SCALE-6 Sensitivity/Uncertainty Methods and Covariance Data

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Computational methods and data used for sensitivity and uncertainty analysis within the SCALE nuclear analysis code system are presented. The methodology used to calculate sensitivity coefficients and similarity coefficients and to perform nuclear data adjustment is discussed. A description is provided of the SCALE-6 covariance library based on ENDF/B-VII and other nuclear data evaluations, supplemented by "low-fidelity" approximate covariances.

I. Introduction

SCALE (Standardized Computer Analyses for Licensing Evaluation) [1] is a modular code system developed by Oak Ridge National Laboratory (ORNL) to perform calculations for criticality safety, reactor physics, and radiation shielding applications. SCALE calculations typically use sequences that execute a predefined series of executable modules to compute particle fluxes and responses like the critical multiplication factor. SCALE also includes modules for sensitivity and uncertainty (S/U) analysis of calculated responses. The S/U codes in SCALE are collectively referred to as TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation).[2] SCALE-6—scheduled for release in 2008—contains significant new capabilities, including important enhancements in S/U methods and data.

The main functions of TSUNAMI are to (a) compute nuclear data sensitivity coefficients and response uncertainties, (b) establish similarity between benchmark experiments and design applications, and (c) reduce uncertainty in calculated responses by consolidating integral benchmark experiments. TSUNAMI includes easy-to-use graphical user interfaces for defining problem input and viewing three-dimensional (3D) geometries, as well as an integrated plotting package.

II. Overview of TSUNAMI Modules

TSUNAMI-1D, -2D, and -3D are SCALE sequences that execute modules to determine response sensitivities and uncertainties. The linked computations are completely automated and perform: (a) cross section self-shielding operations, (b) forward and adjoint transport calculations, (c) computation of sensitivity coefficients, and (d) calculation of the response uncertainty. The computation methodology is described in Section III.

TSUNAMI-IP is a utility module that determines the neutronic similarity of two or more systems, as described in section IV.

TSAR (Tool for Sensitivity Analysis of Reactivity) is a module that computes sensitivity coefficients for reactivity responses.

TSURFER (Tool for S/U analysis of Response Functionals using Experimental Results) is a module that uses the method of generalized linear least squares for nuclear data adjustment in a variety of applications. These are discussed in section V.

III. Computational Methodology

Evaluated data from ENDF/B are processed into continuous-energy nuclear data, indicated as $x_r^{(j)}(E)$ for nuclide *j* and reaction *r*. Continuous-energy data are averaged with a specified smooth weighting function *W*(*E*) into *generic* multigroup (MG) data. Using bracket notation to indicate an inner product over the energy interval for group g, the generic MG value is

$$\alpha_{r,g}^{(j)} = \frac{\left\langle x_r^{(j)}(E)W(E)\right\rangle}{\left\langle W(E)\right\rangle} \quad . \tag{1}$$

For example in the resonance range, $W(E) \rightarrow 1/E$, thus Eq. (1) corresponds to an infinitely-dilute MG cross section.

Changes associated with uncertainties in evaluated data cause the processed data to vary by an amount $\Delta x_r^{(j)}(E)$, and this propagates to changes in the generic MG value:

$$\Delta\alpha_{r,g}^{(j)} = \left\langle \frac{\partial \alpha_{g,r}^{(j)}}{\partial x_r^{(j)}(E)} \Delta x_r^{(j)}(E) \right\rangle = \frac{\left\langle W(E)\Delta x_r^{(j)}(E)\right\rangle}{\left\langle W(E)\right\rangle} \quad . \tag{2}$$

Before performing MG transport calculations, self-shielding calculations convert generic MG values into *problem-specific* MG data, designated as $\sigma_{r,g}^{(j)}$. Unlike generic values, the problem-specific data are weighted with an energy spectrum representative of the neutron environment for the particular application of interest:

$$\sigma_{r,g}^{(j)} = \frac{\left\langle x_r^{(j)}(E)\phi_W(E)\right\rangle}{\left\langle \phi_W(E)\right\rangle} \quad , \tag{3}$$

where ϕ_W approximates the problem-specific flux spectrum which in general exhibits the spectral fine-structure responsible for resonance self-shielding effects. The flux, and thus $\sigma_{r,g}^{(j)}$, is affected by the concentration and nuclear data of *j* as well as other materials present, indicated by primed index *j*' : $\sigma_{r,g}^{(j)} \Rightarrow \sigma_{r,g}^{(j)}[x_r^{(j)}(E)\,;\; x_{r'}^{(j')}(E)]$.

The change in $\sigma_{r,g}^{(j)}$ due to variations in evaluated data of all materials in the system is expressed to first order accuracy by

$$\Delta\sigma_{r,g}^{(j)} = \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial x_{r'}^{(j')}} \Delta x_r^{(j)}(E) \right\rangle + \sum_{j',r'} \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial\phi_w} \frac{\partial\phi_w}{\partial x_{r'}^{(j')}} \Delta x_{r'}^{(j')}(E) \right\rangle \quad . \quad (4)$$

We approximate the changes in processed evaluated data, $\Delta x_r^{(j)}(E)$, by the weighted averaged given in Eq. (2); that is

$$\Delta x_r^{(j)}(E) \rightarrow \Delta\alpha_{r,g}^{(j)} \quad , \quad (5)$$

so that Eq. (4) can be expressed

$$\Delta\sigma_{r,g}^{(j)} = \Delta\alpha_{r,g}^{(j)} + \sum_{j',r'} S_{\sigma_{r,g}^{(j)};\,\alpha_{r'g}^{(j')}} \Delta\alpha_{r'g}^{(j')} \quad . \quad (6)$$

In Eq. (6) we have defined a sensitivity coefficient relating changes in self-shielded data to changes in processed data that alter the generic cross section as shown in Eq. (5):

$$S_{\sigma_{r,g}^{(j)},\alpha_{r',g}^{(j')}} = \sum_{j',r'} \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial\phi_W(E)} \frac{\partial\phi_W(E)}{\partial x_{r'}^{(j')}(E)} \right\rangle \quad . \quad (7)$$

A. Explicit response sensitivities

Assume that the functional k(Φ) is some response calculated using SCALE. The *explicit* sensitivity coefficient of response k with respect to a problem-specific (self-shielded) data parameter $\sigma_{r,g}^{(j)}$ appearing in the transport calculation is defined as

$$\mathrm{S}_{\mathrm{k},\sigma_{\mathrm{r,g}}^{(\mathrm{j})}}^{[\exp]} = \frac{\partial \mathrm{k}}{\partial\sigma_{\mathrm{r,g}}^{(\mathrm{j})}} \Delta\sigma_{\mathrm{r,g}}^{(\mathrm{j})} \quad . \quad (8)$$

The response change due to changes in problem-specific MG data is computed to first-order accuracy from the expression

$$\Delta\mathrm{k} = \sum_{\mathrm{g}} \sum_{\mathrm{j,r}} \mathrm{S}_{\mathrm{k},\sigma_{\mathrm{r,g}}^{(\mathrm{j})}}^{[\exp]} \Delta\sigma_{\mathrm{r,g}}^{(\mathrm{j})} \quad . \quad (9)$$

TSUNAMI uses first order perturbation theory to compute explicit sensitivity coefficients. For a given response, perturbation theory only requires a single forward and adjoint transport calculation to determine sensitivities for all nuclear data; thus, $\mathrm{S}_{\mathrm{k}}^{[\exp]}(\mathrm{x}) \rightarrow \mathrm{S}_{\mathrm{k}}^{[\exp]}[\Phi,\Phi^*]$, where Φ and Φ* are solutions of the forward and adjoint MG transport equations, respectively[3]. TSUNAMI has three techniques to compute Φ and Φ* using SCALE transport modules. TSUNAMI-3D uses the MG Monte Carlo code KENO, TSUNAMI-2D uses the NEWT two-dimensional transport code based on the short characteristics method for arbitrary geometry, and TSUNAMI-1D uses one-dimensional discrete ordinates code XSDRNPM.

B. Implicit and complete response sensitivities

It is also useful to relate the response perturbations to changes in *generic* MG data as these are directly related to changes in the processed evaluated data. Substituting Eq. (6) into Eq. (9) and rearranging the order of summations gives

$$\Delta k = \sum_g \sum_{j,r} \left\{ S_{k,\sigma_{r,g}^{(j)}} + \sum_{j',r'} S_{k,\sigma_{r',g}^{(j')}} S_{\sigma_{r',g}^{(j')};\,\alpha_{r,g}^{(j)}} \right\} \Delta\alpha_{r,g}^{(j)} \quad . \quad (10)$$

The second term in brackets in Eq. (1.10) accounts for the fact that changes in one cross section may affect other problem-specific MG cross sections via self-shielding perturbations, and the latter data variations cause additional response changes. Thus the second term is designated as the "implicit sensitivity coefficient." [4] The entire expression contained in brackets is called the "complete sensitivity coefficient," so that

$$S_{k,\alpha_{r,g}^{(j)}}^{[com]} = S_{k,\alpha_{r,g}^{(j)}}^{[\exp]} + S_{k,\alpha_{r,g}^{(j)}}^{[imp]} \quad , \quad \text{and}$$

$$\Delta k = \sum_g \sum_{j,r} S_{k,\sigma_{r,g}^{(j)}}^{[com]} \Delta\alpha_{r,g}^{(j)} \quad . \quad (11)$$

TSUNAMI uses modified versions of the SCALE self-shielding codes to evaluate the expression in Eq. (7) and computes the implicit and complete sensitivities.[5]

TSUNAMI is the only S/U code system that provides complete sensitivities rather than just the explicit component. Figure 1 shows explicit and complete profiles for the sensitivity of the multiplication factor of a low-enriched hydrogen-moderator critical experiment to the hydrogen elastic cross section. Due to the impact on the self-shielding, the complete sensitivity coefficient of H is substantially lower than the explicit sensitivity for energy groups containing ^{238}U resonances. Hence implicit effects are significant for this case.

C. Response uncertainty

One of the main functions of TSUNAMI is to compute the response uncertainty, defined as the square root of the variance,

Var(k) = E(Δk^2), where E represents the expectation operator. Substituting Eq. (11) into this expression and then expanding the product of summations gives

$$Var(k) = \sum_{g,g'} \sum_{j,j';r,r'} S_{k,\sigma_{r',g'}^{(j')}}^{[com]} Cov(\alpha_{r',g'}^{(j')};\alpha_{r,g}^{(j)})\, S_{k,\sigma_{r,g}^{(j)}}^{[com]} \quad . \quad (12)$$

The covariance in the above equation is defined as

$$Cov(\alpha_{r',g'}^{(j')};\alpha_{r,g}^{(j)}) = E(\Delta\alpha_{r',g'}^{(j')};\Delta\alpha_{r,g}^{(j)}) \quad . \quad (13)$$

Eq. (12) shows that the response variance can be related to the covariance of *generic* MG data by using *complete* sensitivity coefficients. This is significant because uncertainties in the generic MG values depend only on the uncertainties in evaluated data, which have been processed by PUFF into a general covariance library for TSUNAMI applications.[6] The SCALE-6 covariance library is discussed in Section V.

IV Similarity Analysis and Data Adjustment

Another important application of TSUNAMI is for determining the neutronic similarity of two systems. Systems with similar sensitivities to nuclear data uncertainties are expected to be computed to comparable accuracy. Hence for validation studies, it is desirable to select benchmark experiments that are most similar to the desired application. [7] Similarity considerations are also important in designing new integral experiments for testing specific data.

The TSUNAMI-IP module provides techniques to quantify the similarity of two systems, based on several alternative "similarity" parameters. For example, c_k represents the correlation coefficient between two systems, arising from shared nuclear data uncertainties as defined by the covariance information.[7] The value of c_k typically ranges from 0, indicating negligible similarity, to a value of 1, indicating nearly identically systems. Figure 2 shows sensitivity profiles and c_k values for ^{239}Pu fission in two critical benchmark experiments and a hypothetical application. The experiment with $c_k = 0.93$ is more appropriate for validation of this application.

Covariance data are also used in the TSURFER module for generalized linear least squares (GLLS) adjustment. The GLLS procedure provides a consistent approach for "consolidating" integral benchmark measurements with calculated results to improve the final estimates for the response values. The original integral measurements and the MG nuclear data are both adjusted, consistent with data uncertainties and correlations, so that the most self-consistent set of integral and MG data is obtained. GLLS forces the adjusted calculated and measured responses to agree while constraining the data variations to minimize a generalized chi-squared parameter. The resulting nuclear data adjustments can provide guidance to evaluators interested in improving the differential data.

The experiment/calculation consolidation reduces prior uncertainties in the computed responses because additional information is incorporated. The same procedure can also be applied to "passive" responses for which no experimental measurements exist (e.g., design applications). In this case the prior calculated value of the application response is adjusted indirectly due to data adjustments inferred from the GLLS consolidation of experimental responses.

ORNL has a database of pre-calculated sensitivity profiles for several hundred critical benchmark experiments specified in the ICSBEP Handbook.[8] These sensitivities may be input to TSURFER, along with calculated sensitivities for one or more application systems, to determine an updated estimate for the application responses and uncertainty and an estimate of the original computational bias. TSURFER has the capability to filter the set of experiments so that only the responses that meet a desired similarity criterion with the application are used in the GLLS adjustment. A consistency filter may also be applied to identify and eliminate inconsistent experiments in order to obtain a target chi-squared value.

Reference [9] from this workshop shows an example of TSUNAMI-IP and TSURFER applications.

V. SCALE-6 Covariance Library

The S/U applications described in preceding sections require reasonable estimates for nuclear data uncertainties. Historically the lack of sufficient covariance information in nuclear data files such as ENDF/B has limited the use of available S/U computation tools like TSUNAMI.

Nevertheless, S/U analysis has proceeded in some cases even under this impairment. Omitted uncertainty data are treated effectively as having zero uncertainty, causing the calculated uncertainty in integral responses to be underestimated. This deficiency is sometimes acceptable, with the recognition that the computed uncertainty represents a lower bound. A more serious problem may occur in applications of GLLS adjustment tools like TSURFER. If a response is sensitive to some nuclide/reaction with no available covariance information, then the GLLS calculation may adjust other data to compensate for the effect of the omitted information. This can lead to nonphysical data modifications. In some instances the omitted covariance data cause an inconsistency manifested as an excessive chi-square value, but this is not always the case. To circumvent these problems, both TSURFER and TSUNAM-IP modules have options to input values for missing covariances. While this approach provides more flexibility, the user is still confronted with the question of what uncertainty values to use.

Based on the assumption that a crude uncertainty value is preferable to the zero value implied by omission, an applications-oriented covariance library has been created using a variety of sources and approximations for all materials in the SCALE cross section libraries. Available ENDF/B-VII covariances (including completed pre-released evaluations) are used for 16 materials.[10] Evaluated covariances from ENDF/B-VI and JENDL are used for 34 materials. If no evaluated uncertainty files are available for a material (which is the majority of cases), then approximate covariance matrices are constructed. Before the release of SCALE-6, uncertainty data for the thermal and epithermal ranges were generated using the "integral approximation" as follows [11]: (a) uncertainties in integral measurements of capture, fission, and elastic thermal cross sections are applied uniformly with full energy correlation in the range below 0.5 eV; (b) relative uncertainties in measured capture and fission resonance integrals and in the elastic potential cross section are applied uniformly with full energy correlation in the range 0.5 eV–5.5 keV.

SCALE-6 will include a more complete set of approximate uncertainties, the result of a collaborative effort between Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), and ORNL to produce "low fidelity" (lo-fi) covariances spanning the full energy range. The lo-fi data consist of ORNL covariances based on the integral approximation in the thermal and epithermal ranges, combined with approximate uncertainties generated by BNL[12] and LANL in the high energy range above 5.5 keV. The high energy covariance data were generated with nuclear model codes and include uncertainties for inelastic, (n,2n), capture, fission, and elastic reactions. In addition to lo-fi covariances, LANL has provided full range "high fidelity" evaluations for elements lighter than fluorine. This is a significant benefit for addressing moderator materials. Details about the lo-fi covariance project can be found in the paper by Little, et al. in this workshop.[13] Table I summarizes the sources of covariance data in the SCALE-6 covariance library.

TABLE I: Sources of covariance data in the SCALE-6 covariance library.

Source	Materials
ENDF/B-VII	$Gd^{152-158,160}$ Th^{232} Tc^{99} $Ir^{191,193}$
(Pre-release) ENDF/B-VII	$U^{233,235,238}$ Pu^{239}
ENDF/B-VI	Na^{23} Si^{28-29} Sc^{45} V^{51} $Cr^{50,52-54}$ Mn^{55} $Fe^{54,56-58}$ $Ni^{58,60-62,64}$ $Cu^{63,65}$ Y^{89} Nb^{93} $In^{(nat)}$ $Re^{185,187}$ Au^{197} $Pb^{206-208}$ B^{209} Am^{241}
JENDL	$Pu^{240-241}$
LANL Hi-Fi	H^{1-3} He^{3-4} Li^{6-7} Be^{9} B^{10-11} C^{12} N^{14-15} O^{16-17} F^{19}
Lo-Fi	~ 200 materials (mostly fission products and minor actinides)

Figures 3 and 4 show examples of covariance data in the SCALE-6 library. Figure 3 is a high fidelity ENDF/B-VII evaluation for ^{233}U, while Fig. 4 shows lo-fi covariances for several fission products.

VI. Summary

The sixth version of the SCALE nuclear analysis code system will be released during 2008. SCALE-6 has several new computation modules that supplement the current S/U capabilities of TSUNAMI. Complete sensitivity coefficients that account for implicit effects due to perturbations in resonance self-shielding can be calculated using several available transport options, including 3D Monte Carlo. The complete sensitivities allow generic covariance data to be propagated to uncertainties in calculated responses such as eigenvalues and reactivity coefficients. Modules for similarity analysis and data adjustment also are available. A library of full energy range covariances based on a combination of high-fidelity evaluations and approximate representations will be distributed with SCALE-6. The library contains uncertainty information for 277 materials, and is the first comprehensive set of nuclear data covariances generally available for S/U applications.

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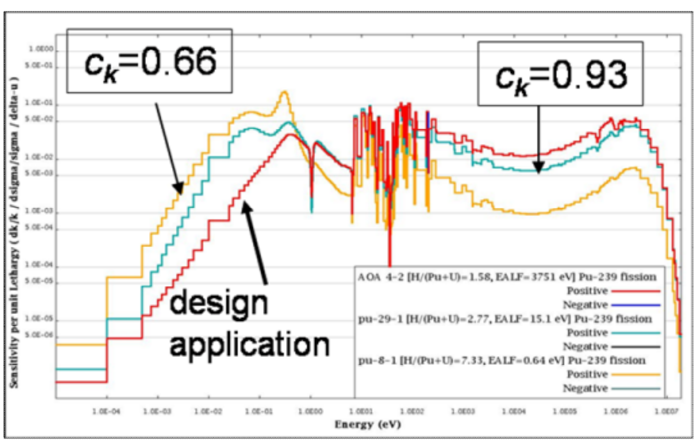

FIG. 2: Correlation coefficients (c_k) between benchmark experiments and application system.

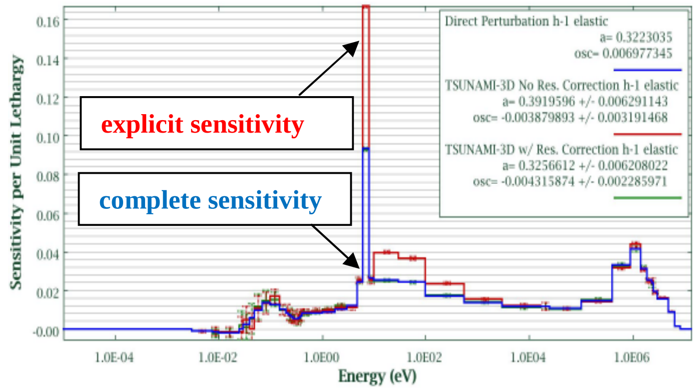

FIG. 1: Explicit and complete sensitivity coefficients.

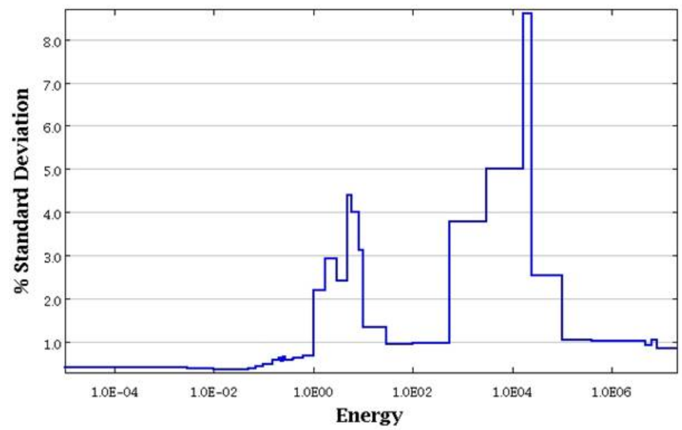

FIG. 3: ENDF/B-VII uncertainty for ^{233}U.

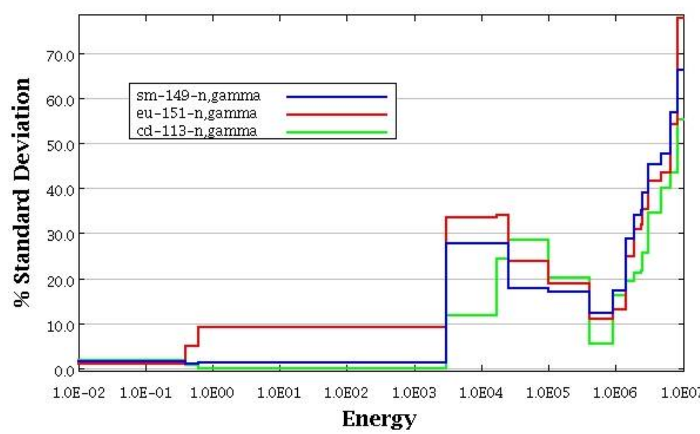

FIG. 4: Approximate uncertainties for three fission products.