DETERMINISTIC UNCERTAINTY ANALYSIS

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INTRODUCTION

Uncertainties of computer results are of primary interest in applications such as high-level waste (HLW) repository performance assessment in which experimental validation is not possible or practical. Because of the complicated nature of the computational structure of large computer models, and because of the large number of input and data parameters associated with such models, to date almost all uncertainty analysis of computer results has been performed using a statistical approach. The purpose of this work is to present an alternate deterministic approach for calculating uncertainties that has the potential to significantly reduce the number of computer runs required for conventional statistical analysis.

DETERMINISTIC UNCERTAINTY ANALYSIS APPROACH

The deterministic uncertainty analysis (DUA) approach proposed in this work relies upon the availability of derivatives of the response of interest to the parameters of interest. The task of calculating these derivatives is the equivalent to calculating sensitivities of a response to the input parameters. Efficient computational techniques for calculating sensitivities, such as the direct and adjoint methods, have received considerable attention. The availability of automated procedures that enhance existing computer models with these analytic capabilities greatly reduces the initial enhancement task to the point where it is now practical to incorporate the calculation of derivatives into the model analysis.

The DUA method constructs a response surface that replaces the computer model with an analytical function relating the response of interest to the parameters of interest. The construction of the response surface is based upon the response value of interest as well as the first derivatives...
of the response to the parameters of interest. In constructing a response surface to a given order of expansion, the use of derivative information reduces the number of computer runs compared to fitting just the response values by a factor of approximately $1/K$, where $K$ is the number of parameters. The advantage is not in using only a few sample runs to construct a global response surface, but to define local response surfaces over subregions of the parameter space. By careful selection of sample parameter space points for which model results will be obtained, the number of computer runs can still be held to a small fraction of the number required for conventional construction of a response surface. Linear expansion in the neighborhood of sampled space points is an example of using local response surfaces.

Unlike conventional use of response surfaces to dramatically increase the number of sampling points, the DUA method propagates probabilities over the entire response surface by completely spanning a discretized parameter space. Only if the entire parameter space is spanned can probabilities be propagated. In probability tree methods\textsuperscript{6}, for example, the probability distributions are typically replaced with the high and low values of the distributions. The DUA method extends the probability tree methods into a more rigorous propagation of probabilities in two ways: (1) Since an analytical expression relates the response to the parameters, the expected value of the response over each discrete mesh can be calculated analytically and thus gives a more meaningful value than just a single sampling point within the mesh; and (2) Because the computer model is replaced with an analytical expression, a finer mesh size can be constructed over the parameter space of most interest.
SAMPLE PROBLEM

The sample problem is taken from Ref. 7, for which the flow through a borehole penetrating two aquifers is calculated based upon eight input parameters. The governing equations, input parameter probability distributions, and resulting statistically determined cumulative probability distribution (CDF) of the flow rate are given in Ref. 7. For this problem, a response surface was constructed using derivative information and used in place of the governing equations to construct a cumulative distribution of the flow rate. Figure 1 compares the CDF of the flow rate for the statistically-determined CDF's based on 10 and 50 sampling points (using Latin Hypercube Sampling) to the deterministic CDF based upon a response surface constructed with only two sampling points. The Figure shows that the DUA method using only 2 sampling points gives an almost identical CDF to the 50-point statistical case.

CONCLUSIONS

The DUA method has been shown to give similar results to the conventional statistical uncertainty analysis method with a considerably reduced number of executions of the calculational model. The method relies upon cost-effective calculation of model derivatives, which is becoming increasingly practical with the development of automated methods to enhance computer models with derivative calculation capability. The DUA method is being evaluated on large-scale computer models being used for design of the HLW salt repository.
Fig. 1. COMPARISON OF DETERMINISTIC CDF BASED ON A 2 POINT EXPANSION TO STATISTICAL CDFS
REFERENCES


