AUTOMATIC DIFFERENTIATION WITH CODE COUPLING AND APPLICATIONS TO SCALE MODULES

Bradley T. Rearden and James E. Horwedel

Oak Ridge National Laboratory*
P.O. Box 2008, Bldg. 5700
Oak Ridge, TN 37831-6170
reardenb@ornl.gov; horwedelje@ornl.gov

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ABSTRACT

An advanced automatic differentiation tool for Fortran 90 software has been developed at Oak Ridge National Laboratory. This tool, called GRESS 90, has a code coupling feature to propagate derivatives relative to the input of one code through a series of codes that utilize the results of one calculation as the input in the next to determine a final result. GRESS 90 has been applied to the resonance self-shielding codes in SCALE to produce the sensitivities of resonance self-shielded neutron cross sections relative to the data input to the calculation for use in the TSUNAMI sensitivity and uncertainty analysis sequences.

Key Words: Automatic differentiation, code coupling, SCALE, TSUNAMI

1. INTRODUCTION

Sensitivity analysis is a necessary component in the evaluation of computer simulation models. Because computational simulation often involves two or more computer programs run in sequence, the calculation of sensitivities using analytic methods requires a code coupling procedure to propagate sensitivities through the entire code sequence. This summary describes a code coupling methodology used in conjunction with automatic differentiation to develop new versions of existing Fortran 90 programs by adding the capability to calculate sensitivities analytically even when the computational simulation is run as a sequence of computer programs. This methodology was successfully used to differentiate and couple the SCALE [1] modules CENTRM and PMC for application in the Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) sequences.

2. GRESS BACKGROUND INFORMATION

Because programmed equations can be differentiated analytically, sensitivities can be precisely defined and calculated using automatic differentiation [2–6]. Furthermore, when computational simulations are implemented as a sequence of computer codes, the automatic differentiation approach can be extended to automate the calculation of sensitivities for the entire sequence.

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In the 1980s, the Gradient Enhanced Software System (GRESS) [5,6] was developed at Oak Ridge National Laboratory to automate the implementation of sensitivity analysis methods into existing Fortran 77 programs. More recently, GRESS was upgraded to allow processing of Fortran 90 programs. The new version of GRESS is named GRESS 90.

An automated code coupling methodology implemented in GRESS 90 extends the automatic differentiation approach to couple a sequence of computer programs. The code coupling procedure involves writing derivatives calculated in one code to a transfer file, along with information identifying parameters of interest for sensitivity calculations. The next code in the sequence reads the transfer file and initializes derivative information needed to calculate derivatives and sensitivities with respect to parameters identified in the first code.

3. GRESS 90 FORWARD CHAINING OPTION

With details that will be provided in the full paper, the GRESS 90 forward chaining option is utilized to calculate and report sensitivities with respect to a subset of the input data. At any given point during execution, the user can retrieve the total first-order derivatives of a calculated variable with respect to all the declared parameters. The steps used to process a code with GRESS 90 are illustrated in Figure 1.

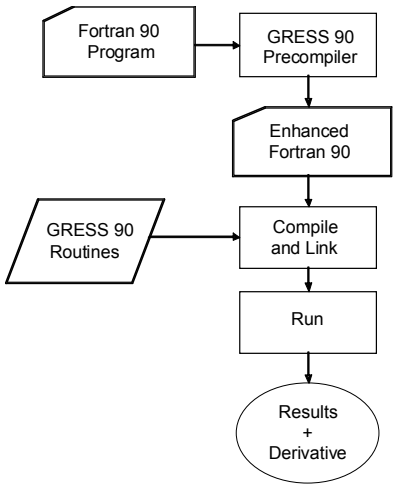

Figure 1. Flowchart showing the processing steps for using GRESS 90.

4. GRESS 90 CODE COUPLING

When a model is implemented as a sequence of computer codes, the code coupling method, illustrated by the flowchart in Figure 2, is used to calculate derivatives with respect to input parameters. For example, assume there are three codes, named A, B, and C, respectively. As shown in Figure 2, both A and B are run first. The input to codes A and B includes sets of parameters of interest, P_A and P_B, respectively. The results from A and B (i.e., R_A and R_B,

respectively) are read as input by code C. The results of interest for derivative calculation, R_C, are output from code C. The independent variables of interest are the inputs P_A and P_B. The derivatives of results from A and B with respect to input parameters can be represented as

$$\frac{d\overline{R_A}}{d\overline{P_A}} \tag{1}$$

and

$$\frac{d\overline{R_B}}{d\overline{P_B}}. \tag{2}$$

Via application of the chain rule, the derivatives of code C with respect to input parameters can be represented as

$$\frac{d\overline{R_C}}{d\overline{P}} = \frac{\partial\overline{R_C}}{\partial\overline{R_A}} \cdot \frac{d\overline{R_A}}{d\overline{P}} + \frac{\partial\overline{R_C}}{\partial\overline{R_B}} \cdot \frac{d\overline{R_B}}{d\overline{P}} + \frac{\partial\overline{R_C}}{\partial\overline{P}}, \tag{3}$$

where $\overline{P} = \overline{P_A} \cup \overline{P_B}$.

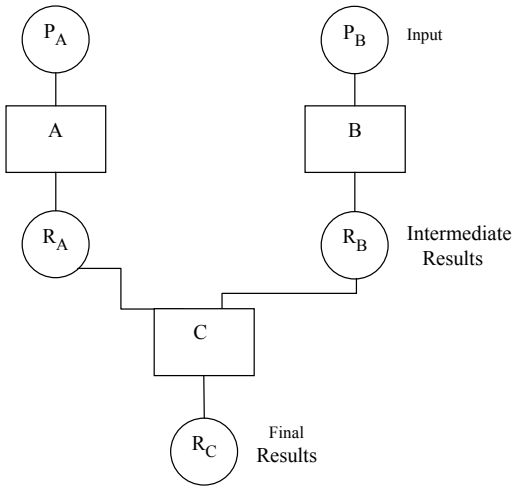

Figure 2. Flowchart illustrating the GRESS 90 code coupling methodology.

The results that are calculated in codes A and B and then read by C are referred to as transfer variables. The parameters of interest from codes A and B are referred to as transfer parameters in C. The user inserts subroutine calls in code C to identify transfer parameters and transfer variables. When code C is executed, derivatives of floating point variables with respect to parameters defined in codes A and B are calculated and may be reported or used for sensitivity calculations.

5. CENTRM AND PMC

Within the SCALE code system, CENTRM and PMC are used in tandem to produce problem-dependent resonance self-shielded multigroup cross sections. CENTRM computes continuous-energy neutron spectra in zero- or one-dimensional systems by solving the Boltzmann Transport Equation using a combination of pointwise and multigroup nuclear data. PMC generates problem-dependent multigroup resonance self-shielded cross sections from an existing AMPX multigroup cross-section library, a pointwise nuclear data library, and a pointwise neutron flux file produced by CENTRM. The continuous-energy solution of CENTRM can accurately model systems with multiple fuel types, overlapping resonances, and Reich-Moore resonance representations. These codes, and the ancillary data formatting code WORKER, were released with SCALE 5.0 in June 2004.

6. PERTURBATION THEORY WITH IMPLICIT COMPONENT

The TSUNAMI sequences of SCALE compute the sensitivity of k_{eff} to each group-wise, nuclide-reaction-specific cross-section data component using adjoint-based, first-order linear perturbation theory. It is important to note that in standard perturbation theory, the sensitivities of k_{eff} are produced relative to the cross sections after the problem-dependent resonance self-shielding calculations have been performed. This is the so-called "explicit" effect.[7] Another first-order sensitivity introduced in thermal and intermediate spectra systems is the "implicit" effect of perturbations in material number densities or nuclear data upon the resonance self-shielded cross sections themselves. For example, a perturbation of the ^{1}H density in a low-enriched uranium system will affect the resonance escape probability in ^{238}U. Thus, the sensitivity of k_{eff} to ^{1}H depends not only on the explicit effect of the ^{1}H but also on the implicit effect of ^{1}H on the ^{238}U cross sections.

7. CENTRMST AND PMCST

To accurately predict the implicit terms from resonance self-shielding calculations performed using CENTRM and PMC, the GRESS 90 system was used to process CENTRM and PMC such that the sensitivities of multigroup resonance self-shielded cross sections output from PMC to the material number densities input to CENTRM could be computed. The sensitivity versions of these codes were named CENTRMST and PMCST. Because the material number densities are input to CENTRMST, and the CENTRMST flux solutions are the input to PMCST, the newly developed GRESS 90 code coupling methodology was used to pass to PMCST the material number densities as independent transfer parameters and the derivatives of the continuous-energy flux solution as a transfer file. When the resonance self-shielding calculation begins in PMCST, the forward chaining of derivatives continues from the values last computed in CENTRMST. The final implicit sensitivities output by PMCST are the sensitivities of the multigroup resonance self-shielded cross sections to the number densities input to CENTRMST. With the addition of these new codes to the TSUNAMI sensitivity analysis sequences, accurate sensitivity coefficients can be generated for systems where resonance self-shielding is important. Several example calculations with and without the implicit contributions will be presented in the full paper.

8. CONCLUSION

The automated GRESS 90 procedure with code coupling was successfully used to add sensitivity capability to SCALE programs CENTRM and PMC. Results demonstrate that the GRESS 90 code coupling methodology can be successfully applied to existing Fortran 90 programs to create new versions of those programs enhanced for sensitivity calculations. Because computational simulations often involve two or more programs run in sequence, the automated code coupling methodology using GRESS 90 is a significant new capability for calculating sensitivities in such simulations.

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