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DETERMINISTIC SENSITIVITY AND UNCERTAINTY ANALYSIS FOR LARGE-SCALE COMPUTER MODELS*

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DETERMINISTIC SENSITIVITY AND UNCERTAINTY ANALYSIS FOR LARGE-SCALE COMPUTER MODELS

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The fields of sensitivity and uncertainty analysis have traditionally been dominated by statistical techniques when large-scale modeling codes are being analyzed. These methods are able to estimate sensitivities, generate response surfaces, and estimate response probability distributions given the input parameter probability distributions. Because the statistical methods are computationally costly, they are usually applied only to problems with relatively small parameter sets. Deterministic methods, on the other hand, are very efficient and can handle large data sets, but generally require simpler models because of the considerable programming effort required for their implementation. The first part of this paper reports on the development and availability of two systems, GRESS and ADGEN, that make use of computer calculus compilers to automate the implementation of deterministic sensitivity analysis capability into existing computer models. This automation removes the traditional limitation of deterministic sensitivity methods. This second part of the paper describes a deterministic uncertainty analysis method (DUA) that uses derivative information as a basis to propagate parameter probability distributions to obtain result probability distributions.

I. INTRODUCTION

Sensitivity and uncertainty analysis are important components of any system performance assessment. The role of sensitivity analysis is to provide a quantitative measure of the effect of system parameters upon key performance indices. Sensitivity analysis also helps limit the scope of the more complicated problem of quantifying uncertainties. Uncertainty analyses is performed to support reliability studies, to produce a cost-benefit analysis in conjunction with cost estimates, to insure compliance with regulatory criteria, and to help identify important research and development needs.

Sensitivity analysis of computer-generated results consists of determining the effect of model data upon the calculated results of interest. Because computer model equations can be differentiated analytically, sensitivities can be precisely defined and calculated in a deterministic fashion using both direct and adjoint methods.[1-8] The deterministic approach is particularly suited to large-scale problems for which direct perturbation of the model data becomes impractical from a cost standpoint. The main drawback to the deterministic approach has been the initial manpower investment to add the computational capability for calculating the necessary derivatives into existing computer models.

For quantification of uncertainties in computer-generated results, the problem can be expressed more precisely as the propagation of input uncertainties through models by the laws of probability to obtain output uncertainties. (The uncertainty associated with whether the computer model accurately reflects the physical phenomena is a problem of model validation and is not addressed in this paper.) Uncertainties of computer results are of primary interest in applications such as 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.[9-12]

This paper presents a comprehensive approach to sensitivity and uncertainty analysis of large-scale computer models that is analytic (deterministic) in principle and that is firmly based on the model equations. The theory and application of two systems based upon computer calculus, GRESS[13-15] and ADGEN[16,17], are discussed relative to their role in calculating model derivatives and sensitivities without a prohibitive initial manpower investment. Storage and computational requirements for these two systems are compared for a gradient-enhanced version of the PRESTO-II[18] computer model. A Deterministic Uncertainty Analysis (DUA) method[19,20] that retains the characteristics of analytically computing result uncertainties based upon parameter probability distributions is then introduced and results from recent studies are shown.

II. DETERMINISTIC SENSITIVITY ANALYSIS

A brief description of general sensitivity theory is given here as an aid to understanding the problem of applying this theory to computer models. The example to be discussed will be that of a general set of non-linear equations given by

$$y = F(y,c) \quad , \tag{1}$$

where y represents the dependent variable being solved for, c represents the user-specified model data or parameter set, and F defines the model equations. The particular form chosen in Eq. (1) is one that can be used generally to represent equations coded in the FORTRAN programming language. The left side of the equation can represent the stored value of the variable calculated from the functional formula on the right side.

Since the number of components of the vector y calculated in any typical large-scale modeling problem is large, it is useful to define a generic result for such a calculation that is of particular interest to the model user. Typically many results will be needed for analysis but in most cases they form a much smaller set than the actual set of y component values. A typical result will be defined as

$$R = h(y) \quad , \tag{2}$$

where R is a single number that is a function of the solution to Eq. (1). For notational ease, the generic parameter α_i will be used to denote any individual parameter. The total number of parameters in the problem will be assumed to be M so that the index on α_i will run from 1 to M.

The basic problem in any sensitivity study is to find the rate of change in the result R arising from changes in any model parameters. For the generic parameter α_i, then, the quantity of interest is the numerical value of $dR/d\alpha_i$ given analytically by

$$\frac{dR}{d\alpha_i} = \frac{\partial h}{\partial y}\frac{dy}{d\alpha_i} \quad . \tag{3}$$

Since the functional dependence of R on y through h(y) is defined analytically by the model user, only $dy/d\alpha_i$ needs to be generated in order to evaluate Eq. (3). The procedure needed to get $dy/d\alpha_i$ is to differentiate Eq. (1) as follows:

$$\frac{dy}{d\alpha_i} = \frac{\partial F}{\partial y}\frac{dy}{d\alpha_i} + \frac{\partial F}{\partial c}\frac{dc}{d\alpha_i} \quad . \tag{4}$$

Rearranging Eq. (4) yields the following set of coupled equations to solve for $dy/d\alpha_i$,

$$\left(I - \frac{\partial F}{\partial y}\right) \frac{dy}{d\alpha_i} = \frac{\partial F}{\partial c} \frac{dc}{d\alpha_i} \quad , \tag{5}$$

or in more compact form,

$$Ay_i' = s_i \quad , \quad i = 1,\ldots,M \quad , \tag{6}$$

where I is the identity matrix and A, y_i', and s_i are given by

$$A = I - \frac{\partial F}{\partial y} \quad , \tag{7}$$

$$y_i' = \frac{dy}{d\alpha_i} \quad , \tag{8}$$

and

$$s_i = \frac{\partial F}{\partial c} \frac{dc}{d\alpha_i} \quad . \tag{9}$$

If Eq. (6) were solved directly for y_i', the result could be used in Eq. (3) to evaluate $dR/d\alpha_i$. This method of sensitivity analysis is called the "direct" approach and is a classical methodology that has received a great deal of attention in the literature.[1,5] Since Eq. (6) must be solved each time a new α_i is defined, the direct approach is most suitable for problems with relatively few input parameters of interest, for problems in which the solution of Eq. (6) is very inexpensive compared to the solution of the model itself, or for analytical problems in which the inverse of A can be explicitly determined.

For large-scale models with a large data base in which the ultimate objective is still the evaluation of $dR/d\alpha_i$ for many α_i, the intermediary step of solving for $dy/d\alpha_i$ and its inherent computational inefficiency can be avoided. For such problems the "adjoint" approach is far more applicable. In this methodology, use is made of the fact that Eq. (6) is linear in y_i', and appropriate adjoint equations can therefore be developed specifically to evaluate Eq. (3).

Defining the matrix adjoint of A as A* and using the usual definition of this adjoint give the identity,

$$u^{tr}Av = v^{tr}A^*u \quad , \tag{10}$$

where u and v are arbitrary vectors and A* is defined as

$$A^* = A^{tr} \quad . \tag{11}$$

Here the tr superscript represents the transpose of the vector or matrix.

If specific vectors for the problem at hand are chosen for u and v, the problem-specific adjoint equation can be set up as follows:

$$A^*y^* = s^* \quad , \tag{12}$$

where

$$A^* = A^{tr} - \left(I - \frac{\partial F}{\partial y}\right)^{tr} \quad . \tag{13}$$

Choosing s* as

$$s^* = (dh/dy)^{tr} \quad , \tag{14}$$

Eq. (3) can now be evaluated as follows:

$$\frac{dR}{d\alpha_i} = y^{*tr}\frac{\partial F}{\partial c}\frac{dc}{d\alpha_i} \quad , \quad i = 1,\ldots,M, \tag{15}$$

where y* is now the solution to

$$\left(I - \frac{\partial F}{\partial y}\right)^{tr} y^* = \left(\frac{dh}{dy}\right)^{tr} \quad . \tag{16}$$

The simplicity of the adjoint approach lies in the fact that Eq. (16) needs to be solved only once to get any and all sensitivities in the problem. This is a result of Eq. (16) being independent of the definition of α_i. The particular choice of α_i is only reflected in the

evaluation of Eq. (15), which involves simple vector products. In essence, the adjoint approach reduces the computational effort needed to evaluate $dR/d\alpha_i$ from solving many coupled linear equations to the evaluation of several vector products. For large-scale systems with many thousands or even millions of parameters, this represents orders of magnitude in computational efficiency.

It should be noted here that both the direct and adjoint equations (i.e., Eqs. (6) and (16)) are in any case far easier to solve than the original model (Eq. (1)). Both Eqs. (6) and (16) are linear while Eq. (1) is nonlinear. The direct and adjoint approaches, however, require the results of the original model equations to be available in order to set up Eqs. (6) and (16), since the **A** matrix and the vectors **s**, and **s*** depend on y.

In order to solve either the direct or adjoint sensitivity analysis, then, the model user must first generate the matrices $\partial F/\partial y$ and $\partial F/\partial c$ from the original nonlinear computer model. For large-scale problems this generally requires a great deal of painstaking human effort. First, the model equations must be extracted from the computer coding. They must then be differentiated with respect to all parameters of interest, and finally direct or adjoint sets of equations must be set up for computational solution. Successful automation of this procedure greatly reduces the human effort involved, potentially by orders of magnitude. The advantage of automation of sensitivity model development is therefore great indeed. The next two sections discuss two automated systems that use calculus precompilers to add capability to existing FORTRAN computer models for solving the direct and adjoint equations procedures.

III. GRESS

An Automated System for Solving the Direct Sensitivity Problem

For large-scale computer models, the equations are usually very complex and tied closely to and embedded in complex model logic and data-handling routines. In addition, for nonlinear problems, the numerical solution procedure often precludes an easy separation of the modeling equations from other parts of the model coding structure. For these reasons, a general system was developed to automate the application of computer calculus in existing codes. The system first developed for solving the direct sensitivity problem was the GRadient-Enhanced Software System (GRESS). Details of the GRESS system are given in Refs. 13,14, and 15, and the underlying ideas are briefly summarized herein.

The basic principle of GRESS is to read the model source program and search for model equations. These are identified uniquely by the appearance in the FORTRAN source program of the "=" symbol. Since all FORTRAN "equations" so identified occur in the form of Eq. (1) (i.e., with a single dependent variable on the left side of such an expression), GRESS can search for and analyze each equation in terms of its functional

dependence on y and c. The basic computer calculus operations of GRESS are then used to compute the successive elements of $\partial F/\partial c$ and $\partial F/\partial y$ as each expression is encountered. The differentiation is carried out analytically using calculus software for all permissible FORTRAN functions and operators and the results are computed and stored numerically using the local (current) values of the independent and dependent variables. GRESS takes advantage of the fact that in solving Eq. (5), the matrix $(I - \partial F/\partial y)$ is lower triangular and the y vector can be computed by forward substitution. The important point is that the components of y are solved successively as each equation is differentiated and that the $(I - \partial F/\partial y)$ matrix does not have to be stored. (The adjoint problem requires the storage of this matrix, as will be discussed in the next section).

GRESS only recognizes real-variable store operations as valid equations (i.e., the left side variable in a FORTRAN equation must be real), since continuous derivatives are to be calculated. Also, the left hand side of an equation is treated as a separate component of y each time it is executed (including each execution in a DO LOOP). The calculation of $\partial F/\partial y$ and $\partial F/\partial c$ in effect means that GRESS can be used to calculate the derivative of any real variable in the model with respect to any other real variable in the model. All derivatives are available for both internal and/or external use. For example, the derivatives $dR/d\alpha_i$ are used in the DUA method to be described later.

The application of GRESS to an existing FORTRAN model consists of a automated precompilation in which the automated code translation necessary to compute derivatives is performed using computer calculus. This step consists primarily of a rearrangement of the program data structure and a substitution of calls to GRESS interpretive software in place of all arithmetic lines of coding. All arithmetic operations of the original model are precompiled into a pseudomachine code (the GRESS P-code) for use during program execution. The two output files of this step are the enhanced model and the binary P-code file. These two files and a set of GRESS software subroutines supporting the enhanced model are compiled and run as a normal FORTRAN program to produce both the reference model results and gradient information. The gradients and reference results are used to calculate the sensitivities.

GRESS has undergone extensive verification during its development. To date, five major computer models of interest to the National High-Level Waste Program have been enhanced using GRESS, with direct comparison of GRESS-calculated derivatives to perturbation-derived derivatives being made for each enhanced model.[21-25]

IV. ADGEN

An Automated System for Solving the Adjoint Sensitivity Problem

The adjoint problem is defined by Eqs. (12-16). As previously mentioned, the calculation of the adjoint solution vector y^* from Eq. (16) is not a function of the selection of input parameter α_i and thus need only be performed once to determine the derivatives of a response of interest with respect to any parameter of interest. The matrix $\partial F/\partial c$ must also be determined but it too is independent of the parameter of interest. The only parameter dependent operation required to calculate the derivative $dR/d\alpha_i$ is the simple matrix multiplication operation $(y^{*tr})(\partial F/\partial c)(dc/d\alpha_i)$ in which the vector $dc/d\alpha_i$ is a function of α_i. A system to automate the calculation of derivatives based upon the solution of the adjoint equations has been developed.[17] The system is named ADGEN (ADjoint GENerator) and uses the GRESS precompiler to calculate all required derivatives of the $\partial F/\partial y$ and $\partial F/\partial c$ matrices.

Recall that GRESS solves Eq. (5), taking advantage of the fact that the matrix $(I - \partial F/\partial y)$ is lower triangular and the solution by forward substitution requires only that the vector $dy/d\alpha$ be stored. However, to solve the adjoint problem, all derivatives that constitute the n x n matrix $(I - \partial F/\partial c)^{tr}$ must be stored, where n = total number of equations, counting each time an equation is solved in a DO LOOP as a separate equation; the left hand side of each equation in a DO LOOP is treated as a separate element of y. Although only the non-zero elements are saved, the storage of the matrix $(I - \partial F/\partial c)^{tr}$ may require a substantial amount of storage capability. The storage difficulties are counterbalanced by features of Eqs. (15) and (16) that make the ADGEN calculation of y^* both practical and cost efficient. Note that the matrix $(I - \partial F/\partial c)^{tr}$ is upper triangular and that the column vector $(dh/dy)^{tr}$ is a simple user-defined vector (for most cases a vector with a single non-zero entry of unity). Thus Eq. (16) is easily solved by back substitution and the values of y^* can be successively stored in the space allocated for the $(dh/dy)^{tr}$ vector. The calculation of $dR/d\alpha_i$ from Eq. (15) must be performed for each α_i but this requires only trivial matrix multiplications and very little computer cost.

The ADGEN system calculates the normal model results as well as the derivatives making up the $\partial F/\partial y$ and $\partial F/\partial c$ matrices. Again, the major difference from the direct approach using GRESS is that the ADGEN system requires that the matrix $(I - \partial F/\partial c)^{tr}$ be stored and includes a post-processor solver routine to calculate the adjoint solution.

V. SAMPLE APPLICATION OF GRESS AND ADGEN

The distinguishing feature is solving Eq. (5) using GRESS is that only the elements of a single row of $\partial F/\partial y$ and $\partial F/\partial \alpha_i$ $[-(\partial F/\partial c)(\partial c/\partial \alpha_i)]$ need be saved in computer memory at any one time. This advantage is very fruitful if one wishes to solve for the derivatives of many LHS

elements (responses) with respect to a data element α_i. The disadvantage is that to calculate derivatives with respect to other data elements, Eq. (5) must be solved for each additional α_i of interest. The computational burden is approximately proportional to the number of α_i. In our experience to date, the computational time for calculating derivatives with respect to m chosen elements of c, denoted by T_m is

$$T_m \approx T_{REF}(\beta_0 + \beta_1 m)$$

where T_{REF} is the execution time of the reference model before derivative enhancement and β_0 and β_1 are constants falling between 1.0 to 20.0 and 0.1 to 1.4 respectively.

Another problem sometimes occurring in practice is that the elements of dy/dx_i must be stored in memory as Eq. (5) is solved for each row. Therefore the number of α_i with respect to which derivatives are calculated in a single execution of the enhanced model may be limited by system memory resources.

As mentioned in Section IV, solution of the adjoint equations, Eqs. (15 and 16), using the ADGEN system reduces the computation effort for calculating derivatives of a single response with respect to many parameters compared to repeatedly solving Eq. (5) for each α_i, as is done in GRESS. The solution to Eq. (16) is straightforward due to the upper triangular structure of $(I - \partial f/\partial y)^{tr}$, but requires storage of the nonzero elements of $(I - \partial f/\partial y)^{tr}$. ADGEN circumvents the necessity to store this matrix in memory by using an efficient scheme for solving Eq.s (15 and 16) based upon retrieval of portions of $(I - \partial f/\partial y)^{tr}$ from off-line storage and segmenting the calculation of derivatives.

The relative computational and storage requirements of the direct and adjoint approaches using GRESS and ADGEN are compared for the derivative enhancement of the PRESTO-II computer model.[18] PRESTO-II is intended to serve as a non site-specific screening model for evaluating possible health effects due to shallow-land disposal of radioactive waste. The model has approximately 6,900 lines of coding.

The sample problem results shown below are for the Barnwell sample problem included in Ref. 18. This problem calculates a time-dependent radiation dose to man from transport of 42 radionuclides over a one thousand year time span. Table 1 summarizes the execution times and storage requirements for the reference and the derivation-enhanced versions of PRESTO-II.

The number of parameters (data) and responses for this problem both number in the thousands. So calculation of derivatives of all responses (thousands) with respect to two data values using GRESS requires an increase in execution time from 44 seconds (Reference PRESTO-II) to 1,560 seconds (GRESS-enhanced PRESTO-II), a factor of 35.5. Conversely, calculation of derivatives of a single response with respect to all the data (thousands of parameters) requires 2,279 seconds (using ADGEN) for the

first response. This time is that required to create the adjoint matrix (1,560 seconds) and to calculate derivatives (299 seconds). For each additional response of interest, 299 seconds are required to calculate derivatives of the response to all the data. The 2,279 seconds and 299 seconds represent factors of 51.8 and 6.8, respectively, over the reference model run time. These factors clearly indicate that the adjoint approach using ADGEN is very cost effective compared to estimating derivatives by parameter perturbations. For evaluating the sensitivities of a large subset of the data base, ADGEN is orders of magnitude more cost effective than direct parameter perturbations.

Table 1. Comparison of execution times and storage requirements for derivative-enhancement of the PRESTO-II computer model by the GRESS direct approach and the ADGEN adjoint approach

PRESTO-II Reference Model

Compilation Time, s	48
Link Time, s	3
Run Time, s	44

PRESTO-II, Derivative Enhancement

Precompilation Time, s	29
Compilation Time, s	49
Link Time, s	4

		Run Time (s)	Direct Storage Access (Mbytes)
ADGEN:	Create $(I - \partial f/\partial y)^{tr}$	1,980	143.5[a]
ADGEN:	Adjoint Solution	299[b]	
GRESS:	2 parameters[c]	1,560	0
GRESS:	8 parameters[d]	1,816	0

[a]This matrix is created only once and can be used for calculating derivatives of one or more responses with respect to all the data or any subset thereof using the adjoint approach.

[b]This is the time required to solve for the derivative of a single response with respect to all the data.

[c]Calculation of derivatives of all responses with respect to two input parameters.

[d]Calculation of derivatives of all responses with respect to eight input parameters.

Note however, that the direct access storage requirements using the ADGEN system can be quite large, evidenced by the 143.5 megabytes needed to store the adjoint matrix for the PRESTO-II sample problem.

The availability of both the GRESS and ADGEN systems allow the analyst to compute model derivatives and sensitivities for a wide range of applications. GRESS is more suited for small data bases and for restricted direct access storage availability. ADGEN is more suited for calculating sensitivities to a large number of parameters. ADGEN becomes much more cost effective than direct parameter increases; GRESS may or may not be more cost effective than parameter perturbation depending upon the actual model being enhanced. In either case, the first derivative and sensitivities are analytically exact and can be printed and/or saved by simple user instructions in addition to normal model results.

VI. DETERMINISTIC UNCERTAINTY ANALYSIS

The analytical propagation of input uncertainties through a calculational model is unfeasible, if not impossible, for all but the most simple models. The difficulty lies in mapping probability density functions from an M-dimensional space of input parameters to the singly dimensioned output distribution function. To circumvent this problem, the most common approach is to randomly sample the input distributions and then calculate the model output of interest, constructing a probability distribution of the output by rerunning the model for each sample set of input parameters. The input probability distributions and any parameter correlations are handled, in a statistical sense, in the sampling procedure.[11,12] But hopefully the sampling procedure will lead to an output distribution that is representative of that which would result from the actual propagation of input probability distributions. As the number of sampling sets increases, the difference between the calculated and "true" output distribution diminishes. The problems occur in practice when the number of runs of the computer model needed to assure a large enough statistical sample becomes too expensive.

Another approach is to discretize the input probabilities into histograms and evaluate the model output of interest for all possibilities of parameter combinations to form a probability tree.[26] All parameter correlations are incorporated into the probability tree structure. This method does not rely on random sampling and probabilities are easily propagated in probability trees by simple multiplication. The histogram probability distributions are not actually propagated, but rather mean or endpoint parameter values are used. This method is quite feasible for models with a small number of parameters or even for a large number of input parameters if the model is simple (inexpensive). Again the problem arises when the computer model has numerous input parameters and/or is expensive to run.

A third approach is the response surface method in which the computer model is replaced with a simple analytical expression.[27] The

expression is constructed by fitting the computed values of the model output to the corresponding input parameters, or more generally, to chosen functions of the input parameters. Traditionally statistical techniques are used to choose the set of computer model runs to be made for this fitting. The uncertainty in the response is then determined by a second, more extensive statistical sampling and evaluation of the response surface. The advantage of replacing the model with the response surface is the drastically reduced computational time to compute the expression result compared to running the computer model. The disadvantage is the introduction of error in the calculated output by replacement of the model with a simple expression.

The Deterministic Uncertainty Analysis (DUA) method[19] combines the characteristics of the response surface method and probability trees. Statistical sampling is not required and probabilities are propagated analytically within discretized numerical meshes that encompass the parameter space. The approach underlying the deterministic calculation of uncertainties in the DUA method relies upon (1) a replacement of the computer model with an analytical function relating the responses of interest to the parameters of interest and (2) discretizing the parameter space and calculating the expected value of the response within each discrete parameter space "mesh." The parameters of interest are chosen to be those that are "uncertain," meaning that they have known or assumed probability distributions. The parameters of interest may often include the entire set of data used by the computer model.

The DUA method replaces the computer model with a response surface by relating the response of interest as calculated by the computer model to the parameter values by techniques that incorporate knowledge of the partial derivatives of the response with respect to the parameters of interest. The simplest form of a response surface is one formed by linear extrapolation from reference space points to each mesh of the discretized parameter space. Within each mesh the response surface is linear with respect to the parameters, and the calculation of the expected value of the response within the mesh, given parameter probability functions, is straightforward. An extrapolation scheme that makes use of the sensitivities is outlined in Ref. 19.

Sensitivity analysis plays an important role in the formation of the response surface by eliminating those parameters that have a negligible effect on the result of interest based on their sensitivities and uncertainty ranges. Also, the derivative information from the reference model runs can be used to identify the occurrence of parameters that occur exclusively in a given combination. Such identification reduces the parameter space by replacement of the individual parameters with the particular combination. For example, if the derivative of the response with respect to each of two parameters is the same at each reference space point sampled, the two parameters most likely appear in the model as a sum of each other, and a single parameter representing the sum of the two can be used in the formation of the response surface in place of the two individual parameters.

The propagation of parameter probability distributions from the multidimensional parameter space to the singly dimensioned result space is determined by the governing system of equations and the input variable probability density functions (pdf's). In theory, this propagation can be performed analytically by convolution of the integral of the parameter space into a discrete number of integrals of the singly-dimensioned response space, in which each integral is over a monotonically changing function representing the result. However, because the identification of the convolution integrals, in particular the limits of the integrals, is virtually impossible for all but the simplest problems, and because the model equations are nonlinear and complexly intertwined in general, the propagation of probability distributions through computer models cannot be treated analytically in the strictest sense.

The propagation of parameter probability distributions in the DUA approach is performed by discretizing the M-dimensional parameter space (M = number of parameters) into L meshes, each mesh denoted by m_ℓ. The probability of mesh m_ℓ occurring within the entire parameter space, $p(m_\ell)$, is calculated as well as the expected value of the response function within the mesh, $E(R_\ell)$, where R_ℓ represents the response function within m_ℓ. The probability $p(m_\ell)$ is assigned to $E(R_\ell)$ to obtain the probability of $E(R_\ell)$ within the discrete space of expected values. The pairs of $p(m_\ell)$ and $E(R_\ell)$ are reordered such that $E(R_1) < E(R_2) < \ldots E(R_L)$ and as such constitute the probability density function of the response R over the parameter space. The cumulative distribution function (CDF) of R, C(R), is the running sum of the reordered $p(m_\ell)$ paired with the corresponding value of $E(R_\ell)$. In the limit as $L \to \infty$, C(R) approaches the true cumulative distribution function of R as calculated using the response function.

Let the functional form of the response within m_ℓ be given by

$$R_\ell = g_\ell(c) \tag{17}$$

where $g_\ell(c)$ is the response surface function within m_ℓ resulting either from a fitting procedure or from a linear expansion from one or more reference space points. The vector c is the M-dimensional parameter vector given by $c = \{\alpha_1, \alpha_2, \ldots, \alpha_M\}_{tr}$. Given the joint probability function of c as $P(c) = P(\alpha_1, \alpha_2, \ldots \alpha_M)$, the probability that $c \subset m_\ell$ is given by

$$P(m_\ell) = P(c \subset m_\ell) = \int_{m_\ell} P(c)dc \quad , \tag{18}$$

and the expected value of the response R within m_ℓ, $E(R_\ell)$, is

$$E(R_\ell) = \int_{m_\ell} g(c)P(c)dc/p(m_\ell) \quad . \tag{19}$$

The values of $p(m_\ell)$ and $E(R_\ell)$ as calculated by Eqs. (18) and (19) are used to construct the probability density function and cumulative distributions function of the response R.

VII. SAMPLE PROBLEM APPLICATIONS OF DUA

The DUA method is demonstrated for two sample problems and the results are compared to a traditional statistical approach. The first sample problem is from Ref. 28, which exemplifies the use of uncertainty analysis in the study of water flow through a bore hole. The sample problem consists of three coupled equations with eight input parameters and three dependent variables. The analysis focuses on one of the three dependent variables, the flow rate, as the response of interest, and statistical techniques are used to calculate the cumulative distribution of the flow rate given probability distributions for the eight input parameters.

Reference 27 describes a statistical uncertainty analysis approach for this problem based upon the Latin Hypercube Sampling (LHS) procedure using a 50 design-point matrix. The DUA method was also applied to this sample problem, the details of which are given in Ref. 19. As a benchmark against which a comparison of the DUA method and the statistical results from Ref. 27 could be compared, the sample problem model was executed 2304 times in order to approximate the "true" CDF of the flow rate for this problem. A comparison of this benchmark 2304-point CDF to the statistical 50-point CDF from Ref. 28 is shown in Fig. 1. The CDF based upon the 50 point LHS design matrix is a fairly accurate representation of the true CDF of Q. DUA method results were obtained by forming a response surface by extrapolation from two reference model runs and propagating parameter pdf's over a discrete mesh consisting of 2304 meshes. As shown in Fig. 2., the CDF of the flow rate calculated deterministically based on the DUA method closely matches the "true" CDF with only two executions of the derivative-enhanced model.

The second sample problem calculates the temperature and brine flow rates in a repository arising from the decay heat produced from buried high-level nuclear waste. In this study (Ref. 20), GRESS was used to enhance the BRINETEMP[29] computer model for calculation of derivatives and sensitivities needed for uncertainty analysis by the DUA method. The CDF of the brine flow rate and the temperature at a specific location of interest were determined given the pdf's of twelve input parameters. The resulting CDF's from the DUA method were compared to the CDF's from a statistical approach based on a 200-point LHS design matrix. The resulting curves are shown in Figs. 3 and 4. The DUA method used 10 runs of the enhanced BRINETEMP model in determining the CDF of the temperature at

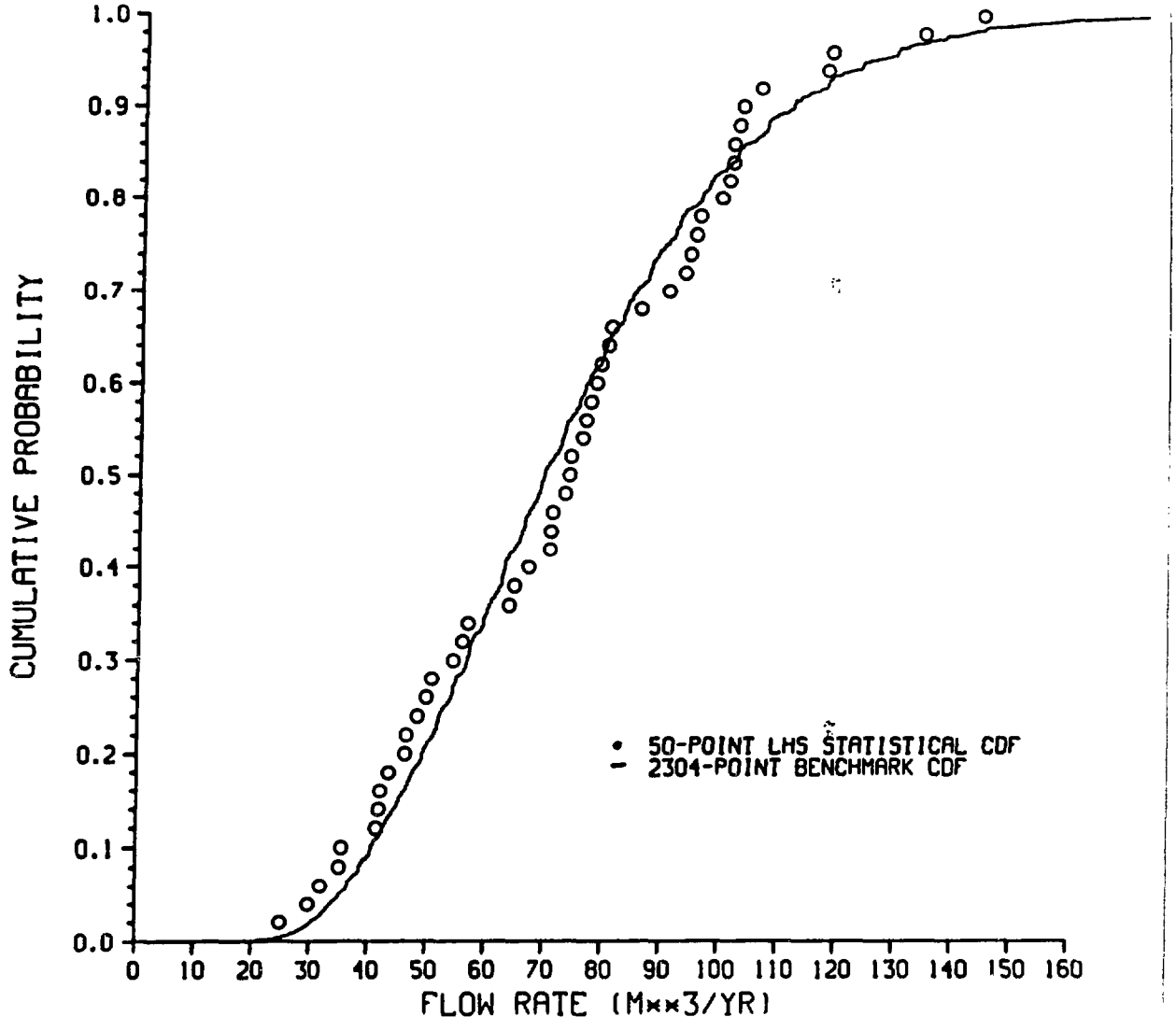

Fig. 1. Comparison of the 50-point LHS statistically calculated CDF to the 2304-point benchmark CDF.

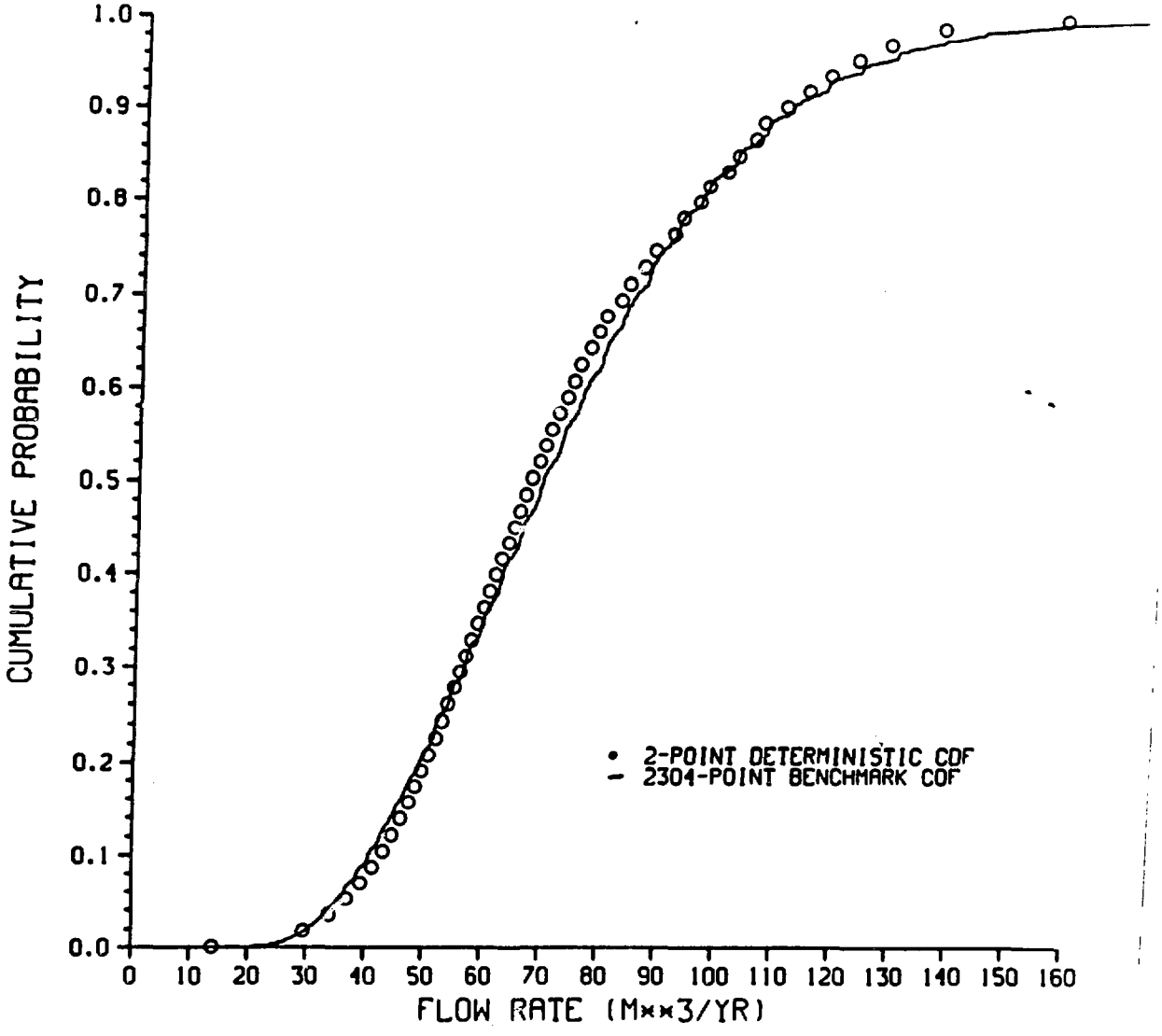

Fig. 2. Comparison of the deterministic CDF based on an extrapolation from two points to 2304 points with the 2304-point benchmark CDF.

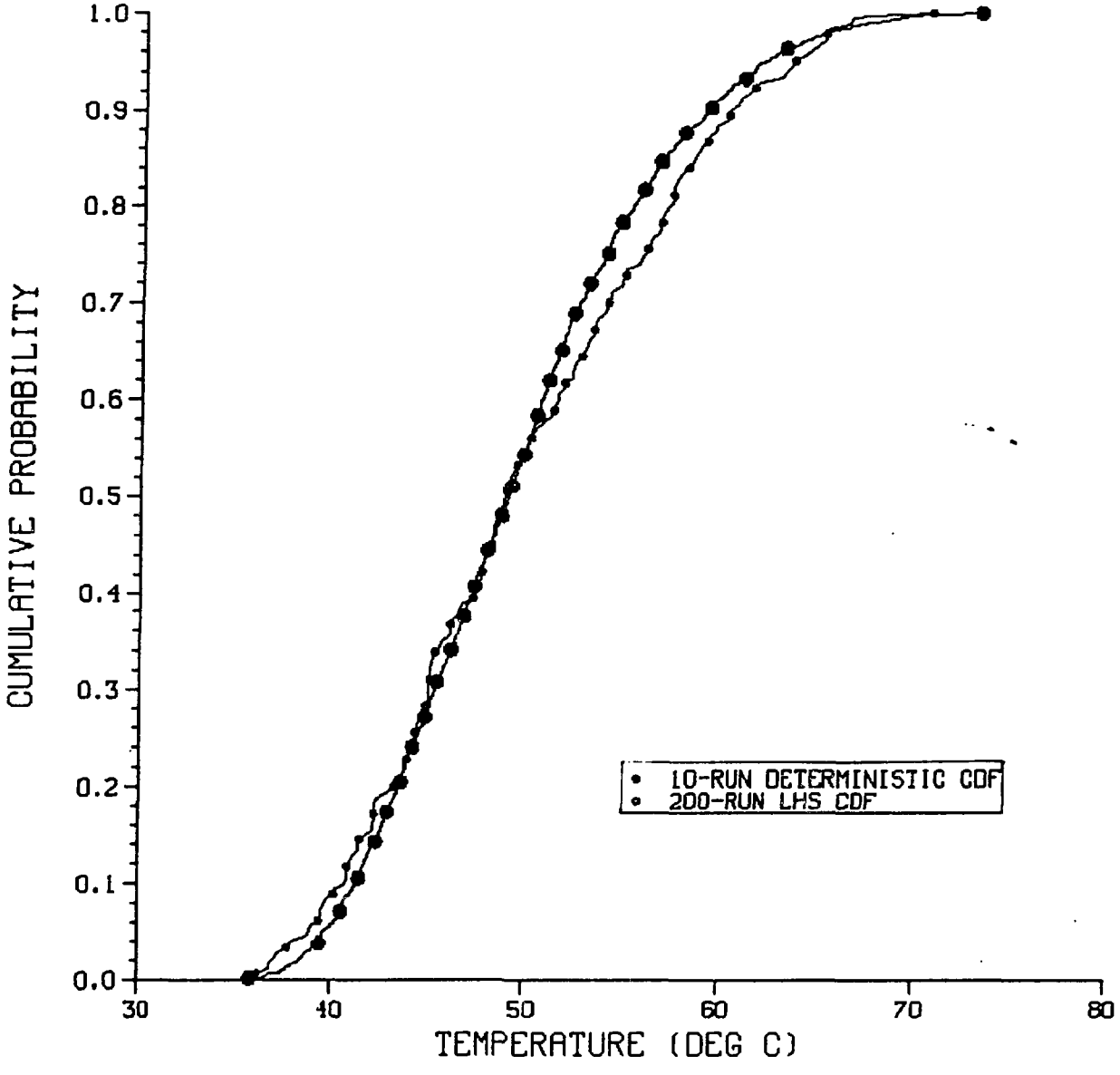

Fig. 3. Comparison of the deterministic CDF for temperature using 10 enhanced reference runs extrapolated to 2400 points with the CDF from 200 statistical runs. Burial time = 1000 years.

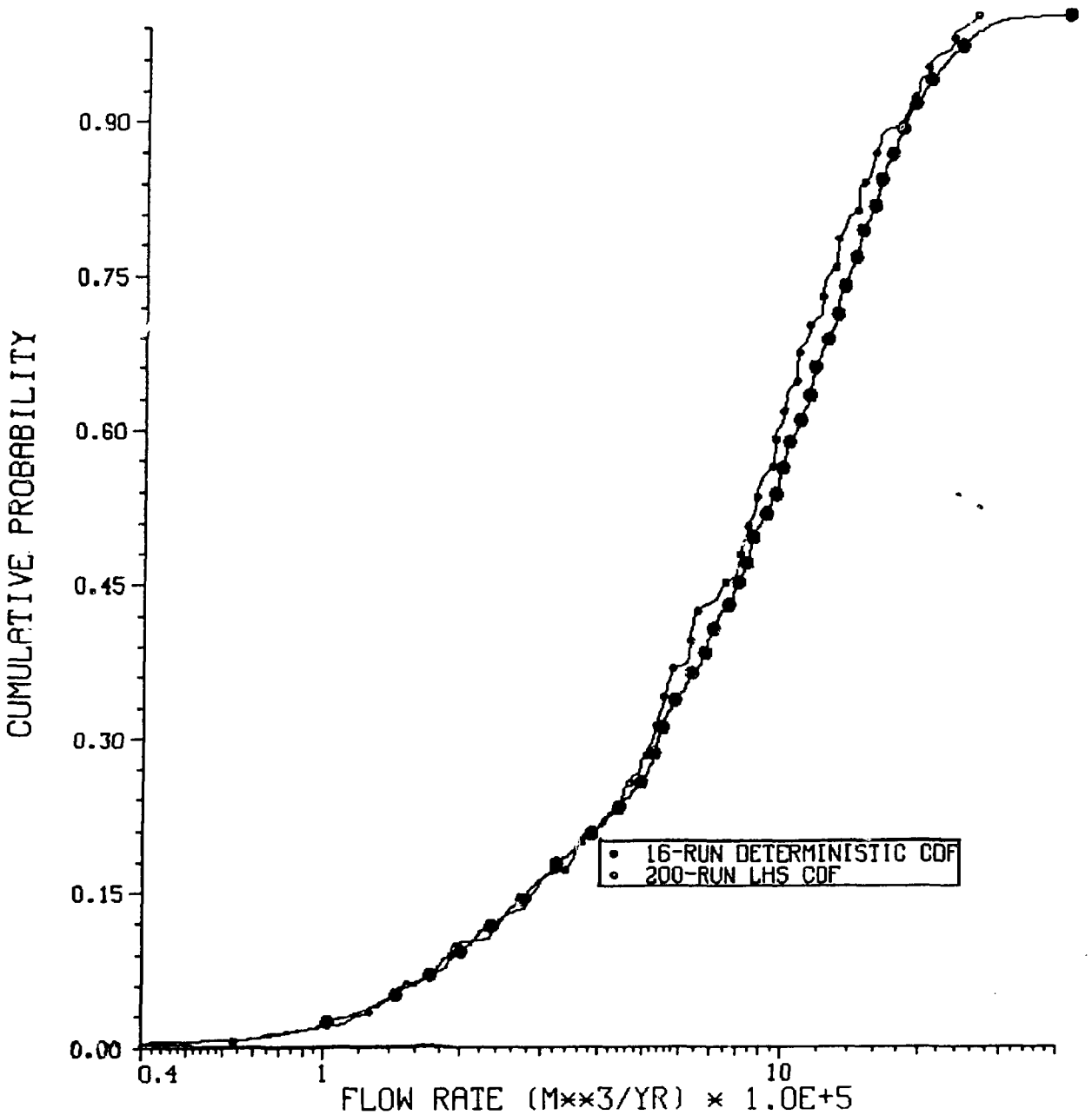

Fig. 4. Comparison of the deterministic CDF for flow rate using 16 enhanced reference runs extrapolated to 3200 points with the CDF from 200 statistical runs. Burial time = 1000 years.

1000 years after burial and 16 for the flow rate. These compare to 200 runs of the reference BRINETEMP model for the LHS statistical analysis. The CDF curves compare closely for the DUA and statistical methods, but the DUA method requires far fewer model runs.

VIII. CONCLUSIONS

A comprehensive, deterministic approach to sensitivity and uncertainty analysis of large-scale computer models is now available. The GRESS and ADGEN systems for automating the calculation of model derivatives and sensitivities have been developed, verified, and applied to several large-scale computer models. The availability of these two systems greatly reduces the man-effort required to add sensitivity capability to existing FORTRAN models.

A deterministic approach to uncertainty analysis (DUA) has been developed, and the availability of derivative information is a key component. The feasibility and advantages of the DUA method is demonstrated by its application to two sample problems. The sample problems show that simple linear extrapolation from a small set of parameter space points produces CDF's of the responses of interest that closely match that produced by statistical analysis using a far greater number of model executions. Although the reduction in model runs for DUA as compared to a statistical approach is offset by the additional cost of calculating derivatives, the Section V timing studies demonstrate that the availability of the GRESS and ADGEN systems for adding derivative-taking capability to existing models makes the DUA approach both practical and computationally advantages for most applications. The strong analytical foundations of propagating probabilities deterministically is another desirable feature of the DUA approach.

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