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TITLE: MULTIGROUP PROCESSING OF ENDF/B DOSIMETRY COVARIANCES

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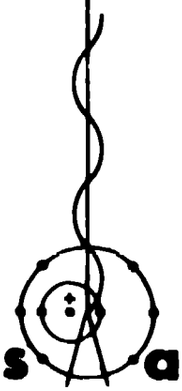

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MULTIGROUP PROCESSING OF ENDF/B DOSIMETRY COVARIANCES

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ABSTRACT

The methodology of multigroup processing of ENDF/B dosimetry covariance (uncertainty) information is discussed, with specific references to the ERRORR covariance module of the NJOY nuclear data processing system. Also discussed is the recent application of ERRORR to the generation of a 137-group, 35-material covariance library for dosimetry applications, and a compact format for storing and transmitting fine-group covariance libraries is introduced.

THE ERRORR COVARIANCE PROCESSING MODULE

The NJOY nuclear data processing system[1] is used at Los Alamos and elsewhere to process data from ENDF/B into forms useful in various applications. A new version, NJOY (10/81), was released to the U. S. code centers in November, 1981. The particular module of NJOY used for preparing multigroup covariance matrices is called ERRORR. In addition, the module COVR is included in the NJOY system to plot and re-format multigroup covariance matrices produced by ERRORR. As with the other NJOY modules, ERRORR and COVR can be operated either as parts of the NJOY system or as stand-alone programs.

Basic Methodology of ERRORR

ERRORR is a flexible program which allows the user several choices in the particular method used to calculate covariances. The first method, the "pointwise" approach, is used when one has access to a data set containing resonance-reconstructed and linearized cross sections in the NJOY "point-ENDF," or PENDF format. The user can produce such a data set using the RECONR and BROADR modules of NJOY. This step is unnecessary for most dosimetry applications, because a PENDF tape containing all of the reactions on the ENDF/B-V dosimetry file, with all resonances reconstruced and Doppler broadedned to 300 K, has been produced recently at Los Alamos and is available from the Los Alamos Nuclear Data Group. In order to keep the size of this data file down to a manageable

size (56 000 card images), a relatively coarse accuracy criterion (1% for non-fissile nuclides, 5% for fissiles) was employed in the resonance-reconstruction calculation.

In this mode of operation, the user can specify a group structure with complete flexibility (up to 620 user groups are allowed) The ERRORR module will determine the union of the user's energy grid and the ENDF/B evaluator's grid for the material of interest. The relationship between these three grids is illustrated in Fig. 1.

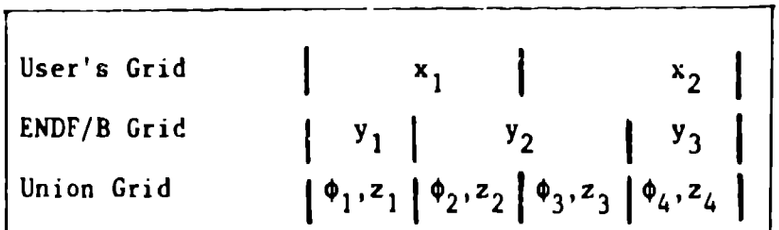

Fig. 1. Illustration of Energy Grid Relations

After forming the union grid, ERRORR integrates $\sigma(E)$ and the user-supplied weight function $\phi(E)$ to obtain the cross sections z_k and "fluxes" ϕ_k, multigrouped on the union grid. These, in turn, are used to calculate multigroup cross sections x_i on the user's grid according to

$$x_i = \frac{\sum_{k \in i} \phi_k z_k}{\sum_{k \in i} \phi_k} \quad . \tag{1}$$

In order to calculate the covariances of x_i, the methodology of ERRORR assumes that the $\phi(E)$ is free of uncertainty, so that the "propagation-of-errors" formula can be used,

$$\mathrm{cov}(x_i, x_j) = \sum_{\substack{k \in i \\ \ell \in j}} a_{ik}\, a_{j\ell}\, \mathrm{cov}(z_k, z_\ell) \tag{2}$$

where the "sensitivity coefficients" a_{ik} are the normalized group fluxes,

$$a_{ik} = \frac{\phi_k}{\sum_{k \in i} \phi_k} \tag{3}$$

The union-grid covariances $\mathrm{cov}(z_k, z_\ell)$ in Eq. (2) are formed from the numerical data in the ENDF/B covariance files by combining them, in the ENDF/B prescribed manner,[2,3] with the union-grid cross sections z_k.

The final step, if the user requests it, is to convert the absolute covariances, Eq. (2), to relative covariances,

$$\text{relcov}(x_i,x_j) = \frac{\text{cov}(x_i,x_j)}{x_i\, x_j} \quad . \tag{4}$$

Group Input Option

A slightly different calculational path is followed if one wishes to start from a multigroup cross section library rather than pointwise data. ERRORR will accept such multigroup cross section input, but only in the format produced by the NJOY group-averaging module GROUPR. Such a library contains both multigroup cross sections and group integrals of the weight function used to produce the cross sections.

In the multigroup input mode, the required union grid cross sections and fluxes are obtained by collapsing (or expanding) the cross sections and fluxes on the input library. At present, no provision is made for replacing the library group fluxes with a set more appropriate for a given application. If a "library" group is subdivided by a union-group boundary, ERRORR assumes the cross section and weighting function are both energy-independent, in order to estimate ϕ_k and z_k above and below the point of subdivision. The remainder of the calculation proceeds as with pointwise input.

A 620-group (SAND-II) GROUPR output library has been produced recently for the ENDF/B-V dosimetry materials, using a constant weight function. This library is also available on request.

Recent Extensions

In some materials, and in certain energy regions, the cross section uncertainty is dominated by the uncertainty in resolved resonance parameters. One noteworthy example is $^{63}Cu(n,\gamma)^{64}Cu$ (ENDF/B-V Material 6435) in the energy range from 10 eV to 15.9 keV, where the entire cross-section uncertainty is represented by means of resonance-parameter uncertainties. The same is true of $^{237}Np(n,f)$ (ENDF/B-V Material 6337) from 0 to 10 eV.

Beginning with the (10/81) version of ERRORR, the resonance-parameter contribution to the uncertainty in infinite-dilution fission and capture cross sections is included automatically when cross section covariances are processed.

This contribution is obtained from the Breit-Wigner formula for the fission and capture areas of a resonance, A_f and A_γ. By differentiating this formula with respect to the resonance parameters, one obtains a set of sensitivities. With these sensitivities and the

covariance matrix of the parameters from ENDF/B, one can apply a propagation-of-errors formula, similar to Eq. (2), to obtain the covariances $cov(A_\gamma,A_\gamma)$, $cov(A_\gamma,A_f)$, and $cov(A_f,A_f)$. These results then are added to the FNDF-specified "long-range" cross section covariances.

The resonance contribution is properly weighted with the isotopic abundance and the ratio of the weight function at the resonance to the average weight in the group. It is assumed, however, that the area of a resonance lies entirely within the group which contains the resonance energy E_r. Because of this assumption, and because ENDF/B provides no correlations between parameters of different resonances, the calculated resonance-parameter contribution affects only the diagonal elements of the affected matrices.

With the implementation of this feature, the uncertainty in the capture cross section of ^{63}Cu, for example, computed for a group which contains the large 577-eV resonance is 3.0%, rather than zero, as in earlier ERRORR versions.

The (10/81) version of ERRORR also handles explicit cross-material covariances. The only explicit cross-material covariances appearing in ENDF/B-V pertain to fission $\bar{\nu}$ values, but there is a clear need for more information of this type in future versions of the Dosimetry File.

A third, more recent, extension of the program allows the processing of covariances in cases when one cross section is measured relative to a well-known "standard" cross section. In such a case, the evaluator may represent the uncertainty in the first cross section as being the sum of two components. The first component is described by an explicit statement of the uncertainty in the measured ratio, whereas the second component, due to uncertainty in the standard, is represented implicitly, with the details provided only in the ENDF/B evaluation for the standard reaction.

In the dosimetry file, this situation occurs for the $^{238}U(n,\gamma)$ reaction (ENDF/B Material 6398), which was measured relative to $^{10}B(n,\alpha)$ from 4 keV to 20 keV, and the $^{239}Pu(n,f)$ reaction (ENDF/B material 6399), which was measured relative to $^{235}U(n,f)$ from 0.2 to 15 MeV. When ERRORR was modified to include the uncertainty in the standard, there was little effect for $^{233}U(n,\gamma)$, but there was a noticeable increase in the uncertainty of $^{239}Pu(n,f)$, from about 2% to 4-5% in the MeV region. This ratio-to-standard capability is not implemented in the distributed version of ERRORR, but a set of code changes to accomplish this is available from the authors on request.

PRODUCTION OF FINE-GROUP COVARIANCE LIBRARIES

In the above discussion, it is assumed that ERRORR is being used to generate the needed covariances directly in the user's group structure, which is the normal use of the program.

However, one can also use ERRORR to generate a library in a fine-group structure, and then use auxiliary collapsing programs to produce coarse-group libraries later. Such auxiliary programs would duplicate the parts of ERRORR which perform the sums shown in Eqs. (1) and (2). However, such auxiliary programs could be much smaller than ERRORR because they need not deal with the considerable complexities of the ENDF/B-V covariance formats.

In order to study the feasibility of generating and using fine-group covariance libraries, we have used ERRORR to produce a 137-group covariance library (containing energy group boundaries, cross sections, relative standard deviations, and relative covariance matrices) containing all of the materials and reactions in the ENDF/B-V Dosimetry File (Tape 531). A 1/E weight function was used for group averaging.

The energy grid employed is the same for all reactions, and was constructed by forming the union of all of energy grids used by evaluators in the covariance files of Tape 531. The resulting master grid is listed in Table I. For these 137-group calculations, the union grid is in all cases identical to the "user" grid, Fig. 1, because any ENDF energies found in a particular evaluation must match one of the "user" energies.

The choice of this group structure for an archival fine-group covariance library was made on the basis of minimizing the number of energy groups, subject to the constraint that information content of the ENDF/B covariance evaluations be preserved. The use of a coarser group structure would irreversibly average away at least some of the detailed correlation structure.

In addition, there is little economic incentive to go choose a coarser structure for the archival library. The computing time required to generate the 137-group 35-reaction library was rather modest, namely about 5 minutes of CDC-7600 central-processor time. This is only about 20% of the time required to produce the input resonance-reconstructed (PENDF) cross section set.

The library thus produced is, as expected, rather bulky. Even though the normal ERRORR output format suppresses zeros, the library contains over 38 000 card images. For this reason we have developed a new format for compact representation of covariance matrices which eventually will be an output option of the COVR module. The design of this format, called the "Boxer" format, proceeds from a simple fact: the ENDF/B-V covariance evaluations define certain rectangular regions (boxes) in energy space, over which the relative covariance is constant. (The ENDF/B format allowing a constant absolute covariance is rarely used, and is not used at all in the ENDF/B-V Dosimetry File). Thus one expects that an element of a multigroup relative covariance matrix derived from ENDF/B frequently will be identical either to the element before it in the same row, or to the element above it in the same column. Thus, the Boxer format allows a combination of "horizontal" and "vertical" repeat operations. Further details of the format are given in Appendix A.

The amount of data compression achieved by this format change is remarkable; from the original 38 000 card images the final library is reduced to less than 1000 card images. Of these 1000, only about 300 are needed for the covariance matrix data proper, with most of the remaining records containing cross section information. By way of comparison the covariance portion of the ENDF/B Dosimetry File itself occupies over 500 card images.

Table 1. RDC Library 137-Group Structure

Group Index	Lower Energy (eV)	Group Index	Lower Energy (eV)	Group Index	Lower Energy (eV)
1	1.00000E-05	47	2.30000E+05	93	4.10000E+06
2	2.53000E-02	48	2.50000E+05	94	4.50000E+06
3	3.00000E-02	49	3.00000E+05	95	5.00000E+06
4	9.00000E-02	50	3.03000E+05	96	5.50000E+06
5	2.50000E-01	51	3.40000E+05	97	5.75000E+06
6	6.25000E-01	52	3.50000E+05	98	6.00000E+06
7	1.00000E+00	53	4.00000E+05	99	6.25000E+06
8	1.80000E+00	54	4.50000E+05	100	6.40000E+06
9	3.00000E+00	55	5.00000E+05	101	7.00000E+06
10	5.00000E+00	56	5.30000E+05	102	7.50000E+06
11	1.00000E+01	57	5.50000E+05	103	8.00000E+06
12	1.50000E+01	58	6.00000E+05	104	8.50000E+06
13	2.00000E+01	59	6.30000E+05	105	9.00000E+06
14	4.00000E+01	60	6.50000E+05	106	9.28400E+06
15	5.00000E+01	61	7.50000E+05	107	9.50000E+06
16	8.00000E+01	62	8.00000E+05	108	1.00000E+07
17	1.60000E+02	63	8.23000E+05	109	1.00600E+07
18	2.00000E+02	64	8.30000E+05	110	1.04100E+07
19	3.00000E+02	65	8.50000E+05	111	1.05000E+07
20	4.00000E+02	66	9.00000E+05	112	1.06400E+07
21	5.00000E+02	67	9.50000E+05	113	1.06800E+07
22	6.00000E+02	68	1.00000E+06	114	1.10000E+07
23	1.00000E+03	69	1.02000E+06	115	1.15000E+07
24	2.00000E+03	70	1.05000E+06	116	1.16860E+07
25	3.00000E+03	71	1.20000E+06	117	1.20000E+07
26	4.00000E+03	72	1.40000E+06	118	1.24000E+07
27	4.80000E+03	73	1.60000E+06	119	1.24143E+07
28	7.00000E+03	74	1.61940E+06	120	1.25000E+07
29	8.00000E+03	75	1.74210E+06	121	1.30000E+07
30	1.00000E+04	76	1.89900E+06	122	1.31000E+07
31	1.50000E+04	77	2.00000E+06	123	1.35000E+07
32	2.00000E+04	78	2.07545E+06	124	1.40000E+07
33	2.30000E+04	79	2.20000E+06	125	1.42000E+07
34	2.50000E+04	80	2.40000E+06	126	1.45000E+07
35	3.00000E+04	81	2.50000E+06	127	1.50000E+07
36	4.00000E+04	82	2.60000E+06	128	1.55000E+07
37	5.00000E+04	83	2.80000E+06	129	1.60000E+07
38	6.00000E+04	84	2.96550E+06	130	1.65000E+07
39	6.76000E+04	85	3.00000E+06	131	1.70000E+07
40	8.00000E+04	86	3.10000E+06	132	1.75000E+07
41	9.00000E+04	87	3.24800E+06	133	1.80000E+07
42	1.00000E+05	88	3.27500E+06	134	1.85000E+07
43	1.30000E+05	89	3.30000E+06	135	1.90000E+07
44	1.50000E+05	90	3.50000E+06	136	1.92000E+07
45	1.84000E+05	91	3.70000E+06	137	1.96000E+07
46	2.00000E+05	92	4.00000E+06		2.00000E+07

The 137-group library in Boxer format is called the RDC (Reactor Dosimetry Covariance) Library. The library and a short retrieval program, TRIEVR, which reads the library and reconstructs full 137 x 137 matrices, are available on request.

Because of the compactness of the library, the retrieval program runs very fast. For example, to search through to find the last reaction in the library and reconstruct the covariance matrix requires less than 2 seconds of CDC-7600 time. To reconstruct all 35 matrices and write them onto a binary disk file requires only 17 seconds of 7600 time. By adding collapse algorithms (see next section) to TRIEVR, one could avoid the cost of permanently storing the large output file.

Coarse-Group Collapse of the RDC Library

We next consider the subject of "collapsing" the RDC multigroup covariances to a relatively coarse user-defined energy grid. Typically one needs covariances on an energy grid which is not exactly a sub-set of the fine-group grid. Thus, we are back to a situation essentially identical to that shown earlier in Fig. 1, provided that the "ENDF/B Grid" is relabelled the "RDC Grid." While the ENDF grid in Fig. 1 referred to the (material-dependent) evaluator's grid, the RDC grid is a characteristic of the entire fine-group library, being the same for all materials. Thus the union grid is also the same for all materials, and it can be determined in advance of any collapse calculations. Also one can calculate in advance the union group fluxes ϕ_k, using any weighting function $\phi(E)$ of interest. Finally, the y_m values in Fig. 1 can be identified with the fine-group cross sections in the RDC Library.

It is convenient to re-cast Eq. (2) in terms of relative covariances,

$$\frac{\mathrm{cov}(x_i,x_j)}{x_i\,x_j} = \sum_{\substack{k\in i \\ \ell\in i}} f_{ik}\, f_{j\ell}\, \frac{\mathrm{cov}(z_k,z_\ell)}{z_k\, z_\ell} \tag{5}$$

where

$$f_{ik} = \frac{\phi_k\, z_k}{\sum_{k\in i} \phi_k\, z_k} \tag{6}$$

is the fractional contribution to output group constant x_i from union group k.

The fact that the energy grid of the RDC Library includes all energy grids used in the ENDF/B-V dosimetry covariance files implies that the

relative covariance $\mathrm{cov}(z_k,z_\ell)/z_k\,z_\ell$ in Eq. (7) need not be reconstructed from ENDF/B; it is guaranteed to be exactly equal to one of the covariances $\mathrm{cov}(y_m,y_n)/y_m\,y_n$ in the RDC Library. It is only necessary to locate the RDC group m which contains union group k. This can be done, for example, by using a material-independent "pointer" array. For example, in the simple case shown in Fig. 1,

$$\frac{\mathrm{cov}(z_2,z_4)}{z_2\,z_4} = \frac{\mathrm{cov}(y_2,y_3)}{y_2\,y_3} \tag{7}$$

To complete the calculation of the coarse-group relative covariance, Eqs. (5) and (6), one needs only to evaluate the factors f_{ik}. If one has access only to the multigroup cross sections y_m, and not the underlying energy-dependent cross-section shape, one cannot proceed completely rigorously. However, because of the large number of groups in the RDC Library (see Table I), it is a good approximation to ignore the energy dependence here and simply set $z_k = y_m$, where RDC group m contains union group k.

REFERENCES

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APPENDIX A

The RDC Library (Boxer) Format

In the Boxer format, data is stored as a list of numerical data values (for example, relative covariances), together with a list of integers which control the loading of the data into the reconstructed array C(i,j). A negative integer, say -n, indicates that the next value in the data list is to be loaded into the next n j-values of C(i,j). A positive integer m means, for the next m j-values, simply carry down the value from the row above,

$$C(i,j) = C(i-1,j) \quad .$$

When the first row (i = 1) is being loaded, the row "above" is defined to be a row containing all zeroes.

In constructing the compressed data set, the choice between using the "repeat-new-value" method or the "carry-down" method is made dynamically on the basis of taking the longest possible "step." If m = n, the "carry-down" method is chosen, as it does not require an entry in the data list.

As an additional compression feature, one may indicate by a "flag" that the matrix C(i,j) is symmetric, hence only the upper right triangle is given explicitly in the compressed data library. These various aspects of the Boxer format are illustrated by a simple example in Fig. A-1. Here a, b, c, and d are arbitrary non-zero data values.

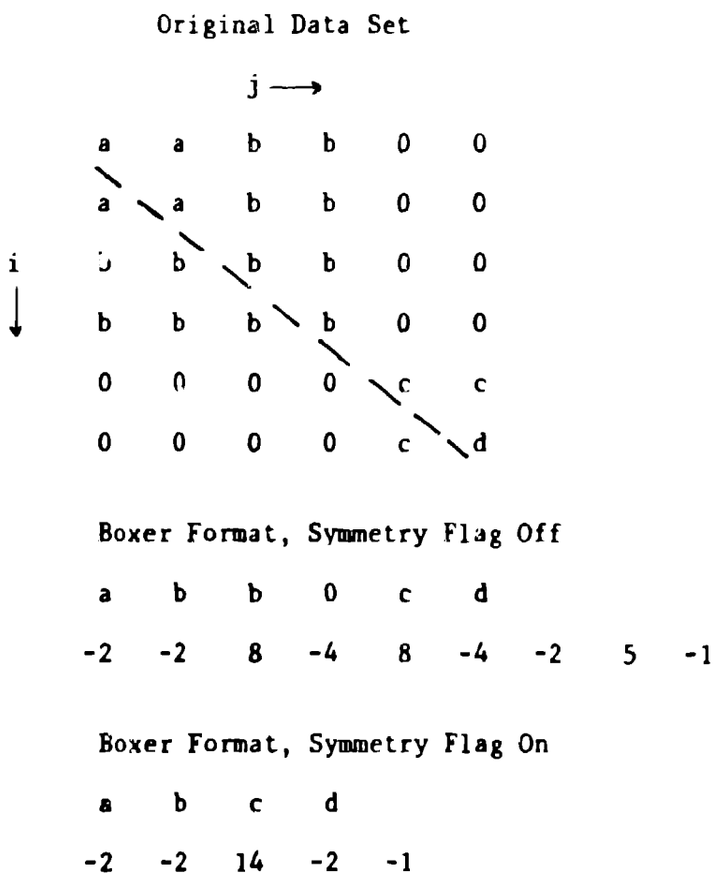

Fig. A-1. Illustration of Boxer Format