APPROXIMATE TECHNIQUES FOR REPRESENTING NUCLEAR DATA UNCERTAINTIES

M. L. Williams, B. L. Broadhead, M. E. Dunn, B. T. Rearden

Oak Ridge National Laboratory,* Nuclear Science and Technology Division, P.O. Box 2008, Bldg. 5700, Oak Ridge, TN 37831-6170, williamsml@ornl.gov

Computational tools are available to utilize sensitivity and uncertainty (S/U) methods for a wide variety of applications in reactor analysis and criticality safety. S/U analysis generally requires knowledge of the underlying uncertainties in evaluated nuclear data, as expressed by covariance matrices; however, only a few nuclides currently have covariance information available in ENDF/B-VII. Recently new covariance evaluations have become available for several important nuclides, but a complete set of uncertainties for all materials needed in nuclear applications is unlikely to be available for several years at least. Therefore if the potential power of S/U techniques is to be realized for near-term projects in advanced reactor design and criticality safety analysis, it is necessary to establish procedures for generating approximate covariance data. This paper discusses an approach to create applications-oriented covariance data by applying integral uncertainties to differential data within the corresponding energy range.

I. INTRODUCTION

Sensitivity/uncertainty (S/U) techniques have been widely used to propagate nuclear data uncertainties to uncertainties in reactor performance parameters.[1,2,3] Recently, S/U methods have begun playing an increasingly important role in criticality safety analysis.[4,5] S/U applications require estimates for nuclear data uncertainties, which are usually specified by a multigroup covariance matrix consisting of variances in the group cross sections for each nuclide-reaction pair, along with correlation coefficients indicating dependencies among the data. Multigroup covariance data can be processed from evaluated nuclear data files such as ENDF/B, JEF, JENDL, etc., which contain descriptions of differential nuclear data as well as, in principle, the covariance information.

In reality, none of the evaluated nuclear files available to the international community currently contain sufficient uncertainty data for many realistic S/U applications. There are plans in the United States to evaluate additional high-quality covariance data for several important materials over the next several years, and this should improve the situation for major nuclides. Nevertheless, there will not be sufficient uncertainty information for the perhaps hundreds of fission products, minor actinides, and impurity materials needed for advanced reactor design, criticality safety, source-term analysis, burnup credit, and shielding calculations. Due to lack of covariance data, S/U applications currently either must neglect the impact of uncertainties in many data or resort to assigning ad hoc values based upon personal experience and preference.[6]

In contrast to the paucity of uncertainty information for differential data, there is a wealth of information available for uncertainties in measured integral data parameters. Extensive compilations of integral data and their uncertainties have been published recently by Mughabghab.[7] Here we examine how uncertainties in measured integral data could be utilized for consistency checking, improving evaluation of uncertainties in differential data, and possibly providing an approximate representation of missing uncertainty data.

II. DIFFERENTIAL AND INTEGRAL DATA

Evaluated differential nuclear data such as contained in ENDF/B are determined typically by combining differential measurements with theoretical expressions from physics models. For example, resolved resonance cross sections may be described by equations of the Reich-Moore formalism. These expressions contain resonance parameters determined by regression of the theoretical equations with one or more differential measurements. Converting the measured results into an evaluated cross section introduces a number of correlated uncertainties into the differential data, caused by background corrections, normalization, etc.[8]

In this paper the term "integral parameter" refers to an *intrinsic* nuclear data parameter, as opposed to an *extrinsic* integral parameter such as the criticality factor k_{eff} that inherently depends upon the facility where the measurement is done. Intrinsic integral parameters are measured experimentally and, in theory, should be independent of the measurement facility; thus, they are

"fundamental" quantities in the same sense as differential nuclear data. Examples of intrinsic integral data are infinitely dilute resonance integrals, Wescott g-factors, and thermal cross sections ["integral thermal cross section" refers to the 2200-m/s value determined by direct measurement or by activation experiments in a standard neutron field, in contrast to values inferred from differential quantities like resonance parameters]. The following are some commonly measured intrinsic integral data, expressed in terms of the differential cross section $\sigma(E)$.

(a) Infinitely dilute resonance integral (RI) from E_L to E_H:

$$I(E_L \rightarrow E_H) \equiv \int_{E_L}^{E_H} \sigma(E) \frac{1}{E} dE . \qquad (2.1)$$

The energy limits are typically selected as $E_L \sim 0.5$ eV (Cadmium cutoff) and $E_H = 5.5$ keV.

(b) Maxwellian-averaged thermal cross section:

$$\langle \sigma_{th} \rangle \equiv \int_0^\infty \sigma(E) M(E,T) dE , \qquad (2.2)$$

where $M(E,T) \equiv$ Maxwellian flux distribution at a temperature of T, normalized to unity.

(c) 2200-m/s thermal cross section (at $E_0 = 0.0253$ eV; $v_0 = 2200$ m/s):

$$\sigma_0 \equiv \int_0^\infty \sigma(E) \delta(E - E_0) dE . \qquad (2.3)$$

Ratios of integral quantities, such as thermal eta $\equiv \frac{\upsilon \sigma_f}{\sigma_a}$, may also be of interest, but the discussion here is limited to linear functionals that have the general form

$$P_m \equiv \int_{E_1}^{E_2} \sigma(E) W_m(E) dE , \qquad (2.4)$$

where $W_m(E)$ is the response weighting function for integral parameter "m." By definition of an intrinsic integral parameter, $W_m(E)$ is an analytical–or at least well-characterized–function with negligible uncertainty. The multigroup form of Eq. (2.4) is

$$P_m \equiv \sum_{g=1}^{G} \sigma_g W_{m,g} , \qquad (2.5)$$

where σ_g = multigroup cross section for group g, a weighted average of the differential data;
$W_{m,g}$ = integrated value of $W_m(E)$ over energy group g;
G = the number of energy groups.

Integral parameters can play an important role in data evaluation by providing normalizations and checks on differential data. The SAMMY [9] computer code for nuclear data analysis allows incorporation of integral constraints during the regression procedure so that integral as well as differential measurements are fit simultaneously. Even when integral parameters are not actively incorporated into the fitting process, they may play a less obvious passive role in data analysis by providing useful checks that the differential and integral data are consistent. Differential data uncertainties should reflect the influence of integral data.

As a hypothetical example, suppose that a differential evaluation of resonance parameters produces a thermal cross section value of 100 ± 10 barns, and that the accepted integral value is 92 ± 2 barns. Since the differential value is significantly outside the uncertainty in the integral value, it is reasonable for the evaluator to modify the initial fitting parameters, consistent with differential measurement uncertainties, so that a revised evaluation gives a thermal cross section of 95 barns. The new cross section still fits the differential data within its 10% uncertainty but is now more consistent with the integral measurement. Although the differential evaluation states an uncertainty of $\pm 10\%$ in the thermal value, the actual uncertainty should be less because it was constrained *passively* to be within the uncertainty of the integral measurement.

Table I shows values of thermal cross sections and resonance integrals determined from ENDF/B-VI.8-evaluated differential data compared with the corresponding integral measurements and their uncertainties.[7] It can be seen that the values obtained from ENDF/B evaluations have a large probability of falling within two standard deviations of the integral parameter values; only 2 of 36–the [241]Pu capture integral and [241]Am thermal capture–are slightly outside of two-sigma. This fact suggests that the uncertainty in the integral measurement is a reasonable estimate for the uncertainty in the calculated parameters obtained with differential data.

Assume that integral measurements of a parameter P_m produce a best-estimate value of $P_m^{(I)}$, with a standard deviation of $Std(P_m^{(I)})$. Define $P_m^{(D)}$ to be the value of P_m calculated from differential data (processed into multigroup form) by using in Eq. (2.5). The variance in $P_m^{(D)}$ is

$$Var(P_m^{(D)}) = \mathbf{W_m^T C_{XX} W_m} , \qquad (2.6)$$

where $\mathbf{W_m}$ is the G dimensional column vector containing $W_{m,g}$ by group; and
$\mathbf{C_{XX}}$ is the (G, G) multigroup covariance matrix determined from differential uncertainties.

TABLE I. Comparison of Calculated and Measured Integral Parameters

Type of Data	Thermal Cross Section (b)		Resonance Integral (b)	
	ENDF/B-VI.8	Measured ± *std*	ENDF/B-VI.8	Measured ± *std*
^{1}H (n, γ)	3.320×10^{-1}	$3.326 \pm 0.007 \times 10^{-1}$	1.49×10^{-1}	$1.49 \pm 0.00 \times 10^{-1}$
^{56}Fe(n, γ)	2.59	2.59 ± 0.14	1.35	1.40 ± 0.20
Zr (n, γ)	1.85×10^{-1}	$1.85 \pm 0.03 \times 10^{-1}$	9.57×10^{-1}	$9.50 \pm 1.50 \times 10^{-1}$
^{113}Cd (n, γ)	2.06×10^4	$2.06 \pm 0.11 \times 10^4$	3.92×10^2	$3.90 \pm 0.40 \times 10^2$
^{135}Xe(n, γ)	2.63×10^6	$2.65 \pm 0.11 \times 10^6$	7.65×10^6	$7.60 \pm 0.50 \times 10^6$
^{149}Sm(n, γ)	4.02×10^4	$4.01 \pm 0.06 \times 10^4$	3.48×10^3	$3.39 \pm 0.20 \times 10^3$
^{155}Gd(n, γ)	6.09×10^4	$6.09 \pm 0.05 \times 10^4$	1.56×10^3	$1.45 \pm 0.10 \times 10^3$
^{235}U (n, γ)	9.87×10^1	$9.83 \pm 0.08 \times 10^1$	1.40×10^2	$1.44 \pm 0.06 \times 10^2$
^{235}U (n, f)	5.85×10^2	$5.83 \pm 0.01 \times 10^2$	2.76×10^2	$2.75 \pm 0.05 \times 10^2$
^{238}U (n, γ)	2.72	2.68 ± 0.04	2.78×10^2	$2.77 \pm 0.03 \times 10^2$
^{237}Np (n, γ)	1.81×10^2	$1.76 \pm 0.03 \times 10^2$	6.60×10^2	$6.40 \pm 0.50 \times 10^2$
^{239}Pu (n, γ)	2.70×10^2	$2.69 \pm 0.03 \times 10^2$	1.81×10^2	$2.00 \pm 0.20 \times 10^2$
^{239}Pu (n, f)	7.48×10^2	$7.48 \pm 0.02 \times 10^2$	3.10×10^2	$3.01 \pm 0.10 \times 10^2$
^{240}Pu (n, γ)	2.87×10^2	$2.89 \pm 0.01 \times 10^2$	8.50×10^3	$8.10 \pm 0.20 \times 10^3$
^{241}Pu (n, γ)	3.62×10^2	$3.58 \pm 0.05 \times 10^2$	1.79×10^2	$1.62 \pm 0.08 \times 10^2$
^{241}Pu (n, f)	1.01×10^3	$1.01 \pm 0.006 \times 10^3$	5.73×10^2	$5.70 \pm 0.15 \times 10^2$
^{241}Am (n, γ)	6.19×10^2	$5.87 \pm 0.12 \times 10^2$	1.39×10^3	$1.43 \pm 0.10 \times 10^3$

In general the covariance matrix can be written as

$$\mathbf{C_{XX}} = \mathbf{s_X^T} \mathbf{R_{XX}} \mathbf{s_X} , \qquad (2.7)$$

where $\mathbf{s_X}$ is a (G, G) diagonal matrix containing group cross section standard deviations, $Std(\sigma_g)$, and R_{XX} is the correlation matrix. Our conjecture is that whenever integral measurements play an active or passive role in constraining evaluated data, the values of $P^{(D)}$ and $P^{(I)}$ should be consistent within the integral measurement uncertainties, and that the uncertainties should be similar; that is,

$$P_m^{(D)} \; \varepsilon \; P_m^{(I)} \pm Std(P_m^{(I)}) , \qquad (2.8)\text{-a}$$

$$Std((P_m^{(D)})) \sim Std(P_m^{(I)}) . \qquad (2.8)\text{-b}$$

Equation (2.8) provides a consistency check for evaluated covariance data. There is no guarantee these relations hold for all cases, since it is not known how (or if) integral measurements were utilized in a particular evaluation. Nevertheless, covariance evaluations that do not satisfy the above inequality should be examined more closely for consistency.

III. INTEGRAL APPROXIMATION FOR DIFFERENTIAL UNCERTAINTIES

Because of the urgent need for covariance data, it is desirable to determine approximations to represent uncertainties for which no high-fidelity evaluation is available. In this section we examine how integral data uncertainties might be used to approximate the covariance matrix for differential data, and under what conditions the approximation is expected to be reasonable. It should be understood at the outset that information concerning correlations among energy ranges, reaction types, and nuclides must be ignored because of insufficient knowledge. Further, we focus only on data for which intrinsic integral parameters with uncertainty estimates are available: capture and fission thermal cross sections and resonance integrals, and potential cross sections. For many applications in criticality safety and thermal reactor analysis, these are the most important data, especially for fission products, minor actinides, and moderators, which are the majority of materials with no evaluated covariances. The proposed method does not provide uncertainties in the energy range above ~5 keV, or for inelastic or other types of data with no integral

measurements. However, other approximate methods currently are being developed to produce low-fidelity covariances in the fast energy range,[10] which can be combined with this work to generate full-energy-range covariances.

It has been observed that the multigroup covariance matrix for many cases consists of several weakly correlated partitions, while group data within a given partition may be correlated. In the integral approximation the covariance matrix is broken into three partitions called the fast, epithermal, and thermal ranges, respectively. The covariance matrix for a nuclide/reaction pair "r" is partitioned as

$$ \mathbf{C_{XX}} = \begin{bmatrix} \mathbf{F^{(r)}} & 0 & 0 \\ 0 & \mathbf{H^{(r)}} & 0 \\ 0 & 0 & \mathbf{T^{(r)}} \end{bmatrix}, \qquad (3.1) $$

where $\mathbf{T^{(r)}}$ is a (G_T, G_T) matrix for thermal range;

G_T = number of thermal energy groups;

$\mathbf{H^{(r)}}$ is a (G_R, G_R) matrix for epithermal range;

G_R = number of epithermal energy groups;

$\mathbf{F^{(r)}}$ is a (G_F, G_F) matrix for fast range;

G_F = number of fast energy groups; and

$G = G_T + G_R + G_F$

The particular energy groups within each range must be specified based upon some criteria. As previously mentioned, the integral approximation is limited to the thermal and resonance ranges, so that only the matrix partitions $\mathbf{T^{(r)}}$ and $\mathbf{H^{(r)}}$ are discussed here. Low-energy absorption cross sections are usually the most important data needed for fission products, impurity nuclides, and many minor actinides in thermalized systems. In the epithermal energy range, the main data needed for applications are usually the capture and fission rates due to resonance reactions, and the elastic scattering reactions of moderators.

III.A Covariances for Absorption Data in the Thermal Range Partition

The low-energy-absorption cross section for many nuclides is described by a 1/v cross section,

$$ \sigma(E) = \sigma_0 \frac{v_0}{v}, \qquad (3.2) $$

where σ_0 is the integral parameter defined in Eq. (2.3) (i.e., the 2200-m/s cross section). A Maxwellian weight function is usually used to process multigroup data in the thermal range. In this case the average cross section for group g is easily shown to be equal to

$$ \sigma_g = \sigma_0 f_g, \qquad (3.3) $$

where $f_g \equiv \dfrac{v_0}{\overline{v}_g}$, and $\dfrac{1}{\overline{v}_g}$ is the Maxwellian-weighted inverse speed for the group.

For a given multigroup energy structure, the value f_g is constant, so that the change in a group cross sections is equal to $\delta\sigma_g = \delta\sigma_0 f_g$. Defining "E" to be the expectation operator, the relative variance in the group cross section is equal to

$$ \frac{Var(\sigma_g)}{\sigma_g^2} = \frac{E(\delta\sigma_g^2)}{\sigma_g^2} = \frac{Var(\sigma_0)}{\sigma_0^2}. \qquad (3.4) $$

The relative covariance for two thermal groups is

$$ \frac{Cov(\sigma_g \sigma_{g'})}{\sigma_g \sigma_{g'}} = \frac{E(\delta\sigma_g \delta\sigma_{g'})}{\sigma_g \sigma_{g'}} = \frac{Var(\sigma_0)}{\sigma_0^2}, \qquad (3.5) $$

and the correlation coefficient for these groups is

$$ R(\sigma_g \sigma_{g'}) \equiv \frac{Cov(\sigma_g \sigma_{g'})}{Std(\sigma_g)\, Std(\sigma_{g'})} = 1.0. \qquad (3.6) $$

The group cross sections are fully correlated since there is only one degree of freedom for 1/v absorbers. Some nuclides do not have 1/v cross sections in the thermal range, for example, due to a low energy resonance. In this case the group cross section can be expressed as a ratio to the Maxwellian-averaged value defined by the integral parameter in Eq. (2.2):

$$ \sigma_g = \frac{\langle \sigma_{th} \rangle}{\sigma_0} \times \frac{\sigma_g}{\langle \sigma_{th} \rangle} \times \sigma_0. \qquad (3.7) $$

The ratio $\dfrac{\langle \sigma_{th} \rangle}{\sigma_0}$, symbolized as "G", is called the "Wescott G-factor" or "non-1/v factor." The Wescott factor is unity for 1/v cross sections but can be greater or less than unity for non-1/v data. Equation (3.7) also can be written in a form identical to Eq. (3.3) by defining

$$ f_g = G \frac{\sigma_g}{\langle \sigma_{th} \rangle}. \qquad (3.8) $$

If the impact of changes in the relative shape of the thermal data is small compared to changes in its normalization, then f_g in the above equation can be assumed constant. In this case the previously derived Eqs. (3.4) and (3.6) are also valid for non-1/v nuclides.

III.B Covariances for Resonance Absorption in the Epithermal Range Partition

The concentrations of absorber impurities, as well as many fission products and minor actinides, are usually

small; hence, their multigroup absorption cross sections are represented adequately by infinitely dilute values. Even cross sections of fissile materials are not heavily shielded in low-enriched systems. Under these conditions it can be shown that the energy distribution of cross sections does not have a large effect on computed multiplication factors for many applications, as long as the group cross sections sum to the correct resonance integrals (RI's). This is illustrated in Table II, which shows the relatively small changes in calculated criticality factors (k_{eff}) due to replacing the ^{235}U multigroup cross sections by a flat value that produces the correct resonance integral; that is, $\bar{\sigma} = \dfrac{RI}{\Delta U_{epi}}$, where ΔU_{epi} is the lethargy width of the resonance range. Note that the infinitely dilute resonance integral approximation is especially accurate for the dilute ^{235}U solutions, as expected. We can take advantage of this behavior to obtain an approximate covariance matrix for the epithermal resonance range. The infinitely dilute RI defined in Eq. (2.1) is written in multigroup form as

$$I = \sum_{g \in epi} I_g ,$$

where $I_g = \sigma_g \Delta u_g$ and where Δu_g is the lethargy width of group "g". The group resonance integral can be expressed as $I_g = f_g I$, where f_g is the fraction of the total integral contributed by group g; hence,

$$\sigma_g = I \frac{f_g}{\Delta u_g} . \qquad (3.9)$$

Whenever changes in group distribution are unimportant compared to changes in magnitude, we can approximate $\delta\sigma_g = \delta I \dfrac{f_g}{\Delta u_g}$. In this case, the relative variance and covariance elements are given by

$$\frac{Var(\sigma_g)}{\sigma_g^2} = \left(\frac{f_g}{\sigma_g \Delta u_g} \right)^2 E(\delta I^2) = \frac{Var(I)}{I^2} . \quad (3.10)$$

As in the thermal range, this approximation has only one degree of freedom, and the correlation coefficient can be shown to be equal to unity for groups in the epithermal matrix partition.

III.C Moderator Scattering Cross Sections

Moderator materials are important in many applications due to their impact on slowing down and resonance escape probability of epithermal neutrons. Within the epithermal range, moderator scattering data are represented by the nearly *constant* potential cross section σ_p, and the secondary energy/angular distributions correspond to s-wave interactions. This assumption can also be used as a first approximation to treat elastic scattering data of resonance absorber materials that do not contribute significantly to the neutron slowing-down process. Therefore the energy transfer element $\sigma_{g \to g'}$ of the multigroup scatter matrix is

$$\sigma_{g \to g'} = \sigma_p f_{g \to g'} , \qquad (3.11)$$

Table II. Impact of Changes in Shape of ^{235}U Epithermal
Cross Section: Flat versus Actual Shape

Critical Benchmark	Benchmark Description	Modified Data	k_{eff}	
			Original	Flat
HST013-1	bare sphere; HEU/water solution	^{235}U: (n,γ), (n,f)	0.99940	0.99932
LST002-1	H$_2$O-reflected sphere; LEU/H$_2$O solution	^{235}U: (n,γ), (n,f)	0.99821	0.99835
PST002-2 (PNL-2)	H$_2$O-reflected sphere; Pu/water solution	^{239}Pu: (n,γ), (n,f)	1.00563	1.00672
PWR pincell	Hot Full Power; UO$_2$ 30 GWD/MT	^{235}U: (n,γ), (n,f)	0.99725	0.99938
PWR pincell	Hot Full Power; UO$_2$ 30 GWD/MT	^{149}Sm,^{143}Nd,^{103}Rh,^{151}Sm, ^{133}Cs,^{155}Gd,^{152}Sm:	0.99725	0.99421
FLATTOP	U-reflector, HEU	^{235}U(n,γ), ^{235}U (n,f)	1.00051	1.00368

where $f_{g \to g'}$ is the fixed group-to-group distribution computed from the analytical s-wave distribution function. Again, there is only one degree of freedom for the uncertainty data. The relative variance is

$$\frac{Var(\sigma_g)}{\sigma_g^2} = \frac{Var(\sigma_p)}{\sigma_p^2} \ , \qquad (3.12)$$

and the covariance matrix is fully correlated.

The free-atom cross section also can be represented by σ_p; thus, the above relations can be extended to the thermal range of materials with free-gas scattering kernels. In the thermal range, the free-gas cross section is proportional to the free-atom value and the group-to-group distribution $f_{g \to g'}$ corresponds to the analytical free-gas scattering kernel.

III.D Examples

Figure 1 compares standard deviations for ^{232}Th and ^{155}Gd capture data in the epithermal and thermal partitions [respectively, groups 13–24 and 25–44 in the 44 group structure of the SCALE code system[11]], based on the integral approximation and the ENDF/B-VII covariance evaluations.[12] The evaluated differential uncertainty for ^{232}Th is ~1.3% throughout the thermal range, while the integral uncertainty is 0.4%. The standard deviation in the ^{155}Gd differential evaluation agrees well with the integral uncertainty of ~1% around 0.025 eV but averages about 5% over much of the thermal range. In the epithermal range, the integral uncertainties seem to be reasonable estimates of the standard deviations for these materials. Figures 2 and 3 show correlation matrices for the thermal partitions. Because the ^{232}Th cross section has 1/v variation, the correlation matrices for the ENDF/B-VII and integral approximation are essentially identical and equal to full correlation. However, ^{155}Gd has a Wescott factor of about 0.84, indicating substantial deviation from 1/v behavior. The ENDF/B-VII correlation matrix of ^{155}Gd shows many thermal groups are highly correlated, but the groups around 0.025 eV tend to have low, or even anti-, correlation with higher energy thermal groups.

III.E Summary of Integral Approximation for Covariance Matrices

The integral approximation divides the covariance matrix into uncorrelated partitions. The relative variance and correlations within a partition have the general form

$$\frac{Var(\sigma_g)}{\sigma_g^2} = \frac{Var(P_m^{(I)})}{P_m^2}, \text{ and } Corr(\sigma_g, \sigma_{g'}) = 1.0 \ , (3.13)$$

where $g \ \varepsilon \ \{G_{min}, G_{max}\}$ is the range of groups in the partition, and

$P_m^{(I)}$ is an integral parameter "m" with a known uncertainty. The integral parameter is defined by response functions W_m over the partition [see Eq. (2.5)].

The integral approximation of the covariance matrix for each partition is equal to

$$\mathbf{C_{XX}} = \frac{Var(P_m^{(I)})}{P_m^2} \ \sigma \mathbf{U_{XX}} \sigma =$$

$$Var(P_m^{(I)}) \left[\frac{\sigma \mathbf{U_{XX}} \sigma}{\mathbf{W_m^T} \left(\sigma \mathbf{U_{XX}} \sigma \right) \mathbf{W_m}} \right] , \qquad (3.14)\text{-a}$$

and the corresponding relative covariance matrix is

$$\mathbf{C_{XX}^{(rel)}} = \sigma^{-1} \mathbf{C_{XX}} \sigma^{-1} = \frac{Var(P_m^{(I)})}{P_m^2} \ \mathbf{U_{XX}} , (3.14)\text{-b}$$

where σ is a (G, G) diagonal matrix whose elements are the group cross section values;
$\mathbf{U_{XX}}$ is a unit matrix containing ones in all positions.

Substituting Eq. (3.14)-a into Eq. (2.6) gives $Var(P_m^{(D)}) = Var(P_m^{(I)})$; thus, the approximate covariance matrix is guaranteed to produce the desired integral parameter uncertainty.

The integral approximation for thermal and epithermal covariances data obviously has limitations. For example, correlations in data of different materials and reactions are not considered. Furthermore there is no correlation between the epithermal and thermal partitions of the covariance matrix; while groups within each partition are fully correlated. Figure 4 shows a recent evaluation of ^{235}U fission covariance data over the energy range of 0–3 keV, obtained by propagating differential resolved resonance parameter uncertainties from SAMMY into multigroup values. [13] The average differential uncertainty in the thermal range is about 0.4% compared to 0.2% in the integral value, and in the epithermal range, it is generally 0.3–1%, while the integral uncertainty is 1.8%. The correlation matrices are significantly different. Because ^{235}U is a non-1/v absorber, thermal groups are less than fully correlated in the differential evaluation, though still highly correlated (>75%) over much of the range. The thermal data also are somewhat correlated to the epithermal data, especially groups near the thermal energy boundary (as expected). However, the most noticeable difference is that the differential evaluation indicates only short-range correlations in the epithermal data, in contrast the long-range (i.e., full) correlations in the integral approximation.
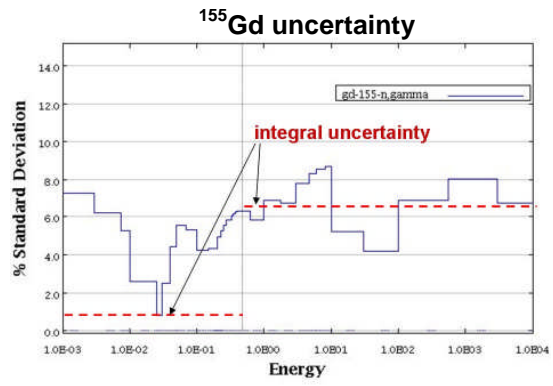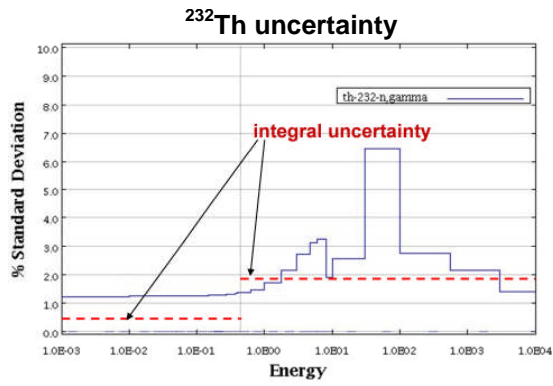
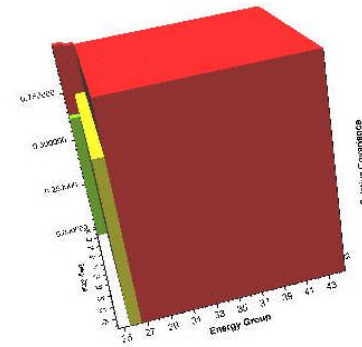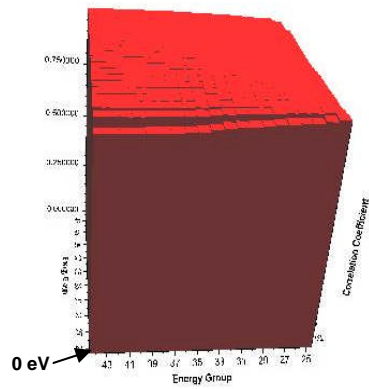Fig. 1. Standard deviation of ^{232}Th and ^{155}Gd capture data in thermal and epithermal: integral approximation vs. ENDF/B-VII.

Fig. 2. Correlation matrix of ^{232}Th capture in thermal range: integral approximation vs. ENDF/B-VII.
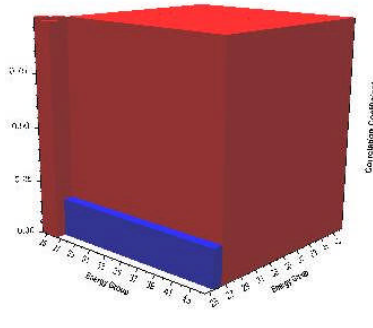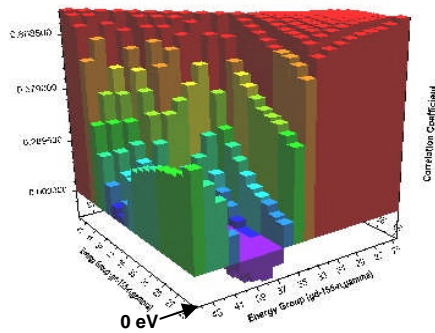
Fig. 3. Correlation matrix of ^{155}Gd capture in thermal range: integral approximation vs. ENDF/B-VII.

Standard Deviation

U-235 fission uncertainty

ENDF/B-VII ^{235}U Correlation Matrix

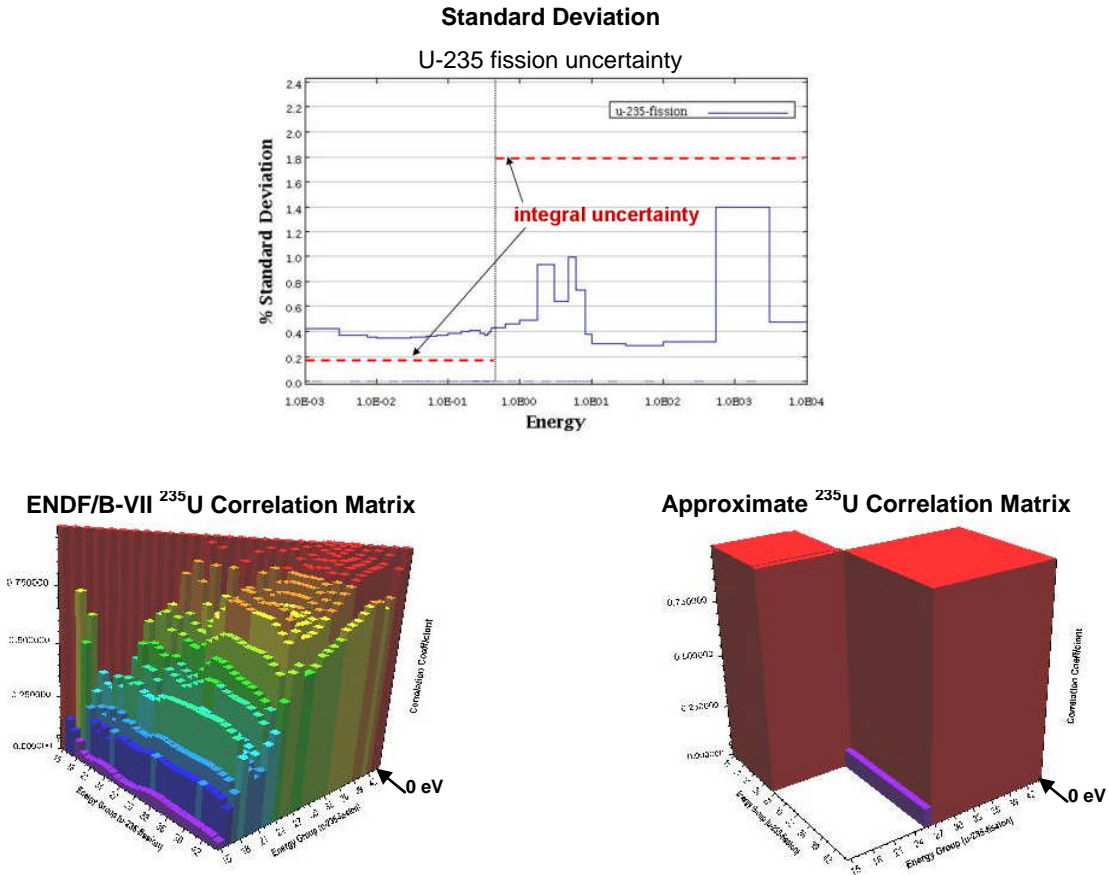Approximate ^{235}U Correlation Matrix

Fig. 4. Covariance data for ^{235}U fission in thermal and epithermal partitions: integral approximation vs. ENDF/B-VII.

The latter behavior is due to the assumption that the integral uncertainty is the only information known about the covariance matrix, so that the state of knowledge is limited to one degree of freedom with fully correlated data. Full correlation causes the maximum estimated uncertainty in calculated application responses. However, if additional information can be incorporated into the covariance matrix, then the application uncertainty could be reduced. For example, suppose that a better estimate is known for the correlation matrix (perhaps based on behavior of known high-fidelity covariances of similar data). The integral approximation of the covariance matrix becomes

$$C_{XX} \; = \; Var(P_m^{(I)}) \left[\frac{\sigma \tilde{R}_{XX} \sigma}{W_m^T \left(\sigma \tilde{R}_{XX} \sigma \right) W_m} \right] , \quad (3.15)$$

where $\tilde{R}_{XX}$ is the approximation for the actual correlation matrix R_{XX}. For example, short-range correlations can be represented by a tri-diagonal matrix; or perhaps a linear combination of tri-diagonal and a unit matrix would suffice.

The above equation still preserves the uncertainty in the measured integral parameter, while modifying the covariance matrix to include a better knowledge of correlations. This approach should be studied further as a possible method to improve the integral approximation.

IV. SUMMARY

The integral approximation provides a simple method to estimate low-fidelity covariances, which is complementary to other covariance evaluation work being performed.[14,15] The primary advantage of this approach is that it provides a practical technique to generate near-term uncertainty information for a wide variety of materials. Three comparisons of the integral approximation with covariance data based on recent differential evaluations indicate that the integral uncertainty is somewhat lower for the thermal standard deviations, and slightly higher for the resonance range of ^{235}U. The ENDF/B-VII correlation matrices for the epithermal range seem to indicate primarily short-range correlations, while the integral approximation assumes full correlation. Although the integral approximation may not be adequate for covariance data of major nuclides that require

higher-fidelity evaluations, it should be sufficiently accurate to provide low-fidelity uncertainties for numerous nuclides of "secondary importance" that appear in many applications.

REFERENCES

1. C. R. WEISBIN, J. H. MARABLE, J. L. LUCIUS, E. M. OBLOW, F. R. MYNATT, R. W. PEELLE, and F. G. PEREY, *Application of FORSS Sensitivity and Uncertainty Methodology to Fast Reactor Benchmark Analysis*, ORNL/TM-5563, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN (December 1976).

2. W. P. POENITZ and P. J. COLLINS, "Utilization of Experimental Integral Data for the Adjustment and Uncertainty Evaluation of Reactor Design Quantities," *Applications of Critical Experiments and Operating Data to Core Design via Formal Methods of Cross Section Data Adjustment*, NEACRP-L-307, Jackson Hole, WY (September 1988).

3. J. H. MARABLE, C. R. WEISBIN, AND G. DE SAUSSURE, "Uncertainty in the Breeding Ratio of a Large Liquid-Metal Fast Breeder Reactor: Theory and Results," *Nucl. Sci. Eng*., **75**, 30–55 (1980).

4. B. L. BROADHEAD, B. T. REARDEN, C. M. HOPPER, J. J. WAGSCHAL, and C. V. PARKS, "Sensitivity- and Uncertainty-Based Criticality Safety Validation," *Nucl. Sci. Eng*., **146(3)**, 340–366 (2004).

5. S. GOLUOGLU, K. R. ELAM, B. T. REARDEN, B. L. BROADHEAD, and C. M. HOPPER, *Sensitivity Analysis Applied to the Validation of the ^{10}B Capture Reaction in Nuclear Fuel Casks*, NUREG/CR-6845 (ORNL/TM-2004/48), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory, Oak Ridge, TN (August 2004).

6. G. ALIBERTI, G. PALMIOTTI, M. SALVATORES, T. K. KIM, T. A. TAIWO, M. ANITESCU, I. KODELI, E. SARTORI, and J. TOMMASI, "Nuclear Data Sensitivity, Uncertainty, and Target Accuracy Assessment for Future Nuclear Systems," *Annals of Nucl. Energy*, **33**, 700 (2007).

7. S. F. MUGHABGHAB, *Atlas of Neutron Resonances: Resonance Parameters and Thermal Cross Sections*, Elsevier, Amsterdam (2006).

8. N. M. LARSON, L. C. LEAL, H. DERRIEN, G. ARBANAS, R. O. SAYER, and D. WIARDA, "A Systematic Description of the Generation Of Covariance Matrices," *PHYSOR-2006: ANS Topical Meeting on Reactor Physics*, Vancouver, Canada, September 10–14, 2006.

9. N. M. LARSON, *Updated Users' Guide for SAMMY Multilevel R-Matrix Fits to Neutron Data Using Baye's Equations*, ORNL/TM-9179/R7, Oak Ridge National Laboratory, Oak Ridge, TN (2006).

10. M. HERMAN, P. OBLOZINSKY, D. ROCHMAN, T. KAWANO, and L. LEAL "Fast Neutron Covariances for Evaluated Data Files," *PHYSOR-2006: ANS Topical Meeting on Reactor Physics,* Vancouver, Canada, September 10–14, 2006.

11. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation,* ORNL/TM-2005/39, Version 5.1, Vols. I–III, Oak Ridge National Laboratory, Oak Ridge, TN (November 2006). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.

12. M. B. CHADWICK et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nuclear Data Sheets*, **107**, No. 12, December 2006.

13. L. C. LEAL, H. DERRIEN, N. M. LARSON, AND R. Q. WRIGHT, *R-matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV*, ORNL/TM-13416, Oak Ridge National Laboratory, Oak Ridge, TN (November 1997).

14. L. LEAL, H. DERRIEN, G. ARBANAS, N. M. LARSON, and D. WIARDA "Covariance Data for ^{232}Th in the Resolved Resonance Region from 0 to 4 keV," *PHYSOR-2006: ANS Topical Meeting on Reactor Physics*, Vancouver, Canada, September 10-14, 2006.

15. D ROCHMAN, M. HERMAN, P. OBLOZINSKY, and S. F. MUGHABGHAB, *Preliminary Cross Section and Nu-bar Covariances for WPEC Subgroup 26*, BNL-77407-2007-IR, National Nuclear Data Center, Brookhaven National Laboratory (2007).