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SENSITIVITY ANALYSIS OF PREDICTIVE MODELS WITH AN AUTOMATED ADJOINT GENERATOR

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ABSTRACT

The adjoint method is a well established sensitivity analysis methodology which is particularly efficient in large-scale modeling problems. Its efficiency comes from the fact that the coefficients of sensitivity of a given response with respect to every parameter involved in the modeling code can be calculated from the solution of a single adjoint run of the code. Sensitivity coefficients provide a quantitative measure of the importance of the model data in calculating the final results. The major drawback of the adjoint method which has prevented its widespread use in computational systems is the requirement for calculations of very large numbers of partial derivatives in order to set up the adjoint equations of the model. ADGEN is a software system which has been designed to eliminate this drawback and automatically implement the adjoint formulation in computer codes. In this paper, the ADGEN system will be described and its use for improving performance assessments and predictive simulations will be discussed.

INTRODUCTION

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. Statistical methods and perturbation analysis have traditionally been used to perform sensitivity analyses. When applied to large-scale studies (e.g., nuclear reactor design, reactor safety, radioactive waste isolation, etc.) these conventional methods have serious drawbacks: not only is their cost prohibitive, but they generally cannot handle all parameters involved in a study. Deterministic methods, on the other hand, such as the adjoint formulation (e.g. see Refs. 1 and 2), 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 (e.g. to calculate the large number of derivatives necessary to set up the adjoint equations). This paper describes a new automated system, named ADGEN, which makes use of the strengths of computer calculus[3,4,5,6] to automate the costly and time-consuming calculation of derivatives in FORTRAN computer codes and automatically generate adjoint solutions of computer codes.

THE ADGEN SYSTEM

The overall automated process can be simply described using the following example. Let

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

represent, in vector form, the set of equations and storage operations programmed in a FORTRAN code. The components of the vector $\bar{y}$ on the left-hand side of the equation are the stored value of the variables being solved for, $\bar{c}$ represents the user-specified model data or parameter set, and $\bar{F}$ defines the model equations. Let $R = h(\bar{y})$ define a typical result, R, where R is a single number and h represents the known functional dependence of R on $\bar{y}$, and let α_i denote a generic parameter which can be a component of the vector $\bar{c}$ or of the vector $\bar{y}$.

The basic problem in any sensitivity study is to find the rate of change in the result R arising from changes in any of the 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

$$\frac{dR}{d\alpha_i} = \frac{\partial h}{\partial \bar{y}} \frac{d\bar{y}}{d\alpha_i} \quad . \tag{2}$$

Since the functional dependence of R on $\bar{y}$ through $h(\bar{y})$ is defined analytically by the model user, only $d\bar{y}/d\alpha_i$ needs to be generated in order to evaluate Eq. (2). Differentiating Eq. (1) and rearranging it yields the following set of coupled equations to solve for $d\bar{y}/d\alpha_i$,

$$\left(I - \frac{\partial \bar{F}}{\partial \bar{y}}\right) \frac{d\bar{y}}{d\alpha_i} = \frac{\partial \bar{F}}{\partial \bar{c}} \frac{d\bar{c}}{d\alpha_i} \tag{3}$$

where I is the identity matrix.

If Eq. (3) were solved directly for $d\bar{y}/d\alpha_i$, the result could be used in Eq. (2) to evaluate $dR/d\alpha_i$. 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.[7,8] Its main drawback arises in large-scale applications where the number of α_i's whose sensitivities need to be evaluated becomes prohibitively large. Since Eq. (3) must be solved each time a new α_i is defined, the practical value of this approach is therefore restricted to smaller-scale analytical problems or other cases where $\left(I - \frac{\partial \bar{F}}{\partial \bar{y}}\right)$ can easily be inverted.

Since the ultimate objective of a large study, however, is still the evaluation of $dR/d\alpha_i$, the intermediary step of solving Eq. (3) for each α_i of interest (and its inherent computational inefficiency) can be avoided. For such problems the adjoint[1,2] approach is far more applicable. In this methodology, use is made of the fact that Eq. (3) is linear in $d\bar{y}/d\alpha_i$, and an appropriate adjoint equation can therefore be developed specifically to evaluate Eq. (2) as

$$\frac{dR}{d\alpha_i} = \bar{y}^{*tr} \frac{\partial \bar{f}}{\partial \bar{c}} \frac{d\bar{c}}{d\alpha_i} \tag{4}$$

where $\bar{y}^*$ is now the solution to

$$\left(I - \frac{\partial \bar{F}}{\partial y}\right)^{tr} \bar{y}^* = \left(\frac{\partial h}{\partial \bar{y}}\right)^{tr} , \tag{5}$$

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

The simplicity of the adjoint approach lies in the fact that Eq. (5) needs to be solved only once to get any and all sensitivities in the problem. 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 obtain the many derivatives represented by $\partial \bar{F}/\partial \bar{y}$ and $\partial \bar{F}/\partial \bar{c}$. This drawback is now eliminated with the automatic differentiation capability demonstrated in the GRESS system.[3,4,5,6] Thus, ADGEN (see Fig. 1) uses a GRESS-like precompiler named EXAP (Extended Arithmetic Processor) which can enhance any FORTRAN code with the computer calculus necessary to calculate all required derivatives in Eqs. (4) and (5). At execution of the enhanced code, ADGEN automatically manages the storage of the derivatives to set up Eq. (5) as a large matrix equation. The solution y^* is then calculated using efficient back-substitution techniques and is used in Eq. (4) to obtain all sensitivities of interest through straightforward vector calculations.

DEMONSTRATION ON A LARGE-SCALE PROBLEM

During the development phase of the ADGEN software, several small sample problems have served as a testbed for the system. A demonstration of the suitability of the overall approach and system for large scale applications has been successfully conducted using the PRESTO-II code. PRESTO-II is a large FORTRAN code which contains approximately 6,900 lines of coding. It is intended to serve as a non site-specific screening model for evaluating possible health effects due to shallow-land disposal of

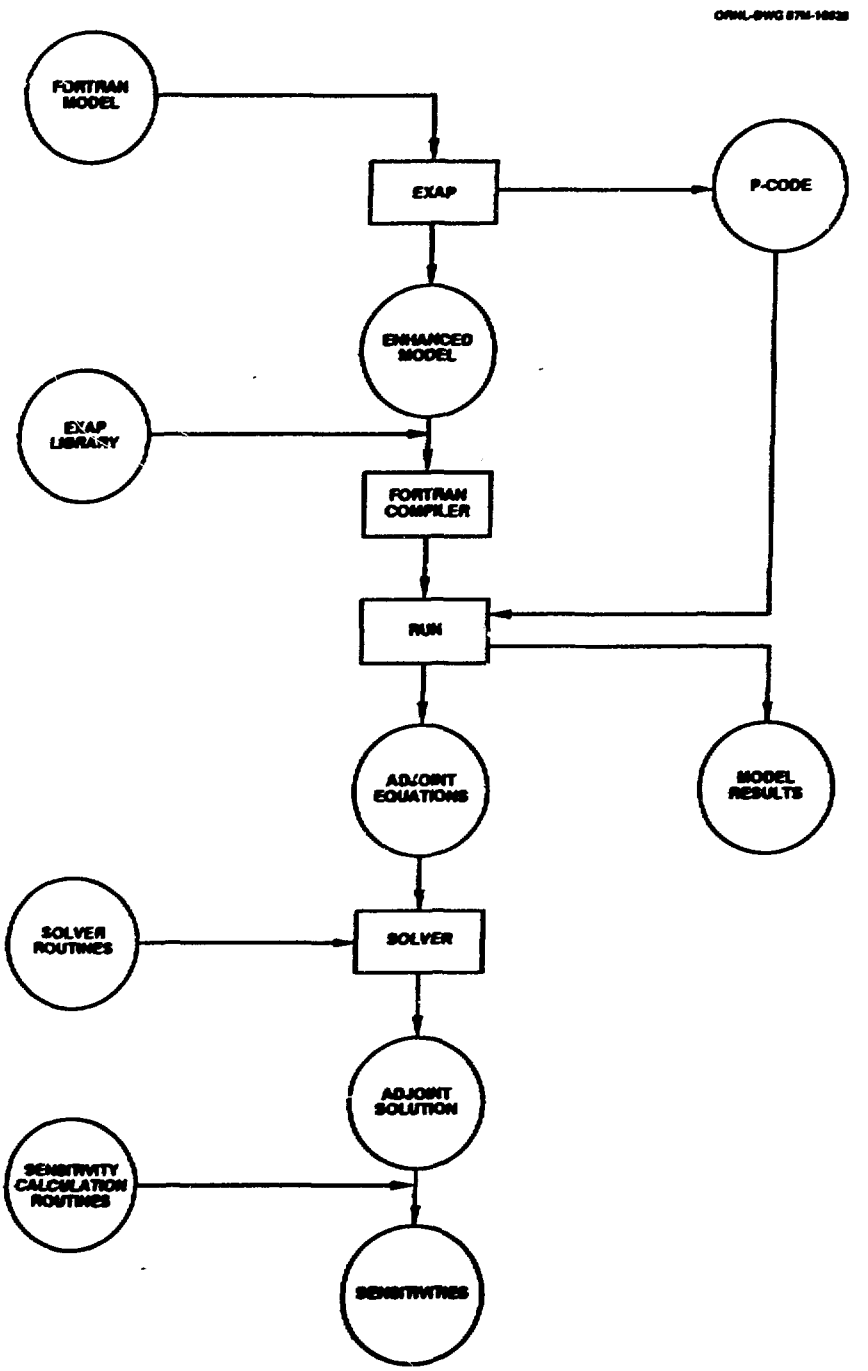

Fig. 1. Flowchart of the ADGEN System.

radioactive waste. In the demonstration study, the entire PRESTO-II code was first transported to our VAX system and then successfully enhanced through the EXAP precompiler (see Fig. 1). The resulting enhanced program was linked to the EXAP library and run on a sample problem. In the sample problem, time dependent radiation doses to man from transport of 42 radionuclides are calculated using a very large data base of approximately 69,000 input parameters. The enhanced code and the adjoint equation solver routines were used to generate, in a single run, the adjoint equation matrix (containing approximately 870,000 rows for this problem) and the derivatives of the doses to all 69,000 parameters. The accuracy of the calculations was verified using perturbation analysis for selected parameters.

CONCLUSIONS

Automated sensitivity analysis using the adjoint approach has been shown to be both feasible and practical. A computer system, named ADGEN, has been developed to automatically generate adjoint solutions of FORTRAN computer codes and efficiently calculate all sensitivities of interest in a numerical problem. The system has been tested on several analytical sample problems and its suitability for large-scale applications has been demonstrated on a code involving approximately 6,900 lines of coding and 69,000 input parameters. The results of the demonstration and the run-timing studies confirmed that 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.

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