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AUTOMATIC DIFFERENTIATION WITH CODE COUPLING AND APPLICATIONS TO SCALE MODULES

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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

The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) computational sequences within the SCALE [1] code package utilize first-order eigenvalue perturbation theory to predict the response of a system k_{eff} value to changes in each constituent group-wise cross-section-data value. A unique capability of the TSUNAMI sequences is the calculation of the sensitivities of the problem-dependent multigroup resonance self-shielded cross sections due to input parameters to the resonance self-shielding calculation and the propagation of these cross-section sensitivities to the final k_{eff} sensitivities. With the release of the SCALE ENDF/B-VI cross-section-data library in SCALE 5.1, new codes for the calculation of problem-dependent resonance self-shielded cross sections and their derivatives have been developed. The GRESS 90 automatic differentiation system with code coupling was developed and implemented in these codes to produce the required sensitivity coefficients.

2. 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. One may show that the relative change in k due to a small perturbation in a macroscopic cross section, Σ , of the transport operator at some point in phase space \vec{r} can be expressed as [2]

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$$S_{k,\Sigma(\bar{r})} \equiv \frac{\Sigma(\bar{r})}{k} \frac{\partial k}{\partial \Sigma(\bar{r})} = -\frac{\Sigma(\bar{r})}{k} \frac{\left\langle \phi^\dagger(\bar{\xi}) \left(\frac{\partial A[\Sigma(\bar{\xi})]}{\partial \Sigma(\bar{r})} - \frac{1}{k} \frac{\partial B[\Sigma(\bar{\xi})]}{\partial \Sigma(\bar{r})} \right) \phi(\bar{\xi}) \right\rangle}{\left\langle \phi^\dagger(\bar{\xi}) \frac{1}{k^2} B[\Sigma(\bar{\xi})] \phi(\bar{\xi}) \right\rangle}, \quad (1)$$

where ϕ = neutron flux,
 ϕ^\dagger = adjoint neutron flux,
 k = k_{eff} , the largest of the eigenvalues,
 A = operator that represents all of the transport equation except for the fission term,
 B = operator that represents the fission term of the transport equation,
 Σ = problem-dependent resonance self-shielded macroscopic cross sections,
 $\bar{\xi}$ = phase space vector, and
 $\langle \rangle$ indicates integration over space, direction, and energy variables.

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-call ‘‘explicit’’ effect [3]. 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 ^1H density in a low-enriched uranium system will affect the resonance escape probability in ^{238}U . Thus, the sensitivity of k_{eff} to ^1H depends not only on the explicit effect of the ^1H on the operators in Eq. (1) but also on the implicit effect of ^1H on the self-shielded ^{238}U cross sections.

The implicit portion of the sensitivity coefficient, the sensitivity of the group-wise data to the input quantities, is defined as [4]

$$S_{\Sigma_{x,g},\omega_i} = \frac{\partial \Sigma_{x,g} / \Sigma_{x,g}}{\partial \omega_i / \omega_i}, \quad (2)$$

where ω_i is some input quantity. The ω_i term could represent the number density of a particular material, a certain nuclear data component, or a physical dimension of a system. If ω_i is a certain cross-section data component for process y of nuclide j in energy group h expressed as $\Sigma_{y,h}^j$, which is sensitive to perturbations in process x in energy group g for nuclide i expressed as $\Sigma_{x,g}^i$, the complete sensitivity of k_{eff} due to the explicit and implicit contributions of $\Sigma_{x,g}^i$ can be defined using the chain rule for derivatives as

$$\left(S_{k,\Sigma_{x,g}^i} \right)_{\text{complete}} = \frac{dk/k}{d\Sigma_{x,g}^i / \Sigma_{x,g}^i} = \frac{\partial k/k}{\partial \Sigma_{x,g}^i / \Sigma_{x,g}^i} + \sum_j \sum_h \frac{\partial k/k}{\partial \Sigma_{y,h}^j / \Sigma_{y,h}^j} \times \frac{\partial \Sigma_{y,h}^j / \Sigma_{y,h}^j}{\partial \Sigma_{x,g}^i / \Sigma_{x,g}^i}. \quad (3)$$

3. 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.

To properly implement the implicit sensitivity theory into the SCALE 5.1 code package, it was necessary to obtain the sensitivity of the resonance self-shielded cross sections generated from PMC to data input to the CENTRM calculation. The methodology chosen to perform these tasks was to produce an advanced automatic differentiation tool with a code-coupling feature such that the sensitivities generated in the CENTRM calculation could be properly reflected in the PMC results.

4. GRESS BACKGROUND INFORMATION

Because programmed equations can be differentiated analytically, sensitivities can be precisely defined and calculated using automatic differentiation [5–9]. Furthermore, when computational simulations are implemented as a sequence of computer codes, the automatic differentiation approach can be extended to enable the calculation of sensitivities for the entire sequence.

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 some Fortran 90 features. 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.

5. GRESS 90 FORWARD CHAINING OPTION

In a Fortran program, calculated left-hand-side variables are a function of previously defined left-hand-side variables and data, with assignments made either through mathematical operations or read statements. This relationship can be expressed as

$$\bar{y} \leftarrow \tilde{f}(\bar{y}), \quad (4)$$

where the symbol \leftarrow indicates a value assignment (i.e., store) operation. The components of the column vector, \bar{y} , are all the terms on the left hand side of real number replacement statements. The column vector, \tilde{f} , represents the right-hand-side mathematical operations. The vector, \bar{y} , includes both calculated results and input data. Read statements are treated in the same manner as setting a variable equal to a constant.

In a Fortran program, a symbol cannot explicitly depend on itself. When a Fortran variable is redefined, mathematically, it is not the same variable. In the statement $X \leftarrow X + 5.0$, the X on the left and the X on the right represent two different locations in the solution vector, \bar{y} .

Mathematically, the equation can be thought of as $X_2 = X_1 + 5.0$. Therefore to represent Eq. (4) mathematically, the dependence of a variable on itself must be considered explicitly. If we define

$$\frac{dy_i}{dy_i} = 1, \text{ for all } i, \quad (5)$$

then Eq. (1) can be rewritten as

$$\bar{y} = \tilde{f}(\bar{y}). \quad (6)$$

Differentiating Eq. (3) with respect to \bar{y} yields

$$\frac{d\bar{y}}{d\bar{y}} = \frac{d\tilde{f}}{d\bar{y}} \cdot \frac{d\bar{y}}{d\bar{y}} + I, \quad (7)$$

where the identity matrix, I , provides the explicit dependence of a variable on itself necessary to make Eq. (7) meaningful. Equation (7) can be rearranged such that

$$\left[I - \frac{d\tilde{f}}{d\bar{y}} \right] \cdot \frac{d\bar{y}}{d\bar{y}} = I. \quad (8)$$

Equation (8) can be represented in a more compact form as

$$AY' = I, \quad (9)$$

where

$$A = \left[I - \frac{d\tilde{f}}{d\bar{y}} \right]$$

and

$$Y' = \frac{d\bar{y}}{d\bar{y}}.$$

Because Fortran equations are solved in a sequential fashion, Fortran variables are dependent on previously defined variables. Therefore,

$$\frac{\partial f_i}{\partial y_j} = 0, \text{ for } j \geq i,$$

such that the matrix, $\frac{d\bar{f}}{d\bar{y}}$, is a lower triangular matrix with zeros on and above the diagonal. This matrix can easily be solved by application of the chain rule of calculus as each row is determined.

The GRESS 90 forward chaining option is utilized to calculate and report sensitivities with respect to a subset of the input data. The method used is to resolve Eq. (9) for selected columns in the matrix, Y' , by forward substitution in memory as each Fortran statement is executed. A fully resolved column in Y' represents the derivatives of every real variable with respect to the user-selected variable or parameter associated with that column. Because selected columns in Y' are resolved by forward substitution in memory, the A matrix is never saved. 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.

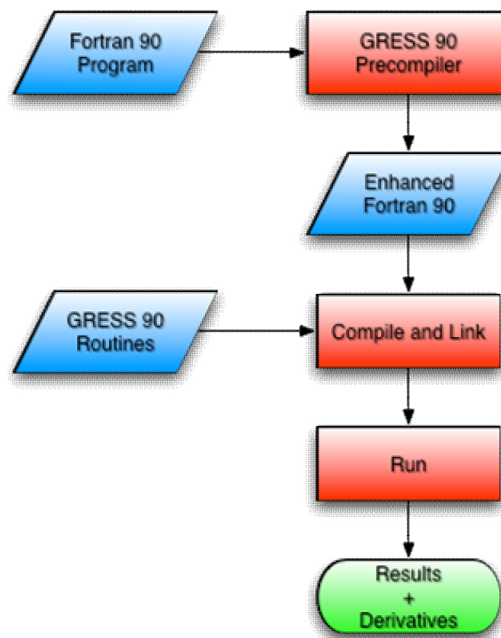


Figure 1. Flowchart showing the processing steps for using GRESS 90.

6. 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 independent of each other and are run first. The input to codes A and B includes sets of parameters of interest, P_A and P_B , respectively. The input to code C includes any new input parameters, P_C , as well as the results from A and B, R_A and R_B , respectively. The results of interest for derivative calculation, R_C , are output from code C. The independent variables of interest are the inputs P_A , P_B and P_C .

The derivatives of results from A and B with respect to input parameters can be represented as

$$\frac{d\bar{R}_A}{dP_A} \quad (10)$$

and

$$\frac{d\bar{R}_B}{dP_B}. \quad (11)$$

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

$$\frac{d\bar{R}_C}{dP} = \frac{\partial\bar{R}_C}{\partial P_A} + \frac{\partial\bar{R}_C}{\partial P_B} + \frac{\partial\bar{R}_C}{\partial P_C} = \frac{\partial\bar{R}_C}{\partial R_A} \cdot \frac{d\bar{R}_A}{dP_A} + \frac{\partial\bar{R}_C}{\partial R_B} \cdot \frac{d\bar{R}_B}{dP_B} + \frac{\partial\bar{R}_C}{\partial P_C}. \quad (12)$$

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, B, and C are calculated and may be reported or used for sensitivity calculations.

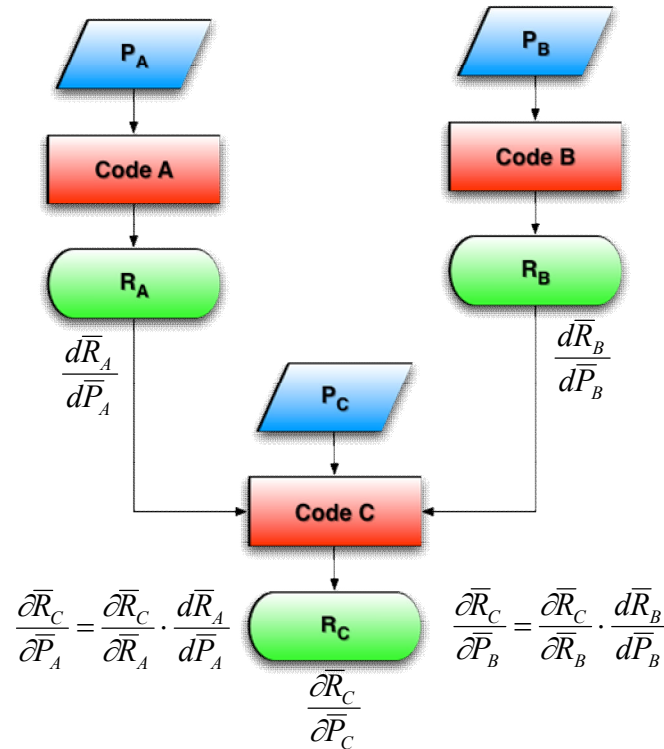


Figure 2. Flowchart illustrating the GRESS 90 code-coupling methodology.

7. CENTRMST AND PMCST

In order to accurately predict the implicit terms defined in Eq. (2) 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 flux derivatives with respect to each nuclide are computed for each energy point in the CENTRM solution mash, typically 50,000-70,000 points. The sensitivity versions of these codes were named CENTRMST and PMCST. Since the material number densities are input to CENTRMST and the CENTRMST flux solutions are 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. It is noted that the CENTRMST solution terminated based on convergence of the flux solution. The convergence of the sensitivities is not explicitly verified.

8. IMPLEMENTATION AND TESTING

The SAMS module of SCALE implements perturbation theory to compute the explicit sensitivity terms and processes the implicit sensitivities output by PMCST to produce the complete sensitivity, as shown in Eq. (3). SAMS is executed as part of the TSUNAMI-1D or TSUNAMI-3D SCALE sequences. TSUNAMI-1D utilizes the one-dimensional discrete ordinates code XSDRNPM for its forward and adjoint flux solutions, where TSUNAMI-3D utilizes the Monte Carlo code KENO V.a. Several sample problems were selected, and the integral sensitivity coefficients were compared to direct perturbation sensitivity values. The direct perturbation values were generated by running several k_{eff} calculations with varied number densities and computing a sensitivity coefficient through central differencing.

The test problems selected for testing the accuracy of the final sensitivity coefficients were critical experiments selected from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [10] and are identified as follows:

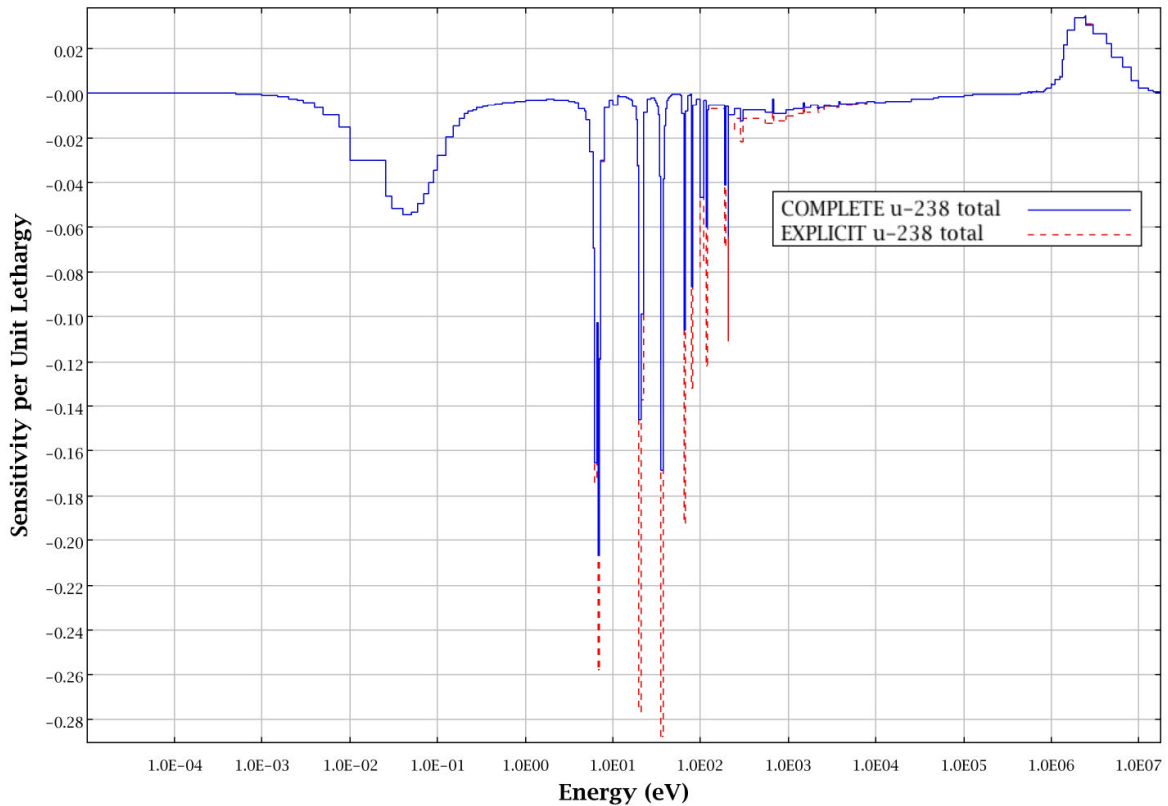
1. LEU-COMP-THERM-033 Case 1 - A TSUNAMI-1D spherical model of well-moderated homogeneous mixture of $\text{U}(2)\text{F}_4$ and paraffin.
2. HEU-MET-FAST-028 – A TSUNAMI-1D spherical model of the Flattop experiment, which consists of a highly enriched uranium core surrounded by a natural uranium reflector.
3. LEU-COMP-THERM-009 Case 10 – A TSUNAMI-3D model of a water-moderated rectangular cluster of $\text{U}(4.31)\text{O}_2$ fuel rods separated by copper plates.

The test problems were all run with the SCALE 238-group ENDF/B-VI cross section data library. The results of the direct perturbation calculations and the explicit and complete sensitivities computed by TSUNAMI using CENTRMST and PMCST are shown in Table I. Note that the TSUNAMI complete sensitivity results agree quite well with the direct perturbation results for all cases. The complete sensitivity values for LEU-COMP-THERM-009 Case 10 match the direct perturbation results within one standard deviation. The TSUNAMI explicit sensitivities, which neglect the contributions of the implicit effect computed by CENTRMST and PMCST, differ from the direct perturbation results by up to 19% for ^{238}U in LEU-COMP-THERM-033 Case 1. For the fast spectrum HEU-MET-FAST-028 system, where resonance self-shielding is insignificant, the effect of the implicit sensitivity calculation is, as expected, negligible.

The effect of the implicit sensitivity computed with CENTRMST and PMCST is further revealed in Fig. 3, where the energy-dependent sensitivity profiles for the sensitivity of k_{eff} to ^{238}U total cross section are shown for the explicit and complete sensitivity calculation. The effect of the resonance self-shielding calculation on the resonance-energy sensitivity coefficients is clearly visible in the difference between these two profiles.

Table I. Comparison of sensitivity results

Test problem	Nuclide	Direct perturbation sensitivity	TSUNAMI explicit sensitivity	TSUNAMI complete sensitivity
LEU-COMP-THERM-033 Case 1	^1H	2.2076E-01	2.5154E-01	2.2091E-01
	^{238}U	-2.0619E-01	-2.4509E-01	-2.0718E-01
HEU-MET-FAST-028	^{235}U in core	5.8050E-01	5.7952E-01	5.7952E-01
	^{238}U in reflector	2.1305E-01	2.1648E-01	2.1654E-01
LEU-COMP-THERM-009 Case 10	^1H Mix 2	2.14E-01 \pm 4.10E-02	2.01E-01 \pm 1.46E-02	2.00E-01 \pm 1.46E-02
	^{238}U	-6.38E-02 \pm 4.10E-03	-7.07E-01 \pm 3.42E-04	-6.24E-01 \pm 4.31E-04

**Figure 3. Energy-dependent explicit and complete sensitivity profiles for ^{238}U total cross section from LEU-COMP-THERM-033 Case 1.**

9. CONCLUSION

The automated GRESS 90 procedure with code coupling was successfully used to add sensitivity capability to SCALE self-shielding 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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