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Bradley T. Rearden and James E. Horwedel

Oak Ridge National Laboratory[*]
P.O. Box 2008, Bldg. 5700
Oak Ridge, TN 37831-6170 USA
Telephone: (865) 574-6085
Fax: (865) 576-3513
E-mail: reardenb@ornl.gov

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

INTRODUCTION

The Tools for Sensitivity and UNcertainty Analysis Methodology Implementation (TSUNAMI) [1,2] computational sequences within the SCALE [3] code package use 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 system with code coupling, discussed in the companion paper [4], was used to develop sensitivity versions of the CENTRM [5] and PMC [6] codes called CENTRMST and PMCST, respectively.

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 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.

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.

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

$$S_{k,\Sigma(\vec{r})} \equiv \frac{\Sigma(\vec{r})}{k}\frac{\partial k}{\partial \Sigma(\vec{r})}$$

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

where ϕ = neutron flux;

$\phi^{\dagger}$ = 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-shield macroscopic cross sections;

$\vec{\xi}$ = phase space vector; and

$\langle\ \rangle$ indicate integration over space, direction and energy variables. [7]

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.[8] 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 on the operators in Eq. (1), but also on the implicit effect of ^{1}H on the ^{238}U cross sections.

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

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

where ω_i is some input quantity. [9] 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 $\Sigma^j_{y,h}$, which is sensitive to perturbations in process x in energy group g for nuclide i expressed as $\Sigma^i_{x,g}$, the complete sensitivity of k_{eff} due to explicit and implicit contributions of $\Sigma^i_{x,g}$ can be defined using the chain rule for derivatives as

$$\left(S_{k,\Sigma^i_{x,g}}\right)_{complete} = \frac{\Sigma^i_{x,g}}{k} \frac{dk}{d\Sigma^i_{x,g}}$$

$$= \frac{\Sigma^i_{x,g}}{k} \frac{\partial k}{\partial \Sigma^i_{x,g}} + \sum_j \sum_h \frac{\Sigma^j_{y,h}}{k} \frac{\partial k}{\partial \Sigma^j_{y,h}} \times \frac{\Sigma^i_{x,g}}{\Sigma^j_{y,h}} \frac{\partial \Sigma^j_{y,h}}{\partial \Sigma^i_{x,g}}. \qquad (3)$$

CENTRMST AND PMCST

To accurately predict the implicit terms defined in Eq. (2) from resonance self-shielding calculations performed using CENTRM and PMC, the GRESS 90 system described in the companion paper [4] 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.

IMPLEMENTATION AND TESTING

The Sensitivity Analysis Module of SCALE (SAMS) [10] 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 uses the one-dimensional discrete ordinates code XSDRNPM for its forward and adjoint flux solutions, whereas TSUNAMI-3D uses 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* [11] and are identified as follows:

1. LEU-COMP-THERM-033 Case 1 – A TSUNAMI-1D spherical model of well-moderated homogeneous mixture of $U(2)F_4$ 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 $U(4.31)O_2$ 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 CENTMST 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, in which 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 PMSCT is further revealed in Fig. 1, in which the energy-dependent sensitivity profiles for the

TABLE I. Comparison of Sensitivity Results

Test Problem	Nuclide	Direct Perturbation Sensitivity	TSUNAMI Explicit Sensitivity	TSUNAMI Complete Sensitivity
LEU-COMP-THERM-033 Case 1	^{1}H	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 ref.	2.1305E-01	2.1648E-01	2.1654E-01
LEU-COMP-THERM-009 Case 10	^{1}H Mix 2	2.14E-01 ± 4.10E-02	2.01E-01 ± 1.46E-02	2.00E-01 ± 1.46E-02
	^{238}U	-6.38E-02 ± 4.10E-03	-7.07E-02 ± 3.42E-04	-6.24E-02 ± 4.31E-04

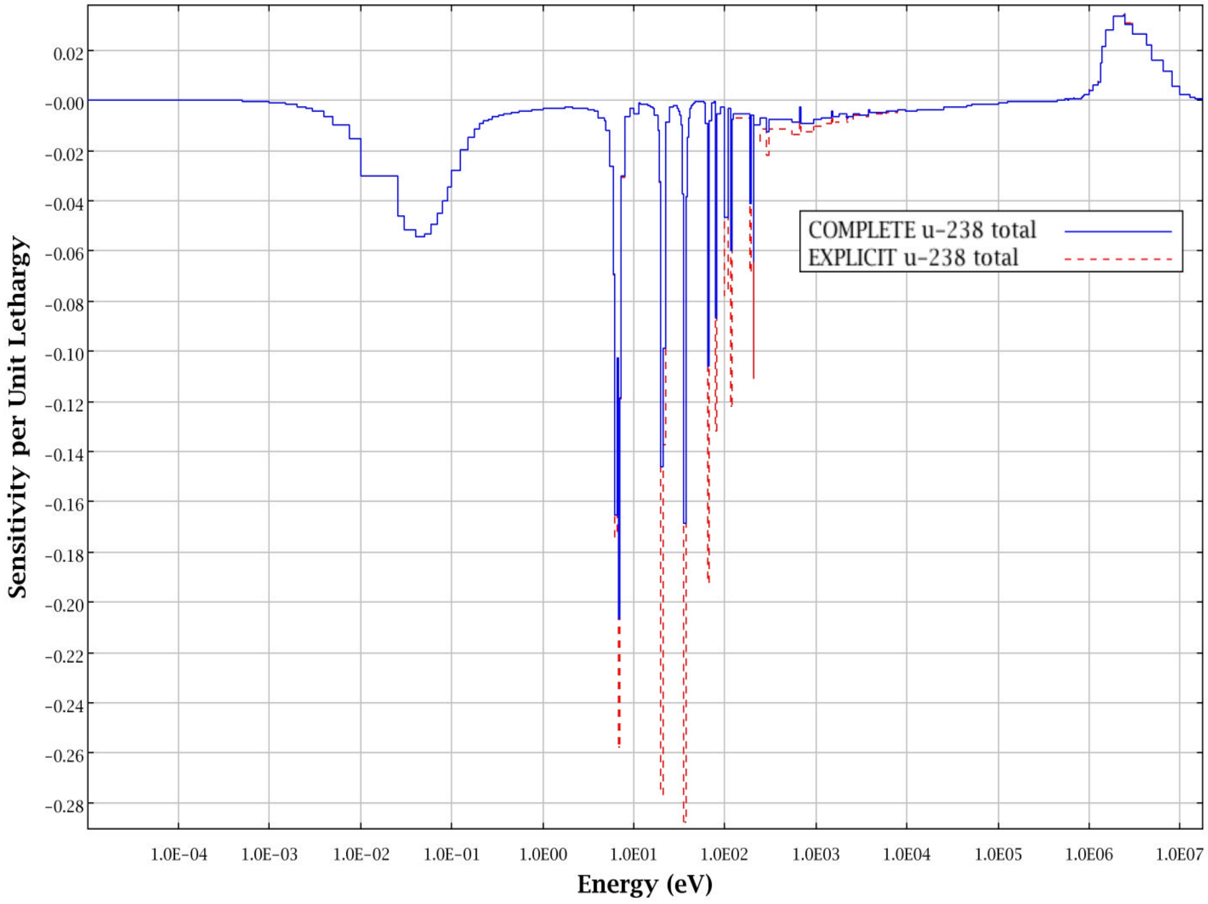

Fig. 1. Energy-dependent explicit and complete sensitivity profiles for ^{238}U total cross section from LEU-COMP-THERM-033 Case 1.

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 sensitivity coefficients is clearly visible in the difference between these two profiles.

CONCLUSIONS

The usefulness and accuracy of the GRESS 90 system with code coupling has been demonstrated through its application to CENTRM and PMC. The complete sensitivity results, including the CENTRMST and PMCST implicit sensitivity coefficients, have been verified through comparison with direct perturbation calculations. The addition of CENTRMST and PMCST to the TSUNAMI software of SCALE provides powerful new capabilities for determining accurate eigenvalue sensitivity coefficients.

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