ANALYTICAL METHODS FOR LARGE-SCALE SENSITIVITY*  
ANALYSIS USING GRESS AND ADGEN

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ANALYTICAL METHODS FOR LARGE-SCALE SENSITIVITY ANALYSIS USING GRESS AND ADGEN

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Sensitivity analysis is an established methodology used by researchers in almost every field to gain essential insight in design and modeling studies and in performance assessments of complex systems. Conventional sensitivity analysis methodologies, however, have not enjoyed the widespread use they deserve considering the wealth of information they can provide, partly because of their prohibitive cost or the large initial analytical investment they require. Automated systems have recently been developed at OKNL to eliminate these drawbacks. Compilers such as GRESS and ADGEN now allow automatic and cost effective calculation of sensitivities in FORTRAN computer codes. In this paper, these and other related tools are described and their impact and applicability in the general areas of modeling, performance assessment and decision making for radioactive waste isolation problems are discussed.

Introduction

The data characterizing geologic media and waste behavior are generally associated with large uncertainties. These uncertainties result from the extreme heterogeneity of the subsurface materials, our lack of understanding of all the complex geochemical and geohydraulic phenomena, and, still today, the inaccuracy of even the most refined state-of-the-art measuring techniques. When these data are used in design studies or performance assessments of large-scale systems, their large uncertainties can propagate through the calculational schemes to lead to very large uncertainties on the performance measures or results of interest. In the case of low level, high level or defense radioactive wastes disposal, large uncertainties generally equate to added risk to the environment or public health. In design studies or risk assessment analyses for waste isolation systems, the uncertainties on the final results or performance measures should, therefore, be evaluated concurrently with the calculated results. Moreover, this evaluation should provide for the assurance, preferably quantitative, that all potential sources of uncertainty in a given problem have been systematically identified and that their effects or sensitivity on the final results have been taken into account in the analysis. Finally, the method for evaluating the sensitivities and uncertainties should provide for the capability to formally perform the inverse problem, i.e., given an unacceptable (i.e., too large) uncertainty on a final performance measure, identify and prioritize all data or input parameters that contribute to that uncertainty, pointing out those needing added attention or research effort in the site characterization or data generating processes, in order to decrease the uncertainty on the calculated values.

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Statistical methods and perturbation analysis have traditionally been used to perform sensitivity and uncertainty analyses. When applied to large-scale studies such as those related to radioactive waste isolation, these conventional methods have serious drawbacks: not only is their cost prohibitive, but they generally cannot handle all parameters involved in a study. They also rely on qualitative expert opinion for selection of "key" parameters, thus preventing formal solution of the inverse problem. Deterministic methods, on the other hand, such as the adjoint formulation, allow systematic and quantitative screening of the parameter space thus providing all the information necessary to perform a complete sensitivity analysis including the inverse problem. These methods, however, have not enjoyed the wide-spread use they deserve, mainly because of the large initial analytical investment they require and their specificity to a given model or code.

Two procedures, making use of the strengths of the adjoint method and of computer calculus, have been designed to automate the costly and time-consuming processes of deterministic sensitivity analysis. These procedures, embodied in two computer precompilers named GRESS (GRadient Enhanced Software System) and ADGEN (Automated Adjoint Generator), will allow cost-efficient, quantitative and systematic sensitivity analyses to be performed which otherwise might not have been undertaken.

The GRESS Precompiler

GRESS (Oblow, 1985, Oblow et al. 1986) is a FORTRAN precompiler that enhances conventional FORTRAN programs with analytic differentiation of arithmetic statements. Basically, GRESS reads the FORTRAN source code text, redefines the variable storage locations, searches for arithmetic statements, enhances these for gradient calculation, and then generates a new FORTRAN source program which can produce derivatives for any real variables if desired. GRESS thus allows any standard FORTRAN code to be enhanced to allow the calculation of any required derivatives, whether they be for use internally (e.g., for iteration acceleration) or externally (e.g., for sensitivity studies).

The use of GRESS is illustrated in Fig. 1. In the preliminary processing step the input program is separated into two subsets. The first, which contains all calculation routines, is hand modified for submission to the GRESS precompiler. The amount and nature of these modifications depend upon the particular application at hand and the limitations of the current version of GRESS. The second subset (possibly null) is composed of subroutines whose only communication with the first subset is through the arguments in their calling sequence. These subroutines have no calculating function in the program and are usually associated with input echoing, output printing or plotting, and peripheral program analysis functions. They do not require GRESS compilation and may usually be submitted unchanged to the FORTRAN compiler.

The GRESS precompilation step is the one in which the code enhancement necessary to compute derivatives is performed using automated computer calculus. A rearrangement of the program data structure and a substitution of calls to GRESS interpretive software are performed automatically by GRESS for all arithmetic lines of coding. The modified
program is then compiled into a pseudo-machine code (the GRESS P-CODE) for use during program execution. The two output files of this step are, therefore, the enhanced FORTRAN subroutines and the binary P-CODE file.

In the enhanced subroutines, the derivatives are calculated according to the chain rule of differential calculus and are propagated from operation to operation analytically by implicit differentiation rules. The application of these well-known mathematical rules to computer logic is, in fact, straightforward due to the sequential structure of computer codes. The parameters with respect to which GRESS will generate partial derivatives are declared by the user at the beginning of the enhanced program. Then, for each storage operation, the lines of coding that have been added by GRESS calculate the derivatives of the stored quantity with respect to any variable used in its computation and, using the chain rule, with respect to the declared parameters. The calculated derivatives can then be output along with the normal results at any stage during enhanced program execution.

The demonstration and extension to large modular codes of these basic concepts as well as the associated GRESS software are described in detail in Ublow (1985), Ublow et al. (1986b), Pin et al. (1986) and Worley et al. (1986).

In the final stage of the GRESS procedure, the enhanced FORTRAN subroutines are combined with the untranslated subset of subroutines and both are submitted to the normal FORTRAN compiler. The relocatable object modules which result from actual compilation are then input to the system link-edit loader, which combines them with appropriate portions of the GRESS interpretive library and the P-code file to form the complete executable program. The library contains the P-code interpreter, a series of support routines, and a set of utility subroutines which may be directly referenced by the enhanced program to display or manipulate derivatives. The resulting enhanced program will execute identically to the original source program with the option of also calculating derivatives.
The ADGEN Precompiler

The ADGEN precompiler has been designed to automatically generate adjoint solutions of computer codes. The overall automated process can be simply described using the following example. Let

\[ \overline{y} = \overline{F}(\overline{y}, \overline{c}) \]  

represent, in vector form, the set of equations and storage operations programmed in a FORTRAN code. The components of the vector \( \overline{y} \) on the left-hand side of the equation are the stored value of the variables being solved for, \( \overline{c} \) represents the user-specified model data or parameter set, and \( \overline{F} \) defines the model equations. Typically, several results which are some function of the solution to Eq. (1) are of particular interest to the model user. Let

\[ \overline{K} = h(\overline{y}) \]  

define a typical result, \( \overline{K} \), where \( \overline{K} \) is a single number and \( h \) represents the known functional dependence of \( \overline{K} \) on \( \overline{y} \). For notational ease, let \( \alpha_i \) denote a generic parameter which can be a component of the vector \( \overline{c} \) or any other variable used in the code.

The basic problem in any sensitivity study is to find the rate of change in the result \( \overline{K} \) arising from changes in any of the model parameters. For the generic parameter \( \alpha_i \), then, the quantity of interest is the numerical value of \( d\overline{K}/d\alpha_i \) given analytically by

\[ \frac{d\overline{K}}{d\alpha_i} = \overline{h} \frac{d\overline{y}}{\overline{y} d\alpha_i} \]  

(3)

Since the functional dependence of \( \overline{K} \) on \( \overline{y} \) through \( h(\overline{y}) \) is defined analytically by the model user, only \( d\overline{y}/d\alpha_i \) needs to be generated in order to evaluate Eq. (3). The procedure needed to get \( d\overline{y}/d\alpha_i \) is to differentiate Eq. (1) and rearrange it to yield the following set of coupled equations to solve for \( d\overline{y}/d\alpha_i \),

\[ (I - \frac{\partial \overline{F}}{\partial \overline{y}} \frac{d\overline{y}}{d\alpha_i} = \frac{\partial \overline{F}}{\partial \overline{c}} \frac{d\overline{c}}{d\alpha_i} \]  

(4)

where \( I \) is the identity matrix.

If Eq. (4) were solved directly for \( d\overline{y}/d\alpha_i \), the result could be used in Eq. (3) to evaluate \( d\overline{K}/d\alpha_i \). This method of sensitivity analysis is called the "direct" approach and is a classical methodology which has received a great deal of attention in the literature (e.g. see Tumovic and Vukobratovic, 1972, Frank, 1978). Its main drawback arises in large-scale applications where the size of the vector \( \overline{c} \) (and therefore the number of \( \alpha_i \)'s whose sensitivities need to be evaluated) becomes prohibitively large. Since Eq. (4) must be solved each time a new
a_1 is defined, the computational expense puts this method out of reach as a practical tool for large-scale sensitivity studies. Its practical value is therefore restricted to smaller-scale analytical problems or other cases where (I - \frac{\partial F}{\partial y}) can easily be inverted.

Since the ultimate objective of a large study, however, is still the evaluation of dK/d\alpha_1, the intermediary step of solving for dy/d\alpha_1 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. (4) is linear in dy/d\alpha_1, and an appropriate adjoint equation can therefore be developed specifically to evaluate Eq. (3) as

\[ \frac{dK}{d\alpha_1} = y^{*\text{tr}} \frac{\partial F}{\partial \alpha} \frac{d\alpha}{d\alpha_1} \]  

where \( y^{*} \) is now the solution to

\[ (I - \frac{\partial F}{\partial y})^{\text{tr}}y^{*} = (\frac{dK}{dy})^{\text{tr}} \]  

and the superscript "tr" represents the transpose of the vector or matrix.

The simplicity of the adjoint approach lies in the fact that Eq. (6) needs to be solved only once to get any and all sensitivities in the problem. This is a result of Eq. (6) being independent of the choice of \( \alpha_1 \). The particular choice of \( \alpha_1 \) is only reflected in the evaluation of Eq. (5) which involves only simple vector products. In essence, the adjoint approach reduces the computational effort needed to evaluate dK/d\alpha_1 from solving many coupled linear equations to the evaluation of several vector products. For large scale systems with many hundreds or even thousands of parameters, this represents orders of magnitude in computational efficiency.

The major drawback of the adjoint approach has traditionally been the large analytical investment necessary to derive the many derivatives represented by \( \frac{\partial F}{\partial y} \) and \( \frac{\partial F}{\partial \alpha} \). This drawback is now eliminated with the automatic differentiation capability of GRESS. Thus, ADGEN uses a GRESS-like procedure to calculate all required derivatives in Eqs. (5) and (6), and automatically sets up Eq. (6) as a large matrix equation. The solution \( y^{*} \) is then calculated using standard back-substitution techniques and is used in Eq. (5) to obtain all sensitivities of interest through straightforward vector calculations. The efficiency of the overall system increases with the number of required sensitivities, i.e., the number of parameters, and problems that were practically unapproachable with the "direct" approach can now be done in routine fashion.
The two general objectives of a performance assessment for a waste isolation system are to evaluate the level of confidence which can be placed in a facility (i.e., estimate the risks involved) in meeting prescribed performance measures, and to pass this level of confidence along to the public and/or the regulatory or licensing authorities. As we mentioned earlier, three aspects of radioactive waste management, which have become increasingly critical with increased public awareness and involvement, require special attention in reaching these objectives. These can be stated as follows: (1) uncertainties in performance assessments equate to risks to public health, (2) remedial actions should be possible to plan and implement (including in the analytical phase) if assessment results are unsatisfactory, and (3) incomplete (or partial) results and qualitative results are insufficient in performance assessments of radioactive waste isolation systems. These concerns became crucial in radioactive waste assessment studies as no methods suitable for large-scale systems such as waste isolation facilities were available to fully answer them.

The following approach which makes use of the new sensitivity analysis tools described earlier and of conventional statistical methods is proposed to solve this problem. The procedure embodying this approach is shown schematically on the diagram of Fig. 2. Following a preliminary data acquisition phase, conceptual models of the site, disposal units, and source terms are developed. These conceptual models generally are refined during the site characterization phase and the data acquisition process should proceed until all data necessary to support the numerical models of the overall system are developed. At this stage of the analysis, all data acquired, be it qualitative or quantitative, is defined as unrefined and is associated with an uncertainty which should both be evaluated and become part of the data base for the site.

Once the numerical models necessary to simulate all site specific phenomena of interest have been developed, appropriate validated computer codes are selected (alternatively developed and verified if necessary) to perform the predictive simulations. To this point, little innovation has been proposed. The next step in the procedure outlined in Fig. 2, however, is the one which has traditionally not been performed in large-scale studies because of cost and time constraints. The complete adjoint sensitivity analysis, now feasible using the CRESS
and ADGEN precompilers described earlier, serves several purposes. First, it allows one to thoroughly check the numerical codes by quantitatively verifying that the influence of each parameter on the results of the analysis corresponds to what was intended in the conceptual models, thus adding to the verification, validation and reliability of the codes. Second, the complete sensitivity analysis allows a formal (i.e., based on systematic and quantitative results) reduction in scope of the uncertainty problem by separating the parameters that have a proven influence on the results from those that have none. Last and most importantly, it allows one, through a ranking of the products of the sensitivities and the data uncertainties, to identify all leading sources of uncertainty for a given result, thus further reducing the uncertainty problem to a reduced set of "key" parameters to be further considered in the detailed treatment of the problem uncertainties. Note that this reduced set of parameters is an exhaustive list of the parameters which have been formally shown to have an influence on the results of interest and that, as opposed to the qualitative expert opinion used for this task in the conventional approaches, the automated sensitivity analysis procedure has provided a systematic and quantitative methodology for the successive reductions in scope of the uncertainty problem.

At this point in the study, preliminary or partial uncertainty calculations generally make it clear if acceptable uncertainties on the final results are obtainable given the current set of data uncertainties. If satisfactory results can be obtained, then the final uncertainty analyses can be completed at minimum cost using the reduced set of parameters and conventional statistical techniques since these methods, whose costs are directly proportional to the number of parameters considered, are practically feasible only for reduced sets of parameters. If, on the other hand, the results are unsatisfactory either because of their actual value or their associated uncertainties, then the results of the complete sensitivity analysis procedure allow the inverse problem to be formally performed since sensitivities with respect to all parameters have been calculated and all leading sources of uncertainty have been identified. The results of the automated procedure, therefore, clearly point out which parameters are the most critical in interpreting the results of a specific performance assessment in the context of regulatory standards or licensing requirements, and where additional research or data acquisition would be most beneficial for the purpose of improving the assessment results or reducing the overall uncertainty in the calculated results.

Since it is not always possible to improve the quality of the data specifically measured for input to a performance assessment, an alternative method, referred to as a "folding procedure" on Fig. 2, can be used to reduce the overall uncertainty in the calculated results. The methodology (see Maerker et al., 1985) allows one to take into account in the system uncertainty analysis any additional knowledge or measured data which may not be explicitly used in the calculational scheme but are related to some physical properties of the system. This folding procedure, described in detail in Maerker et al. (1985), combines the added
knowledge of the data with that used in the calculations by means of a
generalized least-square adjustment procedure, resulting in the reduc-
tion of the uncertainties in the responses as well as in some of the
most important parameters.

Conclusions

A new deterministic procedure for improving large-scale performance
assessment of waste isolation systems has been presented. The procedure
makes use of the GRESS and ADGEN precompilers to provide, in an auto-
mated, systematic and quantitative manner, all the information necessary
to support a complete sensitivity and uncertainty analysis. Because of
its completeness, the procedure allows evaluation of all parameters and
identification of all major sources of uncertainty in a given problem to
support a formal reduction in scope of the uncertainty problem. In this
respect, the procedure allows one to avoid "over collection of data" and
"over modeling" by focussing research and analysis efforts where needed
most. The procedure also allows formal performance of the inverse prob-
lem to improve, if necessary, the assessment results and reduce their
associated uncertainties. To that affect, use can be made of an origi-
nal folding methodology which takes into account in the system uncer-
tainty analysis any additional knowledge of physical properties of the
system which have not been explicitly used in the calculational scheme.
The new deterministic methodologies introduced in the overall procedure
are totally compatible with, and fully complementary to the conventional
statistical methodologies. The conjugated use of these methodologies is
recommended in any complete performance assessment study of large-scale
systems such as waste isolation facilities.

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