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A method to construct covariance files in ENDF/B format
for criticality safety applications

Dimitri G. Naberejnev and Donald L. Smith

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ANL/NDM-148

A Method to Construct Covariance Files in ENDF/B Format for Criticality Safety Applications¹

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June 1999

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Abstract

Argonne National Laboratory is providing support for a criticality safety analysis project that is being performed at Oak Ridge National Laboratory. The ANL role is to provide the covariance information needed by ORNL for this project. The ENDF/B-V evaluation is being used for this particular criticality analysis. In this evaluation, covariance information for several isotopes or elements of interest to this analysis is either not given or needs to be reconsidered. For some required materials, covariance information does not exist in ENDF/B-V: ^{233}U , ^{236}U , Zr, Mg, Gd, and Hf. For others, existing covariance information may need to be re-examined in light of the newer ENDF/B-VI evaluation and recent experimental data. In this category are the following materials: ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , Fe, H, C, N, O, Al, Si, and B. A reasonable estimation of the fractional errors for various evaluated neutron cross sections from ENDF/B-V can be based on the comparisons between the major more recent evaluations including ENDF/B-VI, JENDL3.2, BROND2.2, and JEF2.2, as well as a careful examination of experimental data. A reasonable method to construct correlation matrices is proposed here. Coupling both of these considerations suggests a method to construct covariances files in ENDF/B format that can be used to express uncertainties for specific ENDF/B-V cross sections.

I. Introduction

The information on different types of cross sections, resonance parameters and other quantities of interest in the ENDF (Evaluated Nuclear Data File)¹ is based on the analysis of a variety of measurements as well as on applicable nuclear models. Since the discrepancies between different measurements can be significant and the nuclear models employed are far from being perfect, an interest in covariance information in the ENDF system has developed in recent years. A number of reasons can be advanced to support the notion that such information is often crucial in nuclear data applications.

The construction of covariance information finds its origins at the experimental analysis stage. An experimenter is obliged to provide the most complete information possible on error components related to a particular experiment. Having that information, an evaluator can estimate the degree of "uncertainty" to be assigned to this measurement and others as well in order to provide that information to the users in form of covariance files in ENDF/B format.

Unfortunately, the covariance information in the recent evaluations, such as ENDF/B-V, ENDF/B-VI, JENDL3.2, BROND2.2, and JEF2.2, is either not complete or is absent for a big variety of materials. The only rigorous way to provide that information is to perform a new evaluation incorporating covariance methodology.

Nevertheless, a different, less expensive solution is proposed here which does not require a new evaluation. This solution is based on the idea of considering the covariance information as a measure of confidence in one particular evaluation with respect to the others that are available.

A reasonable estimation of the fractional errors for different neutron cross sections in ENDF/B-V can be based on comparisons between the major existing recent evaluations including ENDF/B-VI, JENDL3.2, BROND2.2, and JEF2.2, as well as a careful examination of pertinent experimental data. A reasonable algorithm for constructing correlation matrices, which is based on this assumption, is proposed. This approach allows the possibility for constructing covariance files in ENDF/B format for a set of selected materials.

II. Covariance Matrices

We discuss here general features of methods used for the construction of a covariance matrix. We follow the approach proposed in the reference 2.

A covariance matrix V_X represents error information for all possible pairs of components X_i and X_j of a vector $\mathbf{X}$ of dimension n . It is derived from a multivariate probability distribution function $p(\mathbf{X})$ as follows:

$$(V_X)_{ij} = \text{cov}(X_i, X_j) = \langle \delta X_i \delta X_j \rangle = \langle X_i X_j \rangle - \langle X_i \rangle \langle X_j \rangle, \quad (1)$$

where $\delta X_i = X_i - \langle X_i \rangle$ and $\langle \rangle$ mean that an average is to be taken with respect to $p(\mathbf{X})$. It is clear that if $i=j$, then the element $(V_X)_{ii}$ simply reflects a variance (standard deviation squared) for the quantity X_i :

$$\text{cov}(X_j, X_j) = \text{var}(X_j) = [\text{stddev}(X_j)]^2 = \langle (\delta X_j)^2 \rangle = \langle X_j^2 \rangle - \langle X_j \rangle^2. \quad (2)$$

Such quantities are commonly used to describe the propagation of errors through the well-known linear *Law of Error Propagation* (LEP). Let us consider a vector $\mathbf{Y}(\mathbf{X})$ of dimension m that is a function of the vector $\mathbf{X}$. This vector has components Y_k . Linear LEP suggests that $\mathbf{Y}$ is a linear combination of all X_j . Nevertheless this approach can be generalized provided that the following conditions are satisfied: a) $\mathbf{Y}$ varies smoothly over all the region of the most probable $\mathbf{X}$; b) the function $p(\mathbf{X})$ is localized in the vicinity of $\langle \mathbf{X} \rangle$, and c) $\mathbf{Y}$ is differentiable with respect to each X_j near $\langle \mathbf{X} \rangle$. In this case $\mathbf{Y}$ can be approximated by a first order Taylor series in the vicinity of $\langle \mathbf{X} \rangle$ as follows:

$$Y_k = Y_k(\langle \mathbf{X} \rangle) + \sum_{j=1,n} \left(\frac{\partial Y_k}{\partial X_j} \right)_{\mathbf{X}=\langle \mathbf{X} \rangle} \delta X_j. \quad (3)$$

Introducing the notation $t_{jk} = (\partial Y_k / \partial X_j)_{\mathbf{X}=\langle \mathbf{X} \rangle}$ and $\langle Y_k \rangle \approx Y_k(\langle \mathbf{X} \rangle)$ we obtain:

$$Y_k = \langle Y_k \rangle + \sum_{j=1,n} t_{jk} \delta X_j, \quad (4)$$

$$\delta Y_k = Y_k - \langle Y_k \rangle = \sum_{j=1,n} t_{jk} \delta X_j. \quad (5)$$

The matrix $\mathbf{T}$, whose components are t_{jk} , is called the sensitivity matrix. In terms of this matrix we can rewrite the preceding formula in its matrix form:

$$\delta Y = T^+ \delta X. \quad (6)$$

From the several preceding formulas it is then easily seen that:

$$\text{cov}(Y_k, Y_l) = \sum_{i=1,n} \sum_{j=1,n} t_{ik} t_{jl} \text{cov}(X_i, X_j). \quad (7)$$

The last expression makes a connection between the $m \times m$ covariance matrix V_Y for Y (with components $\langle \delta Y_k \delta Y_l \rangle$), and the $n \times n$ covariance matrix V_X for X (with components as defined in (1)) through the matrix T :

$$V_Y = T^+ V_X T. \quad (8)$$

In terms of a correlation matrix C , the relative covariance matrix R is defined by the expression:

$$R_{ij} = \frac{V_{ij}}{X_i X_j} = C_{ij} f_i f_j, \quad (9)$$

where f_i and f_j are fractional errors of the quantities X_i and X_j . For convenience we drop the subscript "X" for R , C , and f .

Covariance information in ENDF/B format can be found in file MF=33 and is provided for different types of reactions identified by MT if any error information exists.¹ "Cross" covariances, i.e., cross covariances for different types of reactions or different isotopes may also be provided. Cross covariance information for different isotopes is important in the case where cross sections were deduced from the analysis of ratios of different cross sections. The fission cross section of ^{238}U is an example. Two different flags NC and NI are assigned for such cases. When using NC, the covariances are described indirectly using different values of the flag LTY. To calculate covariances for a particular cross section, a summation has to be performed over all sub-subsections. Different coding methods for covariances in ENDF/B format are used. That is reflected by a LB value. We will not enter into the details of these formats and refer the reader to the manual on ENDF/B formats for details.¹

Here we consider individual isotopes and reactions. "Cross" covariances are therefore ignored. We always use the flag NI for the sake of its simplicity. The issue concerning the use of different covariance formats (reflected by LB value) is still under discussion. The nuclear data community seems now to be agreed that the simplest and the most understandable to a user LB format must be used.³ From the existing options for coding covariances in ENDF files, the most convenient form, in our opinion, is LB=5. This coding corresponds to the formulae (9). Different factors in this formula need to be addressed in order to carry out the covariance generation process. Below, we describe the methods employed to calculate the different factors in (9).

III. A Method to Provide Fractional Errors

How can we get information about fractional errors $f(R, A, e)$ for a particular reaction R , a particular isotope A and a particular evaluation e without carrying out a complete reevaluation procedure? Let us first look at these errors as measure of the degree of confidence that we actually assign to one particular value of one particular cross section. Due to differences in available experimental data and to the difference in the employed methods, cross sections never exhibit the same values for different evaluations (except the trivial cases where one evaluation is a perfect copy of another). Hence, we can begin our analysis by processing different evaluations at temperature of zero degree Kelvin and an infinite dilution cross section for a particular pair (R, A) with a processing code, such as NJOY.⁴ The scatter between these processed cross sections for different evaluations e_i with respect to the evaluation e of present interest (in our case ENDF/B-V) appears to be a reasonable way to estimate those fractional errors for a particular triplet (R, A, e) . The maximum discrepancy between these evaluations e_i and e is the fractional error we chose to select:

$$f(R, A, e) = \max_i \left[\frac{\sigma(R, A, e) - \sigma(R, A, e_i)}{\sigma(R, A, e)} \right]. \quad (10)$$

Obviously, the evaluations, which differ from E by more than 100%, should not be taken into account unless there is strong experimental evidence available to suppose such a large difference. Minimal fractional errors are also imposed in those cases where only very slight changes were found from one evaluation to another.

Since by definition we are interested in providing covariance information for ENDF/B-V, we should compare it for the different types of cross sections processed with all other available evaluations.

We describe here several special cases of interest, which must be treated separately when calculating fractional errors.

- a) Discrepancies between ENDF/B-V and all other evaluations are smaller than the following values: Fission 1%, Capture 5%, Elastic 10%, Inelastic 10%, Nu-bar 1%. In this case we impose those values as the magnitude of fractional errors.
- b) Discrepancies between ENDF/B-V and all other evaluations are bigger than 100%. In this case we impose a conservative fractional error of 70% for each type of reaction.
- c) Discrepancy between ENDF/B-V and at least one evaluation (may be many) is smaller than 100% and the others evaluations differ by more than 100%: In this case we do not take into account those latter evaluations and base our estimation of fractional errors only on the rest of the evaluations.

Since the present interest is in providing covariance files for criticality safety applications, an appropriate energy group structure should be used.

IV. A Method to Construct Correlation Matrices

The relative covariance matrix R_{ij} for the two arbitrary points in energy group structures E_i and E_j is given by the expression:

$$R_{ij} = C_{ij} f_i f_j, \quad (11)$$

where f_i and f_j are the estimated fractional errors of the particular cross section in the groups i and j , and C_{ij} is the correlation matrix which satisfies $-1 \leq C_{ij} \leq 1$. The energies E_i and E_j can be selected for convenience as the midpoint energies of the i^{th} and j^{th} energy groups.

Since we do not enter into details of each particular measurement, the correlation matrix must be reasonably estimated. The principal of construction of the C_{ij} "a priori" is based on the concept of long-, medium- and pair-wise-range correlations. First we assume that C_{ij} is a product of three factors:

$$C_{ij} = L_{ij} M_{ij} S_{ij}, \quad (12)$$

where L_{ij} , M_{ij} and S_{ij} stand for long-, medium- and pair-wise correlations. L_{ij} becomes influential if the points in energy are far from each other. In all cases $0 \leq L_{ij} \leq 1$. M_{ij} takes into account "medium" correlation effects such as correlation between the thermal ($1/v$), resonance, and fast regions. Similarly, $0 \leq M_{ij} \leq 1$. Finally, S_{ij} accounts for correlations between two arbitrary E_i and E_j based on analysis of pair-wise variations, regardless of separation in energy or other physical considerations. The inequality $-1 \leq S_{ij} \leq 1$ holds for pair-wise correlations. Let us consider in greater detail each factor.

Long-range correlation

We make an ad hoc assumption that:

$$L_{ij} = 1 - \alpha \frac{|E_i - E_j|}{\varepsilon}, \quad (13)$$

where ε is the total energy interval of interest (energy range spanned by the evaluations, e. g. 20 MeV). Obviously, $0 \leq L_{ij} \leq 1$. It is seen that the last expression is the first order term in a Taylor's series for the exponential function. Hence, another approach to model L_{ij} can be:

$$L_{ij} = \exp\left(-\alpha \frac{|E_i - E_j|}{\varepsilon}\right), \quad (14)$$

where α is a positive dumping factor which determine the strength of the long-range correlation. Nominally, we estimate $\alpha=1$ to 2. In our calculation we use the expression (14) with $\alpha=1.5$.

Medium-range correlation

The concept of the medium-range correlation in the case of neutron cross sections arises from the fact that there are three distinct regions of energy to consider: Thermal ($1/v$), Resonant and Fast (values due to the unresolved levels) energies. The example of the ^{235}U total cross section (Figure 1) illustrates that fact.

These three regions are generally treated differently in the evaluation process. Hence, while there are common factors between the regions that introduce correlations, these correlations can never be as strong as unity. Roughly these three regions are:

Thermal, based strongly on the $1/v$ shape normalized to measured thermal cross section value;

Resonant, which fits experimental data with different approximation of R-matrix formalism (such as Breit-Wigner multilevel or Reich-Moore formalisms);

Fast, smooth region based on a fit to average experimental data.

Figure 1: Total cross section of ^{235}U .

Therefore, the following gross correlation matrix representing medium range correlations is suggested (Figure 2).

Thermal	1		
Resonant	β	1	
Fast	ξ	γ	1
	Thermal (1/v)	Resonant	Fast

Figure 2: Medium range correlations in three distinct regions in energy.

The introduced quantities β , ξ , and γ satisfy $0 < \beta, \xi, \gamma < 1$. The values of these quantities must be estimated. The thermal cross sections near the resonant region are strongly influenced by the tails of the low-lying resonances, so it is reasonable to assume that the value of β is quite high:

$$\beta \approx 0.75 - 0.9 \text{ (rather strong correlation).}$$

The resonant and fast regions are evaluated differently but the unresolved-resonance region (included in the fast part) imposes a moderate correlation such as

$$\gamma \approx 0.5 \text{ (moderate correlation).}$$

Finally the thermal and fast regions tend to be rather decoupled, so we assume that

$$\xi \approx 0.25 \text{ (weak correlation).}$$

The decomposition of the total energy interval ε into Thermal, Resonant and Fast regions (the values of E_{th} and E_{res}) is isotope dependant and must be examined individually for each particular isotope.

Pair-wise correlation

The pair-wise correlation factor S_{ij} tests for similarity of the error magnitudes f_i and f_j regardless of all other considerations. For this particular correlation component we assume somewhat conservatively that:

$$S_{ij} = \begin{cases} \frac{1}{N} \frac{\sum_n f_i^n f_j^n}{f_i^{\max} f_j^{\max}} & (i \neq j) \\ 1 & (i = j) \end{cases} \quad (15)$$

In the last formula the following notation is introduced:

- f_i^n, f_j^n - fractional errors for the evaluation n and energies E_i and E_j ;
- $f_i^{\max}, f_j^{\max}$ - maximal fractional errors in the energy groups i and j ;
- N - number of the evaluations taken into account.

Keeping the sign of f_i and f_j we can also account for anti-correlation. This approach to correlation estimation technique can be justified as follows: If the errors f_i and f_j are very different from each other then S_{ij} will be small, if they are close then S_{ij} will be bigger. The fact that f_i and f_j may be situated at a long distance in energy from each other will be taken into account through the factors L_{ij} and M_{ij} . Obviously, $-1 \leq S_{ij} \leq 1$. The limiting cases of pair-wise total correlation $S_{ij}=1$ will occur if for each n $|f_x^n| = |f_y^{\max}|$, where x and y stand for all possible combinations of i and j . It is tempting to refer to this type of correlations as short-range since it involves only pairs. However, use of this expression to characterize the correlation could be misleading since E_i and E_j could be very different.

In summary, the strength of correlation or anti-correlation implied by S_{ij} is determined by an assumed common error component which amounts to the average fractional error over all evaluations. It is clear that this approach is ad hoc. The values f_i^n and f_j^n might be similarly small or large for totally different reasons. However, in the absence of other evidence, this approach seems rational. As was mentioned above, the factors L_{ij} and M_{ij} come into play to temper the correlation strength based on other considerations such as energy and region.

V. Calculation Scheme

In this section we describe how our calculations were arranged and performed (Figure 3). Several computer programs were written to perform the necessary operations. Programs **gendfDC** and **pendfDC** helped us to retrieve the information on point- and group-wise cross sections from the **NJOY** output files. The routine **covDD** assembles results from all previous calculations, constructs a covariance matrix for given isotope, and creates the file for MF=33 in ENDF/B LB=5 format for the reactions specified by the user. The routine **graDD** performs some transformations necessary for plotting of the results.

Figure 3: Calculation scheme.

VI. Illustration of the Methods

Let us illustrate the methods described in sections III and IV. We consider here the fission cross section of ^{235}U . First, we processed the files for this isotope with all the available evaluations (ENDF/B-V, ENDF/B-VI, JENDL3.2, BROND2.2, and JEF2.2). The result is plotted in Figure 4. Then we calculated the difference between the fission cross section processed with ENDF/B-V and all other evaluations. The result is shown in Figure 5. Looking for discrepancies over 100% and smaller than a reasonable value for fission (which is of order of 1%), and taking into account only those evaluations, which satisfy this criterion, we obtained fractional errors including signs for this particular reaction (Figure 6). All these figures were generated with the help of the **graDD** routine. The associated correlation matrix, calculated as described in the section IV, is presented on the Figure 7 (planar view) and Figure 8 (3D view).

The covariance matrix obtained in this manner was processed with the code **NJOY**. The results, which summarizes the correlation matrix and the fractional errors, are presented in the Figure 9. In the Figure 10 we show the same information as in the Figure 9 but this time the covariance file, provided with ENDF/B-V evaluation, was used. Note that the covariance information available in ENDF/B-V is minimal. It is for this reason that the present project was initiated. Note that the plotting routine of **NJOY** uses zero values of correlations is the latter are small.

In all our calculations we employed the 44-group structure currently being used in criticality safety applications. This group structure's energy boundaries are presented in Table 1.

Group index	Energy, eV	Group index	Energy, eV	Group index	Energy, eV
1	1.0000e-5	16	3.0000e-3	31	7.5000e-3
2	1.0000e-2	17	2.5300e-2	32	3.0000e-2
3	4.0000e-2	18	5.0000e-2	33	7.0000e-2
4	1.0000e-1	19	1.5000e-1	34	2.0000e-1
5	2.2500e-1	20	2.5000e-1	35	2.7500e-1
6	3.2500e-1	21	3.5000e-1	36	3.7500e-1
7	4.0000e-1	22	6.2500e-1	37	1.0000e+0
8	1.7700e+0	23	3.0000e+0	38	4.7500e+0
9	6.0000e+0	24	8.1000e+0	39	1.0000e+1
10	3.0000e+1	25	1.0000e+2	40	5.5000e+2
11	3.0000e+3	26	1.7000e+4	41	2.5000e+4
12	1.0000e+5	27	4.0000e+5	42	9.0000e+5
13	1.4000e+6	28	1.8500e+6	43	2.3540e+6
14	2.4790e+6	29	3.0000e+6	44	4.8000e+6
15	6.4340e+6	30	8.1873e+6	45	2.0000e+7

Table 1: Group boundaries for 44-group structure being used in criticality safety applications.

Figure 4: Fission cross section of $^{92}\text{U}^{235}$ in 44-group structure used in criticality safety applications.

Figure 5: Comparison of the fission cross section of $^{92}\text{U}^{235}$ for different evaluations.

Figure 6: Fractional errors on the fission cross section of $^{92}\text{U}^{235}$ for ENDF/B-V.

Figure 7: Correlation matrix C_{ij} for $^{92}\text{U}^{235}$ fission (planar view).

C_{ij}

Figure 8: Correlation matrix C_{ij} for $^{92}\text{U}^{235}$ fission (3D view).

Figure 9: Result of generated covariance file for ^{235}U fission cross section processed with the code NJOY.

Figure 10: Result of generated covariance file for $^{235}\text{U}(n,f)$ fission cross section processed with the code NJOY.

VII. Results for different isotopes

We summarize in Appendix A our results for various isotopes. The plots are given as generated with the code **NJOY**. Notice that the **NJOY** plot routine often does not display the small quantities.

In Appendix B, the comparisons between new, generated with **covDD** routine covariances and covariances provided in ENDF/B-V for $^{92}\text{U}^{235}$ are presented.

We also notice that the method used to construct covariance files, as described in sections III and IV, can be applied to any isotopes. We restrict ourselves to displaying only those isotopes of particular interest to the criticality safety applications.

The numerical information used to produce the plots shown in Appendix A can be obtained from Dimitri G. Naberejnev en request.

VIII. Conclusion

A method to construct covariance files in ENDF/B format is described. This method, being based on a reasonable estimation of fractional errors and ad hoc construction of the correlation matrices, allows one to perform an estimation of covariance matrices without performing a new evaluation. Covariance files for several isotopes of interest in criticality safety applications were created.

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Appendix A

$^{92}\text{U}^{233}$: $E_{\text{th}}=1 \text{ eV}$, $E_{\text{res}}=1.\text{e}+4 \text{ eV}$.

Figure 11: Elastic cross section of $^{92}\text{U}^{233}$.

Figure 12: Inelastic cross section of $^{92}\text{U}^{233}$.

Figure 13: Fission cross section of $^{92}\text{U}^{233}$.

Figure 14: Capture cross section of $^{92}\text{U}^{233}$.

Figure 15: Total $\bar{\nu}$ for $^{92}\text{U}^{233}$.

$^{92}\text{U}^{236}$: $E_{\text{th}}=4 \text{ eV}$, $E_{\text{res}} 1.\text{e}+4 \text{ eV}$.

Figure 16: Elastic section of $^{92}\text{U}^{236}$.

Figure 17: Inelastic cross section of $^{92}\text{U}^{236}$.

Figure 18: Fission cross section of $^{92}\text{U}^{236}$.

Figure 19: Capture cross section of $^{92}\text{U}^{236}$.

Figure 20 Total $\bar{v}$ of $^{92}\text{U}^{236}$.

^{40}Zr : $E_{\text{th}}=1.\text{e}+3$ eV, $E_{\text{res}} 1.\text{e}+6$ eV.

Figure 21: Elastic cross section of ^{40}Zr .

Figure 22: Inelastic cross section of ^{40}Zr .

Figure 23: Capture cross section of ^{40}Zr .

^{12}Mg : $E_{\text{th}}=2.\text{e}+3$ eV, $E_{\text{res}} 1.\text{e}+7$ eV.

Figure 24: Elastic cross section of ^{12}Mg .

Figure 25: Inelastic cross section of ^{12}Mg .

Figure 26: Capture cross section of ^{12}Mg .

^{72}Hf : $E_{\text{th}}=1 \text{ eV}$, $E_{\text{res}} 1.\text{e}+4 \text{ eV}$.

Figure 27: Elastic cross section of ^{72}Hf .

Figure 28: Inelastic cross section of ^{72}Hf .

Figure 29: Capture cross section of ^{72}Hf .

Appendix B

$^{92}\text{U}^{235}$: $E_{\text{th}}=4$ eV, $E_{\text{res}}=2.5 \times 10^5$ eV. Results for new generated covariances with covDD.

Figure 30: Elastic cross section of $^{92}\text{U}^{235}$. Results with covDD.

Figure 31: Inelastic cross section of ^{235}U . Results with covDD.

Figure 32: Fission cross section of ^{235}U . Results with covDD.

Figure 33: Capture cross section of $^{92}\text{U}^{235}$. Results with covDD.

Figure 34: Total $\bar{v}$ for $^{92}\text{U}^{235}$. Results with covDD.

$^{92}\text{U}^{235}$. Results with covariances provided in ENDF/B-V.

Figure 35: Fission cross section of $^{92}\text{U}^{235}$. Results with covariances provided in ENDF/B-V.

Figure 36: Fission cross section of $^{92}\text{U}^{235}$. Results with covariances provided in ENDF/B-V.