[7].

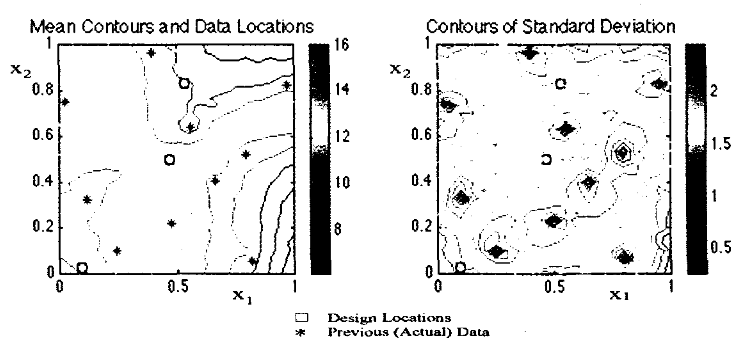

Figure 8. Experimental Design for the Analytical Problem Computed using the Response Modeling Algorithm. New Experimental Points are Indicated by the Squares.

IV. A SIMPLE ENGINEERING DESIGN PROBLEM

Uncertainty analyses based entirely on computational results (as illustrated in the previous example) are possibly the most straightforward application of the response modeling approach to experimental design. Even these more straightforward applications, however, can differ significantly, depending on performance measures used. Estimating reliability, for example, retains only a point estimate (the probability of failure) for each realization in the ensemble as compared with the distributed performance estimate for each realization in the previous section. In this section, another two-dimensional problem is considered where the analysis objective is to locate the minimum response as a function of two inputs that are assumed to be at the designer's control. The inputs do not have a probability distribution associated with them as in the previous example. A brief description of this application follows.

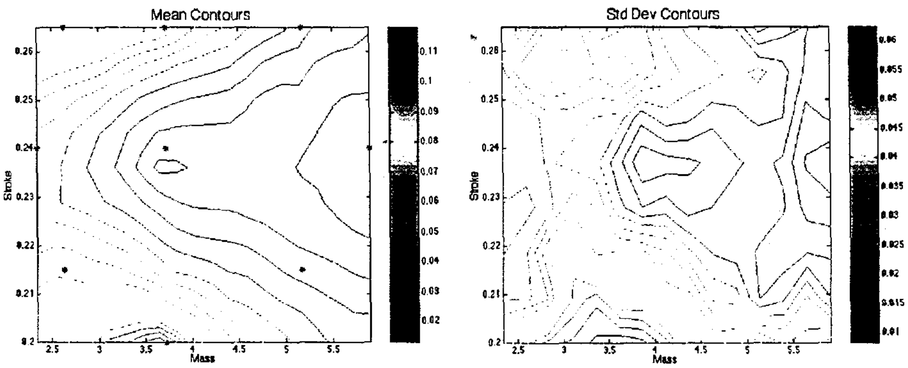

Figure 9. Contours Maps Indicating the Ensemble Mean Values and Standard Deviations.

This application involves the design of rolamites in order to minimize variability in their performance. The available initial data for this application were results from physical testing, rather than computational experiments. While this requires some modeling changes, it can be accommodated through the response modeling approach. Figure 9a gives a contour map of the mean response (standard deviation based on replicate tests) computed from the ensemble. Figure 9b gives the contours of pointwise standard deviation of the response ensemble. The axes are the engineering design variables stroke length and mass. A number of criteria for comparison can be used to select the best candidate design for this application. The criterion used for illustration here is to choose the design that most reduces the expected distance from the minimum to it's expected location in the input space. More specifically $E_r(\|m_r - E_r(m)\|)$ where m_r represents a location for the minimum on response r, $E_r(m)$ is the expected location of the minimum, the norm is Euclidian distance and both expectations, E_r, are taken with respect to the approximate initial response measure. This metric provides a measure of how concentrated (and hence, well understood) these minimum locations are. A good experimental design will discriminate between alternative locations about the input space to find the region of most consistent rolamite performance (and, hence, a good candidate design will indicate substantial differences in the location of this region using results obtained from one set of hypothetical data to another, see Figure 11).

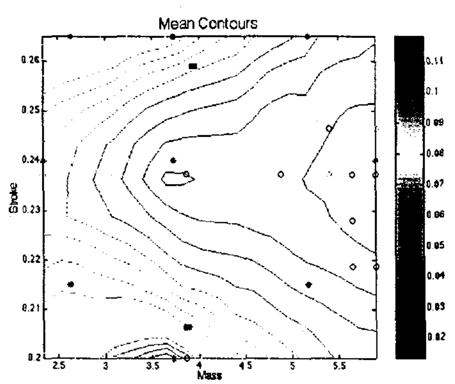

Figure 10. Experimental Design for the Engineering Design Problem Computed using the Response Modeling Algorithm. New Experimental Points are Indicated by the Squares.

Figure 10 illustrates the locations for further experimentation indicated by the squares together with the locations of the initial data (the stars) and the locations of the minimums based on the initial ensemble(the circles). Multiple minima are indicated by colored circles. These points were determined using the response modeling algorithm. The expected reduction in the distance from the average was reduced 12 percent. Figure 11 shows three scenarios that might exist after this further experimentation has been performed. These ensemble averages are computed using response models (similar to the initial model) but including data (determined from the initial model) at the design locations. The values of these "conditioning data" differ in the three figures. Note through comparison with Figure 10 that the likely locations of the minimum have become more concentrated, although the location of the concentration changes from scenario to scenario. This is desirable as the different scenarios are determined based on the probabilistic response model. What is indicative of a good design is that all possible scenarios lead to a better, more concentrated estimate of where the minimum is located.

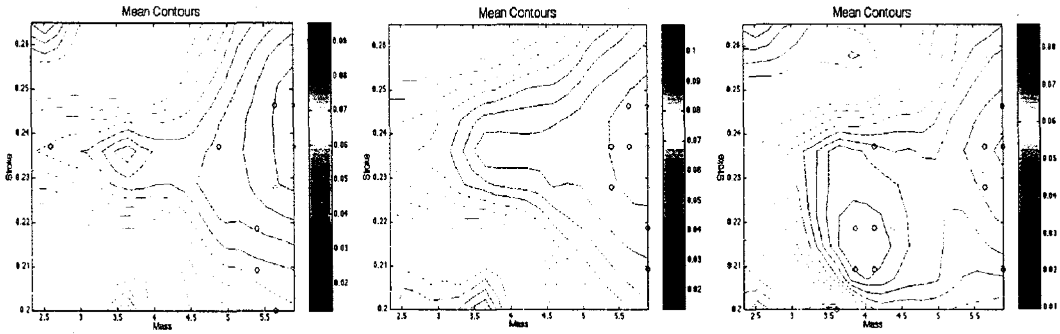

Figure 11. Contours Showing Possible Results After Further Experimentation Using the Experimental Design Selected.

V. AN UNCERTAINTY APPLICATION INVOLVING A COMPLEX RESPONSE FUNCTION

This example illustrates how the basic response modeling approach can be extended to problems where the response of interest is more complicated than those of the previous examples. In this case, the performance measures are based on a continuous output pulse representing current as a function of time. In order to accommodate this additional complexity, a "behavioral model" is constructed. A brief description of this application follows.

A computer model of an explosive firing set is being used to evaluate the possible impact of aging elements of this component and their interfaces to determine an appropriate stockpile lifetime and to estimate their reliability in future application. The objective of the present analysis is to evaluate regions of concern in the input space and determine (if applicable) regions that require further investigation (i.e., where there are valid concerns about aging elements affecting performance). In performing this analysis, only evaluation of the initial data has been accomplished, to date. Figure 12 provides a diagram of the behavioral model. Essentially, the model consists of two components: (1) the probabilistic response modeling component that was described earlier, and (2) a capacitive discharge unit (CDU) computer model. The response model takes as input six aging-related parameters of the computational simulation model. The six inputs were selected through a sensitivity analysis from eleven variables considered initially. A vector of three parameters is generated through the response model. These three "intermediate parameters" capacitance, impedance, and resistance are used as inputs to the CDU computer model that generates the continuous current output pulse. The CDU model was selected because of its flexibility in accommodating output pulses similar to those generated through physical testing or using the computational simulation model.

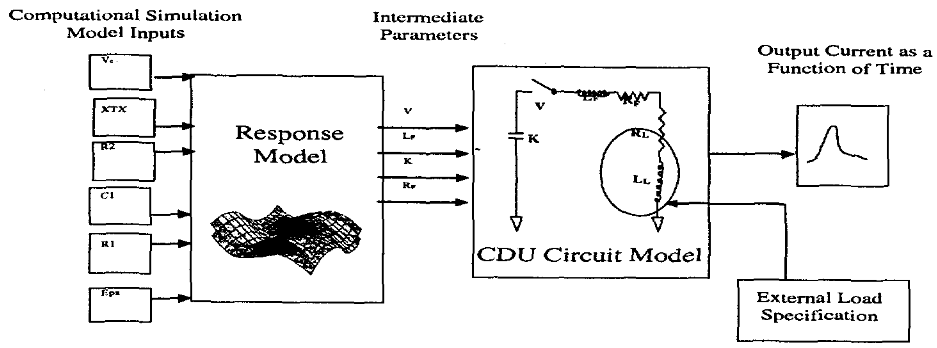

Figure 12. Behavioral Model for the Firing Set Example.

Figure 13 shows the response averages for the inductance intermediate parameter. The axis labels B, C, F, and H represent significant inputs for inductance. The input variables (of the four) that are not included in each plot are set at their average level.

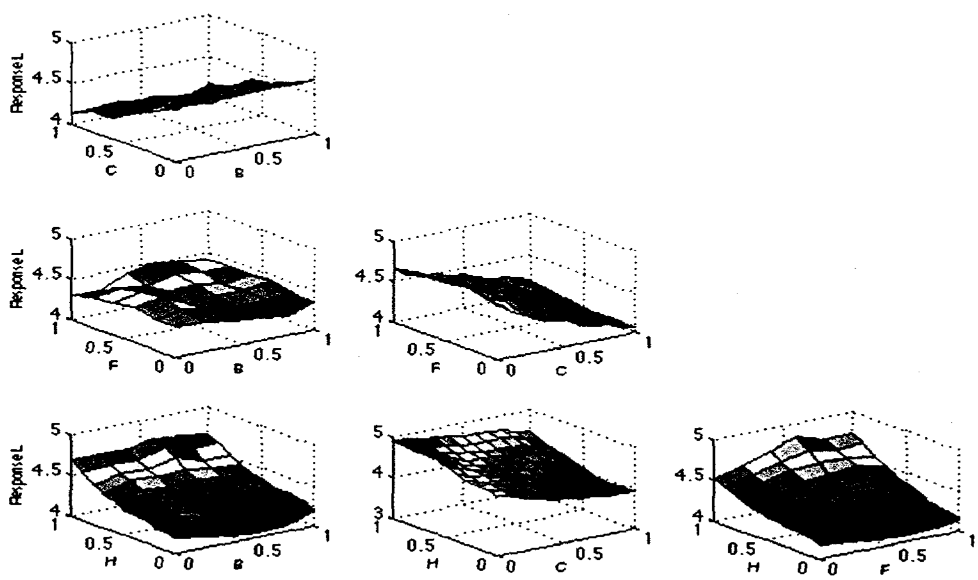

Figure 13. Inductance Response Ensemble Averages. Based on Four Inputs

Figure 14 shows how the behavioral model might be used. A set of inputs has been specified and the plotted curves indicate the range of the response. Because these responses are based on the probabilistic response model using a fixed set of inputs, these curves can be interpreted probabilistically (the probabilities reflect response uncertainty). For example, the probability that the pulse will exceed the amperage indicated by the horizontal line can be estimated by the fraction of curves that exceed that value.

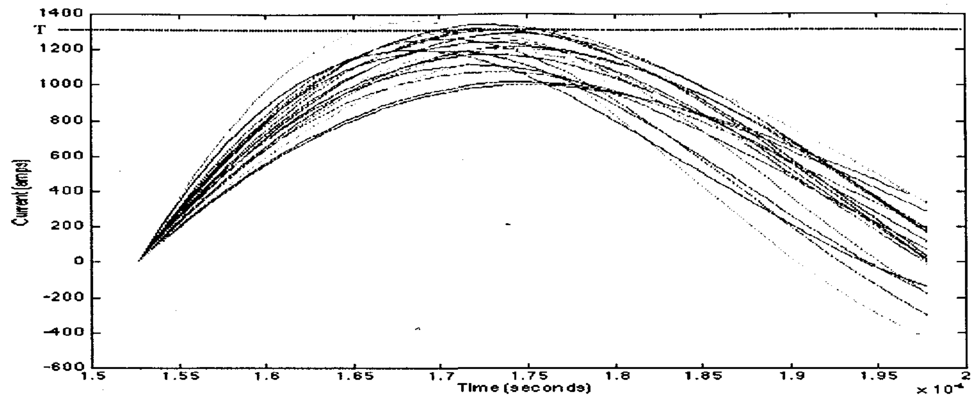

Figure 14. Plot Indicating Output Pulse Variability Based on the Initial Probability Measure.

SUMMARY AND CONCLUSIONS

A response modeling approach to the algorithmic selection of input locations for computer experimentation was described and illustrated. Results on several simple examples demonstrate how the methodology might be used and the wide range of applications to which it might be applied. For the first two examples, designs were constructed that indicate that the approach was working well for these small scale problems. These encouraging results suggest that this approach might be of significant value for higher dimensional problems where the complexities make a solution based entirely on analyst's intuition even more difficult. The primary directions for future research involving the response modeling approach to experimental design include increasing the size of the problem addressed, investigating the use of this approach toward problems of model validation and research into formal methods for constructing the response models.

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