X. ERRORR

A. Introduction

After evaluators have completed their review of the available measurements of various nuclear data (having true values $\sigma_1, \sigma_2, \sigma_3, \cdots$) and the theoretical analysis, they will have formed at least a subjective opinion of the joint probability distribution of the data examined; that is, the probability

$$P(\sigma_1, \sigma_2, \cdots)\, d\sigma_1\, d\sigma_2 \cdots$$

that the true value of σ_1 lies in the range $(\sigma_1, \sigma_1+d\sigma_1)$, and that σ_2 lies in the range $(\sigma_2, \sigma_2+d\sigma_2)$, etc. In the early versions of the ENDF format, only the first moments (expectation values) of this probability distribution could be included in the numerical data files. However, beginning with ENDF/B-IV and expanding significantly in ENDF/B-V and ENDF/B-VI, the second moments of the data probability distributions have been included in many of the files. As discussed in Section B, these second moments (or “data covariances”) contain information on the uncertainty of individual data, as well as correlations that may exist.

Data covariances have many applications. For example, they can be combined with sensitivity coefficients to obtain the uncertainty, due to the data, in calculated quantities of applied interest.[1] This information can be used in turn to judge the adequacy of the data for that application.

The availability of data covariances also makes it possible to use the generalized method of least squares to improve the data evaluation after new integral or differential measurements have been performed.[2] The least-squares method requires only data covariances (not the full probability distribution), and the improved, or adjusted, data are guaranteed[3] to have the smallest possible uncertainties, regardless of the actual shape of the underlying probability distribution function, $P(\sigma_1, \sigma_2, \cdots)$. Thus, the ENDF-formatted covariance files contain, in about as compact a form as possible, a statement about the quality of the data, as well as sufficient information (in principle) to carry out future improvements on an objective basis.

In many of these applications, it is necessary to begin by converting energy-dependent covariance information in ENDF format[4] into multigroup form. This task can be performed conveniently in the NJOY environment, using the ERRORR module. In particular, ERRORR calculates the uncertainty in infinitely dilute multigroup cross sections (or multigroup $\bar{\nu}$ values), as well as the associated correlation coefficients. These data are obtained by combining absolute or relative covariances from ENDF Files 31, 32, and 33 with cross-section or $\bar{\nu}$ data from an existing processed cross-section library, either containing resonance-reconstructed "point" data or containing multigroup data from the GROUPR module of NJOY. ERRORR is coded to treat all approved ENDF-4, -5, and -6 covariance formats for these three files, up to and including a new covariance "law," `LB=8`, <u>except</u> that the processing of File 32 is restricted to Breit-Wigner resolved-resonance parameter uncertainties (`LRF=1` and `2`) in Version-5 format or in the "Version-5 compatible" option of Version 6 (`LCOMP=0`). The present version of ERRORR does not process information[5] from Files 30, 34, 35, and 40, nor from the recently proposed[6] File 36. Work is presently underway to remedy these shortcomings, with the focus being placed on Version-6 format features that are being used by current evaluators.

The methodology of ERRORR assumes that the weighting flux used to convert energy-dependent cross sections into multigroup averages is free of uncertainty. In calculating the effect of uncertainty in resonance parameters on the multigroup cross sections, it is approximated that the entire resonance area is contained in the energy group that contains the peak. Finally, in cases in which the cross-section information is obtained from an existing multigroup library, it is usually necessary to make assumptions about the shape of the cross section and the weight function within certain input energy groups, as discussed below in Section X.E. These are the only approximations or assumptions inherent to the program.

B. Definitions of Covariance-Related Quantities

For convenient reference in discussing the methodology and input requirements of the ERRORR module, we next review the basic definitions of covariance-related quantities. Let x_0 and y_0 be the evaluated values of x and y, respectively:

$$x_0 \equiv \mathrm{E}[x] \; , \tag{1}$$

and

$$y_0 \equiv \mathrm{E}[y] \; . \tag{2}$$

Here E is the expectation operator, which performs an average over the joint probability distribution of x and y. The second moment of this distribution is called the covariance of x with y:

$$\mathrm{cov}(x,y) \equiv \mathrm{E}[(x - x_0)\,(y - y_0)] \; . \tag{3}$$

Covariance is a measure of the degree to which x and y are both affected by the same sources of error. The covariance of x with itself is called the variance of x:

$$\mathrm{var}(x) \equiv \mathrm{cov}(x, x) = \mathrm{E}[(x - x_0)^2] \,. \tag{4}$$

The more familiar standard deviation Δx (also called the "uncertainty") is simply

$$\Delta x \equiv [\mathrm{var}(x)]^{1/2} = [\mathrm{cov}(x, x)]^{1/2} \,. \tag{5}$$

The correlation between x and y (also called the correlation coefficient) is defined as

$$\mathrm{corr}(x, y) \equiv \frac{\mathrm{cov}(x, y)}{\Delta x \; \Delta y} \,. \tag{6}$$

The absolute value of a correlation coefficient is guaranteed to be less than or equal to unity. Another useful quantity is the relative covariance of x with y,

$$\mathrm{rcov}(x, y) \equiv \frac{\mathrm{cov}(x, y)}{x_0 \; y_0} \,. \tag{7}$$

Unlike $\mathrm{cov}(x, y)$, the relative covariance $\mathrm{rcov}(x, y)$ is a dimensionless quantity. Closely related to the relative covariance is the relative standard deviation,

$$\frac{\Delta x}{x_0} = \frac{[\mathrm{cov}(x, x)]^{1/2}}{x_0} \,, \tag{8}$$

which, from Eq. (7), can be written as

$$\frac{\Delta x}{x_0} = [\mathrm{rcov}(x, x)]^{1/2} \,. \tag{9}$$

Combining Eqs. (6) and (7), we have another useful result,

$$\mathrm{corr}(x, y) = \frac{\mathrm{rcov}(x, y)}{(\Delta x / x_0)(\Delta y / y_0)} \,. \tag{10}$$

While it is customary to speak of uncertainties and correlations as separate entities, these are actually just two different aspects of the covariance. If one has a set of absolute covariances for various reactions, including the self-covariance, then Eqs. (5) and (6) can be used to calculate Δx and $\mathrm{corr}(x, y)$. Similarly, if one has a set of relative covariances, one can use Eqs. (9) and (10) to calculate $\Delta x / x_0$ and $\mathrm{corr}(x, y)$.

Consider now a set of nuclear data σ_i with uncertainties characterized by the covariances $\mathrm{cov}(\sigma_i, \sigma_j)$. Let A and B be two linear functions of the σ_i,

$$A = \sum_i a_i \, \sigma_i$$

$$B = \sum_j b_j \, \sigma_j \ ,$$

where the a_i and b_j are sets of known constants. The above definitions can be used to calculate the covariances of the functions A and B induced by the covariances of the data. From Eq. (3),

$$\begin{aligned} \mathrm{cov}(A, B) &= \mathrm{E}\left\{ \left(\sum_i a_i \, \sigma_i \; - \; \sum_i a_i \mathrm{E}(\sigma_i) \right) \left(\sum_j b_j \, \sigma_j - \sum_j b_j \, \mathrm{E}(\sigma_j) \right) \right\} \\ &= \sum_{i,\,j} a_i \, b_j \, \mathrm{E}\left\{ \left(\sigma_i - \mathrm{E}(\sigma_i) \right) \left(\sigma_j - \mathrm{E}(\sigma_j) \right) \right\} \ , \end{aligned}$$

so that

$$\mathrm{cov}(A, B) = \sum_{i,j} a_i \, b_j \, \mathrm{cov}(\sigma_i, \sigma_j) \ . \tag{11}$$

This result, called the "propagation of errors" formula, is fundamental to the subject of multigroup processing of ENDF covariance data and will be referenced frequently in later sections of this chapter.

C. Structure of ENDF Files 31 and 33: Energy-Dependent Data

Data in ENDF format are stored in various numbered "files," where the file number depends on the type of information contained. For example, the covariances of $\bar{\nu}(E)$ (the average number of neutrons per fission, which is a function of the incident neutron energy) are stored in File 31, where the possible "reaction" types are prompt $\bar{\nu}$, delayed $\bar{\nu}$, and total $\bar{\nu}$. File 32 describes the uncertainty in the shape and area of individual resonances. File 33 contains the covariances of energy-dependent cross sections. Within the resolved-resonance energy range, File 33 includes any "long-range" covariances in the reconstructed cross sections, such as covariance components that are highly correlated over many neighboring resonances. The structures of Files 31 and 33 are identical and will be described first.

Files 31 and 33 describe the covariances of energy-dependent data. To expand on this point, we recall that the full energy dependence of a cross section $\sigma(E)$, for example, is described in the ENDF File 3 by specifying the cross-section values at a relatively small number of energy points and then providing a set of interpolation laws to be used in reconstructing the actual cross section at any intermediate energy. Somewhat the same philosophy is used to describe the two-dimensional energy dependence of data covariances in Files 31 and 33. That is, one specifies a set of numerical data and a set of formulae, which together can be used to compute $\text{cov}(x, y)$ for any desired pair of energies, E_x and E_y. Although the interpolation laws are presently restricted to the simple forms described below, it is not true (as sometimes stated) that ENDF contains multigroup covariances. The expression "multigroup covariance" refers to the covariance of one multigroup-averaged quantity with another averaged quantity, whereas ENDF contains the covariances between point-energy data. It is precisely the task of ERRORR to compute multigroup covariances, starting from point covariances.

Files 31 and 33 of an evaluation for material `MAT` are divided into "sections," indexed by the reaction type `MT`. A section `(MAT,MT)` is further subdivided into "subsections." As described in Ref. 4, a subsection is the repository for all explicit statements of the two-dimensional energy dependence of the covariances of reaction `(MAT,MT)` with another reaction `(MAT1,MT1)`. Because covariances are symmetric, a subsection with `MAT1=MAT` and `MT1<MT` would be redundant with a subsection in an earlier section, and such data are, by convention, omitted from the ENDF files.

Subsections are further divided into "sub-subsections." Two different types of sub-subsections are used in the ENDF-5 and ENDF-6 formats. (Although ERRORR also treats data covariances in the earlier ENDF-4 format, this is of little practical interest since only three covariance evaluations were released in Version-4 format.) "NI-type" sub-subsections are used to express covariances explicitly, while "NC-type" sub-subsections are used to indicate the existence of connections between various data that result in "implicit" covariance contributions for various reaction pairs. We shall return to this point in NC-Type Sub-Subsections, Section X.C.2.

1. NI-Type Sub-Subsections. Multiple NI-type sub-subsections are used to describe multiple, statistically independent sources of uncertainty for a given reaction pair. If $\text{cov}(x, y)_n$ is the covariance computed from the data in one sub-subsection, then, because the uncertainties in different sub-subsections are uncorrelated,

$$\text{cov}(x, y) \;=\; \sum_{n=1}^{\text{NI}} \text{cov}(x, y)_n \;,$$

where NI is the number of NI-type sub-subsections in the current subsection. The numerical content of one NI-type sub-subsection consists of either one or two energy grids, a collection of constants, and a parameter LB. The parameter LB governs how the energies and constants are to be used in constructing the covariance in various rectangular regions of $E_x{-}E_y$ space. For LB=0, 1, 2, and 8, a single table containing pairs (E_i, F_i) is given. For LB=3 and 4, two such tables are given. For LB=5, a single set of energies E_i is given, along with an associated square matrix of constants G_{ij}. Finally, for LB=6, two energy grids are given, along with an associated rectangular matrix of constants G'_{ij}.

The first of these tables (E_i, F_i) defines a function $f(E)$ that is constant except for discrete steps at energies E_i,

$$f(E) = F_i, \text{ if } E_i \le E < E_{i+1} . \tag{12}$$

Similarly, if there is a second table,

$$f'(E) = F'_i, \text{ if } E'_i \le E < E'_{i+1} . \tag{13}$$

The LB=5 matrix data G_{ij} also define a function,

$$g(E_x, E_y) = G_{ij}, \text{ if } E_i \le E_x < E_{i+1} \text{ and } E_j \le E_y < E_{j+1} , \tag{14}$$

and similarly for LB=6

$$g'(E_x, E_y) = G'_{ij}, \text{ if } E_i \le E_x < E_{i+1} \text{ and } E'_j \le E_y < E'_{j+1} . \tag{15}$$

These functions are simply histograms in either one or two dimensions. Using the functions f, f', g, and g' thus defined, we can list the formulae in Eq. (16), which are used to specify energy-dependent covariances for the different allowed values of LB. Thus, if x is the value of the cross section or of the $\bar{\nu}$ value for the reaction (MAT,MT) that determines the ENDF/B <u>section</u>, and if y is the value for the reaction (MAT1,MT1) that determines the <u>subsection</u>, then for

$$\begin{array}{lclll}
\text{LB} & = & 0, & \text{cov}(x,y)_n & = f(E_x)\,\delta(E_x,E_y) \\
\text{LB} & = & 1, & \text{rcov}(x,y)_n & = f(E_x)\,\delta(E_x,E_y) \\
\text{LB} & = & 2, & \text{rcov}(x,y)_n & = f(E_x)\,f(E_y) \\
\text{LB} & = & 3, & \text{rcov}(x,y)_n & = f(E_x)\,f'(E_y) \\
\text{LB} & = & 4, & \text{rcov}(x,y)_n & = f(E_x)\,\delta(E_x,E_y)\;f'(E_x)\,f'(E_y) \\
\text{LB} & = & 5, & \text{rcov}(x,y)_n & = g(E_x,E_y) \\
\text{LB} & = & 6, & \text{rcov}(x,y)_n & = g'(E_x,E_y) \;.
\end{array} \tag{16}$$

The symbol $\delta(E_x, E_y)$ has the following meaning: $\delta(E_x, E_y)$=1 if E_x and E_y fall in the same energy interval of the first table (E_i, F_i), and $\delta(E_x, E_y)$=0 otherwise.

The final covariance law, `LB=8`, is an exceptional case that cannot be expressed in terms of point covariances. `LB=8` is used primarily to represent uncertainty effects due to suspected, but unresolved, energy-dependent structure in a given cross section. If ΔE_j is the energy width of the j-th "union" energy group (see the discussion of union groups in Section X.E), and if this group lies within the k-th range (E_k, E_{k+1}) of an ENDF `LB=8` energy grid, then the effect of the `LB=8` subsection is to trigger the addition of an uncorrelated contribution of $F_k\,(E_{k+1} - E_k)/\Delta E_j$ to the (absolute) variance of the j-th union-group cross section. No contributions to off-diagonal elements of the multigroup covariance matrix are generated by an `LB=8` sub-subsection.

2. NC-Type Sub-Subsections. NC-type sub-subsections, which describe covariances indirectly, are used in several evaluation situations, which are flagged by different values of the parameter `LTY`. The first situation, `LTY=0`, occurs when the following two conditions are met: (a) the covariances of a given reaction `MT`, both with itself and with other reactions, can be deduced in an energy range `(E1,E2)` solely from the application of a cross-section "derivation relation,"

$$x(\mathtt{MAT},\mathtt{MT};E) = \sum_i C_i\, x(\mathtt{MAT},\mathtt{MT}_i;E), \tag{17}$$

and (b) the covariances of all of the reaction cross sections on the right-hand side of Eq. (17) have been given directly (that is, using only NI-type sub-subsections) throughout the range `(E1,E2)`. The energy boundaries `E1` and `E2`, the constants C_i, and the reaction identifiers $\mathtt{MT}_i$ are specified in an NC-type sub-subsection with `LTY=0`. This format is widely used in the ENDF/B library, and it makes possible the elimination of large volumes of otherwise redundant data. It also introduces considerable complexity in the multigroup processing, as discussed in Section G, and adds to the computer running times. The presence of this one short sub-subsection affects the calculation of the covariances for many different reaction pairs, such as x`(MAT,MT)` with $x(\mathtt{MAT},\mathtt{MT}_i)$. Less widely used are NC-type sub-subsections with `LTY=1`. These are employed when a reaction `MT` in material `MAT` is evaluated in some energy range `(E1,E2)` as a ratio to a standard reaction `MTS` in some other material `MATS`. That is,

$$x(\mathtt{MAT},\mathtt{MT};E) = R(E)\, x(\mathtt{MATS},\mathtt{MTS};E). \tag{18}$$

In practical evaluation situations, the uncertainty of R is almost never correlated with that of x(MATS,MTS). Because of this, the relative uncertainty in R is treated simply as one independent component of the relative uncertainty in x(MAT,MT), and it is described using normal NI-type sub-subsections. On the other hand, the contribution from uncertainty in x(MATS,MTS) is represented with an NC-type sub-subsection with LTY=1, which contains, in ENDF/B-V, only E1, E2, MATS, and MTS. The actual numerical covariance information must be read from the evaluation for the standard material MATS, which usually resides on an entirely different ENDF tape. An NC-type sub-subsection with LTY=1, which occurs in a given subsection (MAT,MT; MAT,MT), affects the calculation of the covariances only for the current reaction pair (reaction MT with itself) and, in this respect, is more like an NI-type sub-subsection than, for example, an NC-type sub-subsection with LTY=0. This similarity is exploited in the processing of ratio covariances, as discussed in Section X.H.

An NC-type sub-subsection with LTY=2 is used, in a similar way, to describe the covariances of x(MAT,MT) with x(MATS,MTS). As in the LTY=1 case, an LTY=2 sub-subsection contains only E1, E2, MATS, and MTS.

An NC-type sub-subsection with LTY=3 is included in material MATS to describe the (redundant) covariances of x(MATS,MTS) with x(MAT,MT). The numerical information contained here is the same as for LTY=1 and 2. As discussed in Section X.H, an important function of LTY=3 data is to help locate reactions other than (MAT,MT) that have been measured relative to the same standard (MATS,MTS).

D. Resonance-Parameter Formats—File 32

File 32 contains covariances of resonance parameters from File 2. ERRORR processes File 32 in the following limited sense: when infinite-dilution cross-section covariances are processed (see previous section) from File 33, the diagonal elements of the resulting (self-reaction) multigroup covariance matrices are augmented by contributions based on the parameter covariances in File 32.

For evaluations produced in ENDF-5 format, all approved covariance format options are treated. For ENDF-6, many new possibilities were created,[5] including the capability of specifying uncertainty in unresolved-resonance parameters (LRU=2) and to represent correlations between the resolved parameters of different resonances (LCOMP$\neq$ 0). At present ERRORR treats the ENDF-6 File-32 format only in the case where resolved parameters are treated in the "Version-5 compatible" format (LCOMP=0, LRU=1, LRF=1 or 2 only). This restriction is not as serious as it may sound, because, as of the issue date of Release 2 of ENDF/B-VI, all

ENDF/B-VI evaluations containing File 32 use the simple "Version-5 compatible" format. The following discussion, therefore, is limited to this option.

For either of the permitted resolved resonance formalisms (`LRF=1` or `2`), the parameters considered in File 32 are the resonance energy E_r, the neutron width Γ_n, the radiative capture width Γ_γ, the fission width Γ_f, and (in Version 5 only) the total angular momentum J. All cross-parameter relative covariances, such as rcov(Γ_n,Γ_γ), are included, with the exception of the covariances of E_r with the remaining parameters, which are assumed to be negligible. Cross-resonance covariances, such as cov(E_r^i, E_r^j), where i and j refer to different resonances, are omitted in the `LCOMP=0` option.

E. Calculation of Multigroup Fluxes, Cross Sections, and Covariances on the Union Grid

As mentioned before, the main function of the ERRORR module is to calculate the uncertainty in group-averaged cross sections at infinite dilution due to uncertainty in the ENDF point data. In this and the following sections, we describe the procedures used in performing this task.

In order to proceed, it is necessary to introduce into the discussion three different energy grids, namely, the user grid, the ENDF grid, and the union grid. The relationship of these three grids is shown in Fig. 1. The user grid is the multigroup structure in which the output multigroup covariances are to be produced. The ENDF grid is the collection of energies obtained (in subroutines `GRIDD` and `GRIST`) by forming the union of (a) all energy "lists" appearing in any NI-type sub-subsection of any subsection to be processed in the current ENDF material, and (b) all energy pairs used to define the range of effectiveness of any NC-type sub-subsection of any subsection to be processed. The union grid, on the other hand, is simply the union of the user grid and ENDF grid. The utility of the union grid is that (a) the covariances are particularly simple to calculate in this grid, as discussed below, and (b) the multigroup covariances needed by the user are then easily obtainable by a straightforward collapse from this to the user grid. In fact, the design of the current ENDF covariance format was strongly influenced by the desire to employ this particular procedure for multigroup processing.[7, 8]

After the union grid is formed in `SUBROUTINE UNIONG`, the cross sections $x(E)$ and weighting flux $\phi(E)$ are integrated to produce x_I and ϕ_I, multigrouped on this grid. If point cross sections are supplied, an exact integration is done in `SUBROUTINE GRPAV`. If, on the other hand, a multigroup cross-section library is supplied, then `SUBROUTINE COLAPS` is used. If a library group is subdivided by

User Grid	ϕ_1, X_1		ϕ_2, X_2	
ENDF Grid	F_1	F_2		F_3
Union Grid	ϕ_1, x_1	ϕ_2, x_1	ϕ_3, x_3	ϕ_4, x_4

Figure 1: Illustration of energy grid relations.

a union-group boundary, then over the span of that library group, the unknown energy dependencies of $x(E)$ and $\phi(E)$, which are needed to calculate x_I and ϕ_I, are approximated in `SUBROUTINE COLAPS` by constants. Normally, the effect of this approximation is not large and, in any case, can be reduced or eliminated by increasing the number of groups in the input library.

We next consider the theoretical basis for the calculation of union-grid multigroup covariances, as performed in `SUBROUTINE COVCAL`. By definition, x_I is just the average of $x(E)$ over union group I,

$$x_I \equiv \frac{\int_I \phi(E)\, x(E)\, dE}{\int_I \phi(E)\, dE} \; , \tag{19}$$

where $\phi(E)$ is the flux "model" assumed for the multigroup calculations. Let y_J denote similarly the average of $y(E)$ over union group J.

Let us imagine that these groups are subdivided into many subintervals of infinitesimal width, so that in the i-th subinterval of group I, for example, $x(E)$ can be well approximated by the constant x_i. By this device, the integrals that define x_I and y_J can be converted to discrete sums:

$$x_I = \frac{\sum_{i \in I} \phi_i\, x_i}{\phi_I} = \sum_{i \in I} \alpha_{Ii}\, x_i \; , \tag{20}$$

where

$$\phi_i = \int_i \phi(E)\, dE \; , \tag{21}$$

$$\phi_I = \sum_{i \in I} \phi_i = \int_I \phi(E)\, dE \; , \tag{22}$$

and

$$\alpha_{Ii} \equiv \frac{\phi_i}{\phi_I} \; . \tag{23}$$

From these definitions, clearly

$$\sum_{i \in I} \alpha_{Ii} \;=\; 1 \; . \tag{24}$$

Similarly for y,

$$y_J = \sum_{j \in J} \alpha_{Jj} \; y_j \; , \tag{25}$$

and

$$\sum_{j \in J} \alpha_{Jj} = 1 \; . \tag{26}$$

The methodology of ERRORR assumes that $\phi(E)$ in Eq. (19) is free of uncertainty. Under this assumption, the terms α_{Ii} and α_{Jj} are simply known constants. The covariance of x_I with y_J can then be calculated using the propagation-of-errors formula, Eq. (11), together with Eqs. (20) and (25).

$$\begin{aligned} \mathrm{cov}(x_I, y_J) &= \sum_{\substack{i \in I \\ j \in J}} \alpha_{Ii} \; \alpha_{Jj} \; \mathrm{cov}(x_i, y_j) \\ &= \sum_{\substack{i \in I \\ j \in J}} \alpha_{Ii} \; \alpha_{Jj} \; \sum_n \mathrm{cov}(x_i, y_j)_n \; , \end{aligned} \tag{27}$$

where the summation over n results from the different independent contributions to the ENDF point covariances coming from the different NI-type sub-subsections. Changing the order of summation, we obtain

$$\mathrm{cov}(x_I, y_J) \;=\; \sum_n \; \mathrm{cov}(x_I, y_J)_n \; , \tag{28}$$

where

$$\mathrm{cov}(x_I, y_J)_n \;=\; \sum_{\substack{i \in I \\ j \in J}} \alpha_{Ii} \; \alpha_{Jj} \;\; \mathrm{cov}(x_i, y_j)_n \; . \tag{29}$$

To evaluate the sum in Eq. (29), we make use of the fact that union groups I and J do not cross any ENDF grid boundaries. Recalling the discussion of NI-type sub-subsections in Section X.C (and excluding for the moment the case where sub-subsections with `LB=8` are present), there are only two possibilities for the energy dependence of the covariance between ENDF grid points; thus, over the limits of the sum, either $\mathrm{cov}(x_i, y_j)_n$ is independent of i and j (if `LB=0`) or $\mathrm{rcov}(x_i, y_j)_n$ is independent of i and j (if $1 \leq$ `LB` ≤ 6). We consider first the constant-absolute-covariance case, `LB=0`. Eq. (29) can then be rewritten as follows:

$$\mathrm{cov}(x_I, y_J)_n \;=\; \mathrm{cov}(x, y)_n \sum_{\substack{i\in I\\ j\in J}} \alpha_{Ii}\, \alpha_{Jj} \;=\; \mathrm{cov}(x, y)_n \left(\sum_{i\in I} \alpha_{Ii}\right) \left(\sum_{j\in J} \alpha_{Jj}\right) . \tag{30}$$

Invoking Eqs. (24) and (26), we obtain

$$\mathrm{cov}(x_I, y_J)_n \;=\; \mathrm{cov}(x, y)_n \qquad (\mathtt{LB} = 0)\,. \tag{31}$$

For `LB`-values ranging from 1 to 6, the relative covariance is constant over each union group, so we rewrite Eq. (29) in the form

$$\begin{aligned}
\mathrm{cov}(x_I, y_J)_n \;&=\; \sum_{\substack{i\in I\\ j\in J}} \alpha_{Ii}\, \alpha_{Jj}\; x_i\; x_j\; \mathrm{rcov}(x_i, x_j)_n \\
&=\; \mathrm{rcov}(x, y)_n \sum_{\substack{i\in I\\ j\in J}} (\alpha_{Ii}\; x_i)\, (\alpha_{Jj}\; y_j) \\
&=\; \mathrm{rcov}(x, y)_n \left(\sum_{i\in I} \alpha_{Ii}\; x_i\right) \left(\sum_{j\in J} \alpha_{Jj}\; y_j\right) .
\end{aligned} \tag{32}$$

Substituting here from Eqs. (20) and (25), we obtain

$$\mathrm{cov}(x_I, y_J)_n = x_I\; y_J\; \mathrm{rcov}(x, y)_n \qquad (1 \leq \mathtt{LB} \leq 6)\,. \tag{33}$$

The final union-group multigroup covariance is obtained by inserting these results, Eqs. (31) and (33), back into Eq. (28)

$$\mathrm{cov}(x_I, y_J) = \sum_{\mathrm{n(LB=0)}} \mathrm{cov}(x, y)_n \;+ \sum_{\mathrm{n(LB=1,6)}} x_I\; y_J\; \mathrm{rcov}(x, y)_n\,, \tag{34}$$

where the first sum runs over all sub-subsections with `LB=0` and the second runs over all sub-subsections with `LB=1` through `6`. The quantities $\mathrm{cov}(x, y)_n$ and $\mathrm{rcov}(x, y)_n$ here are simply the point-energy covariances from the ENDF covariance file, as described in Eqs. 12 through 16. Equation (34) then is the basic equation used in `SUBROUTINE COVCAL` to calculate the desired union-group covariances.

The final step, if sub-subsections with `LB=8` are present, is to increment the diagonal elements (variances) as follows:

$$\mathrm{cov}(x_I, x_I) = \mathrm{cov}(x_I, x_I) + F_k\, (E_{k+1} - E_k)/\Delta E_I\,, \tag{35}$$

where k indexes the range of the `LB=8` energy grid that includes union group I.

F. Basic Strategy for Collapse to the User Grid

The union-group fluxes ϕ_I are used, in `SUBROUTINE SIGC`, to collapse the union-group cross sections to the coarser user grid. Changing notation slightly, let us denote by $x_I(a)$ the cross section in union group I for reaction a, and similarly let $X_K(a)$ be the cross section in user group K for the same reaction. In complete analogy with Eq. (20)

$$X_K(a) = \frac{\sum\limits_{I\in K} \phi_I \, x_I(a)}{\phi_K} = \sum_{I\in K} A_{KI} \, x_I(a) \; , \tag{36}$$

where

$$\phi_K = \sum_{I\in K} \phi_I \; , \tag{37}$$

and

$$A_{KI} = \frac{\phi_I}{\phi_K} \; . \tag{38}$$

Applying the propagation-of-errors formula again gives

$$\mathrm{cov}\,[X_K(a), X_L(b)] = \sum_{\substack{I\in K\\ J\in L}} A_{KI} \, A_{LJ} \, \mathrm{cov}[x_I(a), x_J(b)] \; . \tag{39}$$

An alternative expression, obtained by simply rearranging coefficients, is

$$\mathrm{cov}\,[X_K(a), X_L(b)] = \frac{1}{\phi_K \phi_L} \sum_{\substack{I\in K\\ J\in L}} T_{IJ}(a,b) \; , \tag{40}$$

where

$$T_{IJ}(a,b) = \phi_I \, \phi_J \, \mathrm{cov}[x_I(a), x_J(b)] \; . \tag{41}$$

Eqs. (40) and (41) provide the basic framework in the ERRORR module for the production of multigroup covariances in the coarse user-group structure. Finally, if the user requests it, the absolute covariances from Eq. (40) are converted to relative form,

$$\mathrm{rcov}[X_K(a), X_L(b)] = \frac{\mathrm{cov}[X_K(a), X_L(b)]}{X_K(a) \, X_L(b)} \; . \tag{42}$$

G. Group-Collapse Strategy for Data Derived by Summation

The procedure described in the previous section must be modified if, in some energy range, either reaction a or b is a "derived" quantity in the sense of Eq. (17) or Eq. (18). In such a case, one cannot apply Eq. (34) directly to the calculation of $\mathrm{cov}[x_I(a), x_J(b)]$, because the covariances on the right-hand side of Eq. (34) will be missing from the ENDF file in the affected energy region.

We consider first the case in which some cross sections are evaluated ("derived") by simply summing other evaluated cross sections, as in Eq. (17). Equation (35) can then be rewritten as

$$X_K(a) = \sum_{I \in K} A_{KI} \left\{ \sum_{\text{all c}} C_I(a,c)\, x_I(c) \right\} , \tag{43}$$

where the quantity in curly brackets is the value of the derived cross section "a" in union group I, as reconstructed from the directly evaluated cross sections $x_I(c)$. The derivation coefficients $C_I(a,c)$ depend on the union-group index I, because the evaluator is permitted to employ different derivation strategies in different energy ranges in order to simplify and shorten the covariance files.

To expand on this last point, suppose there are only three reactions, and suppose that the cross sections $x(1)$ and $x(2)$ rigorously sum to $x(3)$ at all energies. Further suppose that within the energy range covered by the first union group, the cross-section evaluator has used this logical connection in order to "derive" $x(3)$, that is to evaluate $x(3)$, by summing the existing evaluations for $x(1)$ and $x(2)$,

$$x_1(3) = x_1(1) \ + \ x_1(2) \, . \tag{44}$$

Further suppose that in the range of union group 2, $x(1)$ is derived by employing the same logical connection, but in a different way,

$$x_2(1) = x_2(3) - x_2(2) \, , \tag{45}$$

and in union group 3, all three reactions are directly evaluated.

In this example $C_I(a,c)$ has the following values:

$$
\begin{array}{ccc}
\begin{array}{rcl}
C_1(1,1) & = & 1 \\
C_1(2,1) & = & 0 \\
C_1(3,1) & = & 1
\end{array} &
\begin{array}{rcl}
C_1(1,2) & = & 0 \\
C_1(2,2) & = & 1 \\
C_1(3,2) & = & 1
\end{array} &
\boxed{\begin{array}{rcl}
C_1(1,3) & = & 0 \\
C_1(2,3) & = & 0 \\
C_1(3,3) & = & 0
\end{array}}
\end{array}
$$

$$
\begin{array}{ccc}
\boxed{\begin{array}{rcl}
C_2(1,1) & = & 0 \\
C_2(2,1) & = & 0 \\
C_2(3,1) & = & 0
\end{array}} &
\begin{array}{rcr}
C_2(1,2) & = & -1 \\
C_2(2,2) & = & 1 \\
C_2(3,2) & = & 0
\end{array} &
\begin{array}{rcl}
C_2(1,3) & = & 1 \\
C_2(2,3) & = & 0 \\
C_3(3,3) & = & 1
\end{array}
\end{array}
$$

$$
\begin{array}{ccc}
\begin{array}{rcl}
C_3(1,1) & = & 1 \\
C_3(2,1) & = & 0 \\
C_3(3,1) & = & 0
\end{array} &
\begin{array}{rcl}
C_3(1,2) & = & 0 \\
C_3(2,2) & = & 1 \\
C_3(3,2) & = & 0
\end{array} &
\begin{array}{rcl}
C_3(1,3) & = & 0 \\
C_3(2,3) & = & 0 \\
C_3(3,3) & = & 1
\end{array}
\end{array}
$$

Note that in all cases we have formally considered the evaluated cross sections to be derived from themselves, $C_I(a,c)|_{\text{eval}}{=}\delta_{ac}$. This device allows us to use Eq. (42) for all reactions, regardless of whether they are derived or evaluated. Note that, in every case where reaction c is derived in group I, $C_I(a,c){=}0$. (See boxed submatrices.) This null "sensitivity coefficient" is important, because it means that Eq. (42) remains a linear relation involving only dependent quantities with known covariances (the evaluated subset of the union-group cross sections) on the right. This allows us once again to use the propagation-of-errors formula to obtain the desired user-group covariances.

$$
\mathrm{cov}[X_K,(a),X_L(b)] = \sum_{\substack{\text{all c}\\ \text{all d}}} \sum_{\substack{I\in K\\ J\in L}} A_{KI}\,C_I(a,c)\,A_{LJ}\,C_J(b,d)\,\mathrm{cov}[x_I(c),x_J(d)]\;, \tag{46}
$$

or, alternatively,

$$
\mathrm{cov}[X_K,(a),X_L(b)] = \frac{1}{\phi_K\phi_L} \sum_{\substack{\text{all c}\\ \text{all d}}} \sum_{\substack{I\in K\\ J\in L}} C_I(a,c)\,C_J(b,d)\,T_{IJ}(c,d)\;, \tag{47}
$$

where

$$
T_{IJ}(c,d) = \phi_I\;\phi_J\;\mathrm{cov}[x_I(c),x_J(d)]\;. \tag{48}
$$

In `SUBROUTINE COVCAL`, the flux-covariance product T_{IJ} is calculated for all evaluated reaction pairs and written to a "scratch" binary disk file, unit 11. (For diagnostic purposes, it is possible to change this to a formatted scratch file by manually resetting the variable `IMODE` to +1 in the main program.) In the subsequent collapse to the user's group structure in `SUBROUTINE COVOUT`, the user-group covariances $\text{cov}[X_K(a), X_L(b)]$ for one specific a-b reaction pair, for all "MT1" energy groups L, and for as large a range of "MT" energy groups K as possible, are calculated simultaneously in memory.

In `COVOUT`, the disk file (unit 11) is rewound and read completely through, once in each range of MT groups for each a-b reaction pair, to access the union-group covariances for the evaluated reactions. As the union-group data pass through memory, contributions to the user-group covariances are accumulated using Eq. (46). To minimize the number of disk reads and the amount of running time, the dimension of the array in `COMMON/ESTORE/` (and the value of the associated variable `NAMAX`) should be set as large as possible.

In the fairly common situation where cross sections $x(a)$ and $x(b)$ are directly evaluated over the whole energy range of the data file,

$$C_I(a,c) = \delta_{ac}, \text{ for all } I, \tag{49}$$

and

$$C_J(b,d) = \delta_{bd}, \text{ for all } J. \tag{50}$$

In this case, Eq. (46) can be greatly simplified.

$$\begin{aligned} \text{cov}[X_K(a), X_L(b)] &= \frac{1}{\phi_K \phi_L} \sum_{\substack{\text{all c} \\ \text{all d}}} \sum_{\substack{I \in K \\ J \in L}} \delta_{ac}\, \delta_{bd}\, T_{IJ}(c,d) \\ &= \frac{1}{\phi_K \phi_L} \sum_{\substack{I \in K \\ J \in L}} T_{IJ}(a,b)\,. \end{aligned} \tag{51}$$

This result, which is identical to Eq. (39), suggests a shortcut calculational path, which is followed in `SUBROUTINE COVOUT` whenever both reactions are directly evaluated. In preparation for this situation, a second copy of the `COVCAL` binary output file is generated when `COVOUT` is first called. The second copy, on unit 12, is read only in the trivial derivation cases just described (flagged in the code by setting `ISD=1`). Unit 12 is not rewound before processing a given reaction pair a-b, since earlier reaction pairs on the file do not contribute to the sum in Eq. (46) in these cases. Reading of the second copy stops after the union-group covariances for reaction pair a-b are found, because the later reaction pairs do not contribute either.

H. Processing of Data Derived from Ratio Measurements

The treatment of implicit covariances that arise from ratio measurements, as in Eq. (18), is totally different from the treatment of data derived by summation, Eq. (17), discussed in the previous section. Before discussing the processing details, it is helpful first to review the subject of ratio evaluations generally. Returning to the "x-y" notation of Section X.B, let $x(E_x)$ be the value of the cross section for reaction x at energy E_x, and $y(E_y)$ the cross section for reaction y at energy E_y. In some energy region (L_x, H_x), suppose that the best knowledge of $x(E_x)$ is obtained through the application of a measured ratio, $u(E_x)$:

$$x(E_x) = u(E_x)\, z(E_x), \text{ if } L_x \le E_x \le H_x \ , \tag{52}$$

where reaction z is some well-known cross section, possibly one of the official ENDF/B standard cross sections. Similarly, suppose y is derived from the same standard, over a possibly different energy range:

$$y(E_y) = v(E_y)\, z(E_y), \text{ if } L_y \le E_y \le H_y \ . \tag{53}$$

By performing a first-order Taylor-series expansion and then applying the formula for propagation of errors, one can obtain an expression for the contribution to the relative covariance $\mathrm{rcov}[x(E_x), y(E_y)]$ that is attributable to these ratio measurements. In the usual case, where the ratios u and v are only weakly correlated with the standard cross section z, the result is quite simple:

$$\mathrm{rcov}[x(E_x), y(E_y)]_{\mathrm{ratio}} = \mathrm{rcov}[u(E_x), v(E_y)] + \mathrm{rcov}[z(E_x), z(E_y)] \ , \tag{54}$$

if $L_x \le E_x \le H_x$ and $L_y \le E_y \le H_y$, and

$$\mathrm{rcov}[x(E_x), y(E_y)]_{\mathrm{ratio}} = 0 \ \text{ otherwise.} \tag{55}$$

Thus, in this fairly common evaluation situation, the covariance separates naturally into a part involving only the measured ratios and a part involving only the standard. Because the second contribution, $\mathrm{cov}(\mathrm{MT}_z, \mathrm{MT}_z)$, can be read directly from the NI-type sub-subsections in evaluation for the standard, it is not included explicitly in the ENDF subsections for the derived quantities, $\mathrm{cov}(\mathrm{MT}_x, \mathrm{MT}_x)$ or $\mathrm{cov}(\mathrm{MT}_y, \mathrm{MT}_y)$. Instead, the existence of this additional contribution to the covariance is signalled by the presence of an NC-type sub-subsection, as discussed in Section X.C.

The strategy adopted for processing this information in `SUBROUTINE STAND` is to load the NI-type sub-subsections from the evaluation of the standard into the same storage array that is used to store NI-type covariances from the evaluation for reaction x. From that point on, the data from the standard are handled just as if they had come from the evaluation for x, but with one exception. As indicated by Eq. (55), the covariance contribution $\mathrm{cov}[z(E_x), z(E_y)]$ is <u>not</u> added into the total covariance matrix for the current reaction pair if either E_x or E_y lies outside the corresponding energy "window" (L_x, H_x) or (L_y, H_y), respectively.

As discussed in Section X.C, in addition to identifying the standard reaction, the NC-type sub-subsection contains a control parameter `LTY` and two energies `EL` and `EH` whose significance depends on `LTY`. `LTY` is used to identify particular evaluation scenarios: reaction x is the same as reaction y (or at least they are derived from z over the same energy range) (`LTY=1`); y is identical to the standard (`LTY=2`); or x is identical to the standard (`LTY=3`). A fourth possibility, namely, that x, y, and z are entirely distinct, cannot presently be treated with a single NC-type sub-subsection; that is, there is no `LTY` value defined for this case. However, as discussed later, it is still possible to process covariances for this situation by combining information from sub-subsections in two different evaluations. For convenience, we shall refer to this fourth case as `LTY=4`.

The interrelationship of `LTY`, `EL`, `EH`, and the windows (L_x, H_x) and (L_y, H_y) used in ERRORR for the "zeroing-out" operation of Eq. (55), is summarized below:

$$
\begin{aligned}
&\mathtt{LTY} = 1 \\
&\qquad (L_x, H_x) = (L_y, H_y) = (\mathtt{EL}, \mathtt{EH}) \\
&\mathtt{LTY} = 2 \\
&\qquad (L_x, H_x) = (\mathtt{EL}, \mathtt{EH}) \\
&\qquad (L_y, H_y) = (10^{-5}\ \mathrm{eV},\ 20\ \mathrm{MeV}) \\
&\mathtt{LTY} = 3 \\
&\qquad (L_x, H_x) = (10^{-5}\ \mathrm{eV},\ 20\ \mathrm{MeV}) \\
&\qquad (L_y, H_y) = (\mathtt{EL}, \mathtt{EH}) \\
&\mathtt{LTY} = 4 \\
&\qquad (L_x, H_x) = (\mathtt{EL}, \mathtt{EH}) \\
&\qquad (L_y, H_y) = (\mathtt{EL}', \mathtt{EH}')\ .
\end{aligned} \tag{56}
$$

If the user requests covariance data $\mathrm{cov}(x, y)$, where x and y are different and both

Table 1: Covariance Matrices Affected by Ratio Measurements In ENDF/B-V

	^{10}B (n,α)	^{238}U (n,γ)	^{235}U (n,f)	^{239}Pu (n,f)	^{239}Pu (n,γ)	^{241}Am (n,f)	^{242}Pu (n,f)
^{10}B(n,α)	$*$	3					
^{238}U(n,γ)	2	1					
^{235}U(n,f)			$*$	3	3	3	3
^{239}Pu(n,f)			2	1	1	4	4
^{239}Pu(n,γ)			2	1	1	4	4
^{241}Am(n,f)			2	4	4	1	4
^{242}Pu(n,f)			2	4	4	4	1

$*$ = standard
Integer = `LTY` value (see text)

are distinct from the standard (`LTY=4`), the ERRORR module obtains (`EL,EH`) from the `LTY=2` subsection in the evaluation for x that "points" to z. Then, the covariance file for z is read to obtain both (a) the explicit covariances cov(z,z) and (b) the second energy window (`EL`$'$, `EH`$'$), the latter being found in the `LTY=3` sub-subsection that points back to y.

Table 1 lists all ENDF/B-V reactions that contain ratio-to-standard covariance data. The symbols entered in the reaction-by-reaction matrix indicate which reactions are referenced as standards ($*$), and which reaction pairs have implicit nonzero covariances (`LTY`). ERRORR will produce multigroup covariances for any of the reaction pairs in Table I that are marked with ($*$) or (`LTY`). The cross-material covariances (`LTY=2`, `3`, or `4`) must be requested individually using the `IREAD=2` option (see Section X.K, especially the discussion of Cards 10 and 11). An attempt to process covariances for any of the cases `LTY=1` through `4` without supplying a separate ENDF tape containing the needed standard will result in an error stop in `SUBROUTINE GRIDD`. The error diagnostic, however, will supply the details of the corrective action required. (See general discussion of diagnostic messages in Section X.M.)

As an example of the ratio-data capabilities of ERRORR, Fig. 2 shows the covariances between the fission cross sections of ^{239}Pu (reaction x) and those of the important actinide ^{241}Am (reaction y). This is an `LTY=4` case where (L_x, H_x)= (0.2 MeV, 15 MeV) and (L_y, H_y)=(0.2 MeV, 20 MeV). The effect of using two different windows is apparent in the lower right corner of the correlation matrix. The plot itself was produced with the COVR module, which is described in Chapter

XX of this report. The complete NJOY input needed to compute and plot these data is given below at the end of Section X.K.

I. Multigroup Processing of Resonance-Parameter Uncertainties

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,γ)^{64}Cu (ENDF/B-V dosimetry material, `MAT6435`) 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) (`MAT6337`) from 0 to 10 eV and approximately so for the ENDF/B-VI evaluation of ^{23}Na(n,γ) (`MAT1125`) in the neighborhood of the large resonance at 2.81 keV.

In 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. (See the discussion of the input option `MFCOV=33` in Section X.K.) Following a procedure suggested in Ref. 8, the contribution is obtained from the Breit-Wigner formulae for the fission and capture areas of a resonance, A_f and A_γ. By differentiating these formulae with respect to the resonance parameters, one obtains a set of sensitivities. With these sensitivities and the covariance matrix of the parameters from MF32, one can apply the propagation-of-errors formula to obtain the covariances $\mathrm{cov}(A_\gamma, A_\gamma)$, $\mathrm{cov}(A_\gamma, A_f)$, and $\mathrm{cov}(A_f, A_f)$. In `SUBROUTINE RESCON`, these results are added directly into the user-group cross-section covariances calculated from MF33.

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 that contains the resonance energy E_r. Because of this assumption, and because ENDF-5 and the `LCOMP=0` option of ENDF-6 provide no correlations between parameters of different resonances, the calculated resonance-parameter contribution affects only the diagonal elements of the affected matrices, $\mathrm{cov}[X_K(a), X_K(b)]$.

With the inclusion of resonance-parameter covariances, the uncertainty in the capture cross section of ^{63}Cu, for a group that contains the large 577-eV resonance, is 3.0%, rather than zero, as it would be if the MF32 contribution were omitted.

With regard to the above-mentioned example of the important reactor coolant ^{23}Na (`MAT1125`), in an energy group extending from 1.235 to 3.350 keV, the addi-

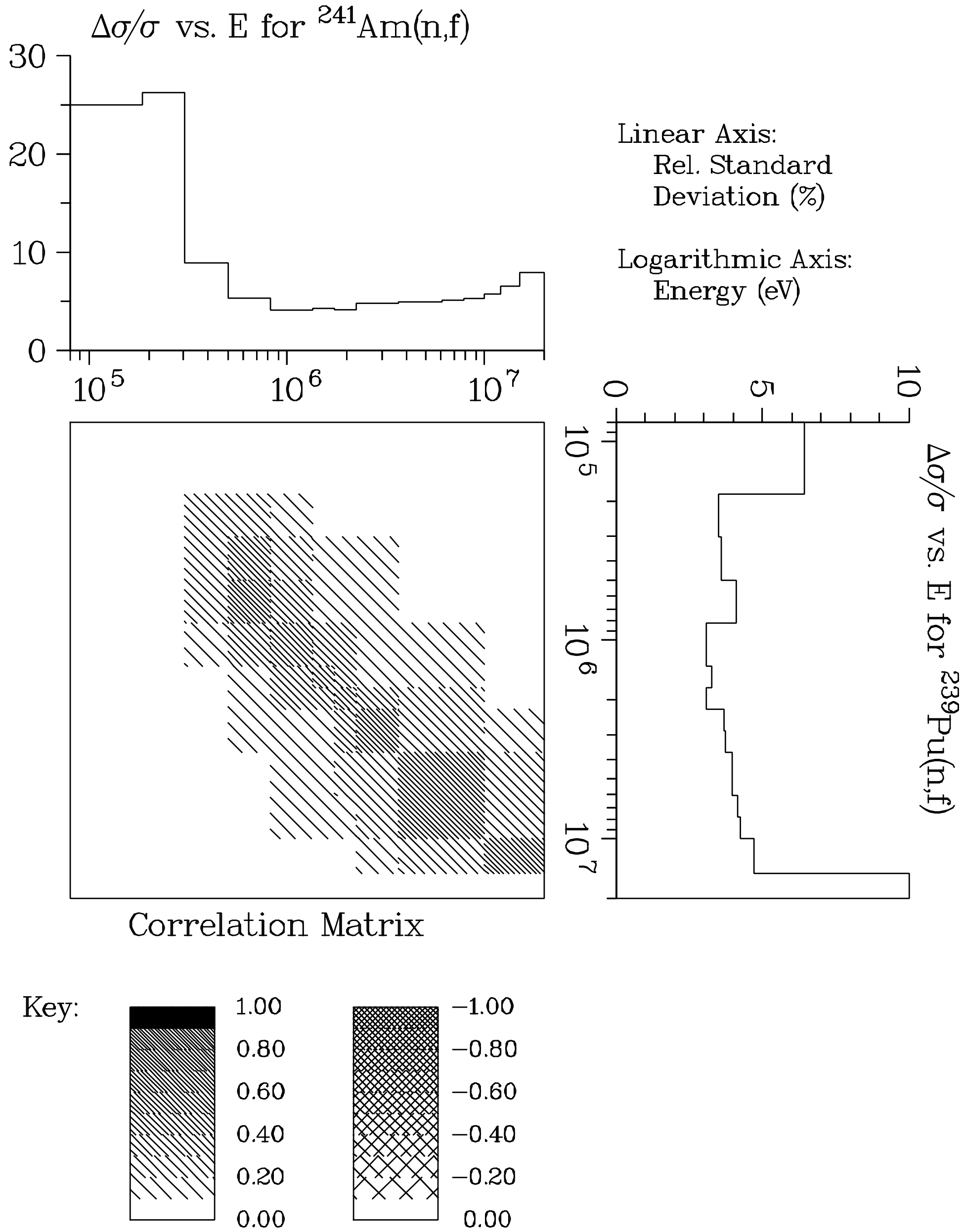

Figure 2: Covariance data for ^{239}Pu(n,f) with ^{241}Am(n,f).

tional uncertainty coming from resonance parameters raises the uncertainty of the capture cross section from 10% to 19%.

J. Processing of Lumped-Partial Covariances

The lumped-partial covariance format, allows the evaluator to specify a group of nuclear reactions and to give the uncertainty only in the sum of the cross sections for that group of reactions. One can, for example, replace 30 or 40 discrete-level inelastic cross sections with 5 or 6 lumped cross sections when constructing the covariance files. Because the volume of the covariance data varies, in general, as the square of the number of reactions, this lumping can greatly reduce the size of the files.

The first ENDF evaluation to employ the lumped-partial format was P. Young's evaluation[9, 10] for ^{7}Li (ENDF/B-V, Rev. 2). All covariance data for this evaluation have been successfully processed into multigroup form using ERRORR. The covariances for `MT854` (a single real level with an excitation energy of 4.63 MeV) with `MT855` (6 lumped pseudo-levels, with excitation energies ranging from 4.75 MeV to 6.75 MeV) have been plotted in Fig. 3. The large negative correlations along the diagonal result from the fact that, below 10 MeV, these inelastic reactions are the major contributors to the relatively well-known tritium production cross section. An upward variation in one reaction at a given energy must be accompanied by a downward change in the other reaction. As shown in the plot, the magnitude of this negative correlation diminishes at higher energies, as other reactions begin to contribute significantly to the tritium-production cross section. Plots of this type, prepared using ERRORR and COVR, have proved to be useful tools in the validation of the covariance files of new evaluations.[11]

K. Input Instructions and Sample Input for ERRORR

As an aid to discussions of the user input to ERRORR, we list below the input instructions that appear as comment cards at the beginning of the current version of this module. Since the code and, hence, the instructions change from time to time, it is always advisable to consult the comment-card instructions contained in the version of the code actually being used and not to rely on the instructions published in any document, including this one. Note that the word "tape" is used in the instructions to refer to an input or output file, regardless of the actual storage medium.

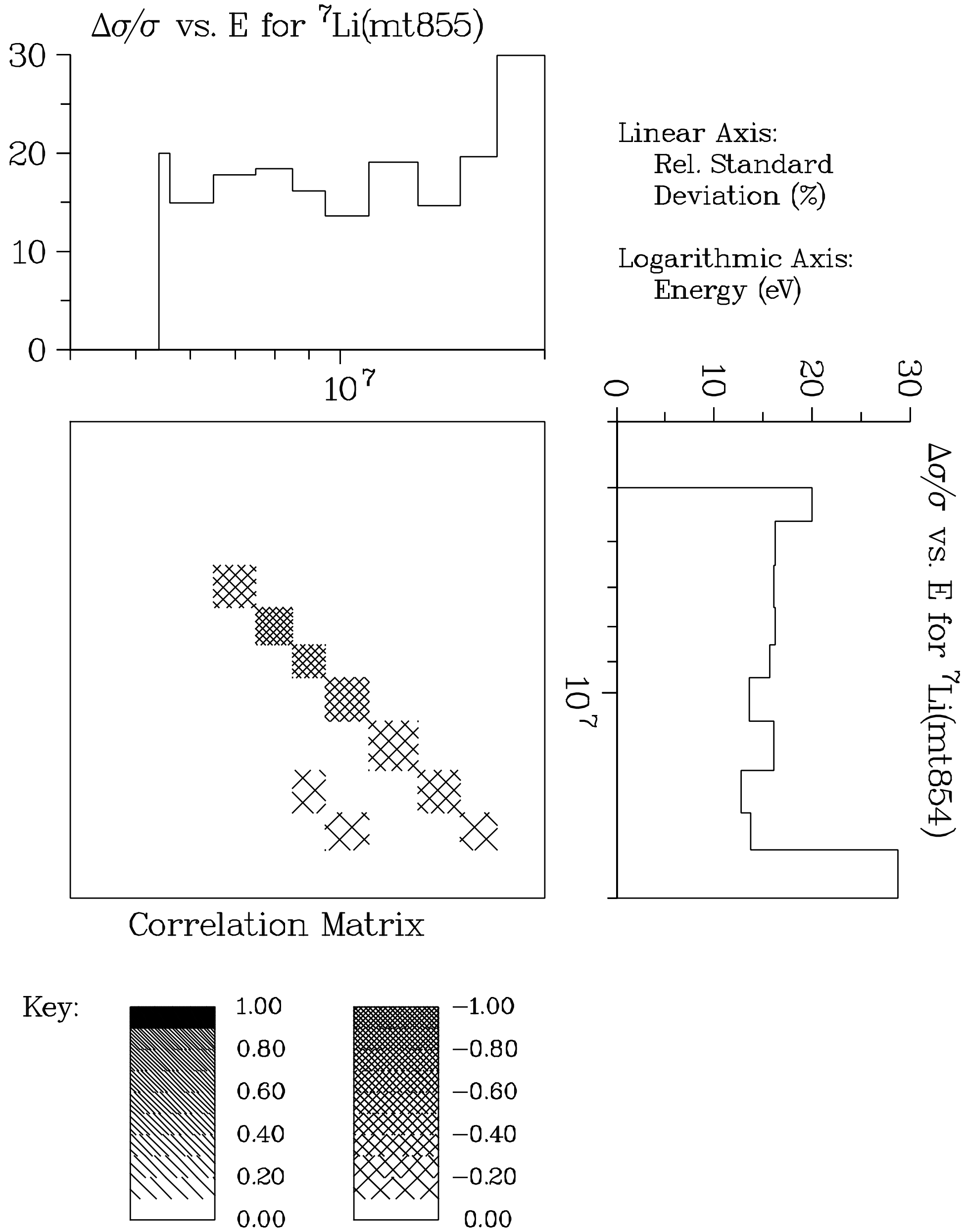

Figure 3: Covariance data for ^{7}Li (MT854) with ^{7}Li (MT855).

```
*---INPUT SPECIFICATIONS (FREE FORMAT)---------------------------*
*                                                               *
*  CARD 1                                                       *
*    NENDF   UNIT FOR ENDF/B TAPE                               *
*    NPEND   UNIT FOR PENDF TAPE                                *
*    NGOUT   UNIT FOR INPUT GROUP XSEC (GENDF) TAPE             *
*            (IF ZERO, GROUP XSECS WILL BE CALCULATED)          *
*            (IF IREAD EQ 2 OR IF MFCOV EQ 31 (SEE CARD 7),     *
*            NGOUT CANNOT BE ZERO)                              *
*            (DEFAULT=0)                                        *
*    NOUT    UNIT FOR OUTPUT COVARIANCE TAPE (DEFAULT=0)        *
*    NIN     UNIT FOR INPUT COVARIANCE TAPE (DEFAULT=0)         *
*            (NIN AND NOUT MUST BE BOTH CODED OR BOTH BINARY)   *
*    NSTAN   UNIT FOR RATIO-TO-STANDARD TAPE (DEFAULT=0)        *
*  CARD 2                                                       *
*    MATD    MATERIAL TO BE PROCESSED                           *
*    IGN     NEUTRON GROUP OPTION                               *
*            (IGN DEFINITION SAME AS GROUPR, EXCEPT IGN=19,     *
*            WHICH MEANS READ IN AN ENERGY GRID, AS IN IGN=1,   *
*            AND SUPPLEMENT THIS WITH THE ENDF COVARIANCE GRID  *
*            WITHIN THE RANGE OF THE USER-SPECIFIED ENERGIES)   *
*            (DEFAULT=1)                                        *
*    IPRINT  PRINT OPTION (0/1=MINIMUM/MAXIMUM) (DEFAULT=1)     *
*    IRELCO  COVARIANCE FORM (0/1=ABSOLUTE/RELATIVE) (DEFAULT=1) *
*  CARD 3    (OMIT IF NGOUT.NE.0)                               *
*    IWT     WEIGHT FUNCTION OPTION                             *
*    MPRINT  PRINT OPTION FOR GROUP AVERAGING (0=MIN., 1=MAX.)  *
*    TEMPIN  TEMPERATURE (DEFAULT=300)                          *
*                                                               *
*---FOR ENDF/B VERSION 4 (IVERF=4) ONLY-------------------------*
*                                                               *
*  CARD 4                                                       *
*    NEK     NUMBER OF DERIVED XSEC ENERGY RANGES               *
*            (IF ZERO, ALL XSECS ARE INDEPENDENT)               *
*  CARD 5    (OMIT IF NEK=0)                                    *
*    EK      NEK+1 DERIVED XSEC ENERGY BOUNDS                   *
*  CARD 6    (OMIT IF NEK=0)                                    *
*    AKXY    DERIVED CROSS SECTION COEFFICIENTS, ONE ROW/LINE   *
*                                                               *
*---FOR ENDF/B VERSION 5 (IVERF=5) ONLY-------------------------*
*                                                               *
*  CARD 7                                                       *
*    IREAD   0/1/2=PROGRAM CALCULATED MTS/INPUT MTS AND EKS/    *
*            CALCULATED MTS PLUS EXTRA MAT1-MT1 PAIRS FROM INPUT *
*            (DEFAULT=0)                                        *
*    MFCOV   ENDF COVARIANCE FILE (31, 32, OR 33) TO BE         *
*            PROCESSED (DEFAULT=33).                            *
*            NOTE--CONTRIBUTION TO GROUP CROSS SECTION          *
*            COVARIANCES FROM RESONANCE-PARAMETER UNCERTAINTIES *
*            (MF=32) IS INCLUDED WHEN MFCOV=33 IS SPECIFIED.    *
*                                                               *
*  FOLLOWING CARDS ONLY IF IREAD EQ 1                           *
```

```
*  CARD 8                                                          *
*    NMT     NO. MTS TO BE PROCESSED                               *
*    NEK     NO. DERIVED CROSS SECTION ENERGY RANGES               *
*            (IF ZERO, ALL XSECS ARE INDEPENDENT)                  *
*  CARD 8A                                                         *
*    MTS     NMT MTS                                               *
*  CARD 8B   (OMIT IF NEK=0)                                       *
*    EK      NEK+1 DERIVED CROSS SECTION ENERGY BOUNDS             *
*  CARD 9    (OMIT IF NEK=0)                                       *
*    AKXY    DERIVED CROSS SECTION COEFFICIENTS, ONE ROW/LINE      *
*                                                                  *
*  FOLLOWING CARD ONLY IF IREAD EQ 2                               *
*  CARD 10                                                         *
*    MAT1    CROSS-MATERIAL REACTION TO BE ADDED TO                *
*    MT1         COVARIANCE REACTION LIST.                         *
*            REPEAT FOR ALL MAT1-MT1 PAIRS DESIRED                 *
*            TERMINATE WITH MAT1=0.                                *
*                                                                  *
*  FOLLOWING CARD ONLY IF NSTAN NE 0                               *
*  CARD 11                                                         *
*    MATB    STANDARDS REACTION REFERENCED                         *
*    MTB         IN MATD.                                          *
*    MATC    STANDARDS REACTION TO BE                              *
*    MTC         USED INSTEAD.                                     *
*            REPEAT FOR ALL STANDARD REACTIONS TO BE REDEFINED.    *
*            TERMINATE WITH MATB=0.                                *
*  NOTE.  IF MATB(1) AND MTB(1) ARE NEGATIVE, THEN MATC(1) AND     *
*    MTC(1) IDENTIFY A THIRD REACTION, CORRELATED WITH MATD THRU   *
*    THE USE OF THE SAME STANDARD.  COVARIANCES OF ALL REACTIONS   *
*    IN MATD (WHICH REFERENCE THE STANDARD) WITH THE REACTION      *
*    MATC(1)-MTC(1) WILL BE PRODUCED.  THE STANDARD REACTION       *
*    MUST BE IDENTIFIED ON CARD 10 AND REPEATED AS THE NEGATIVE    *
*    ENTRIES ON CARD 11.  THE GROUP XSEC TAPE NGOUT MUST INCLUDE   *
*    ALL COVARIANCE REACTIONS IN MATD, PLUS MATC(1)-MTC(1).        *
*------------------------------------------------------------------*
*                                                                  *
*  CARD 12A (FOR IGN EQ 1 OR IGN EQ 19)                            *
*    NGN     NUMBER OF GROUPS                                      *
*  CARD 12B                                                        *
*    EGN     NGN+1 GROUP BOUNDS (EV)                               *
*  CARD 13 (FOR IWT EQ 1 ONLY)                                     *
*    WGHT    WEIGHT FUNCTION AS A TAB1 RECORD                      *
*                                                                  *
********************************************************************
```

Further details on many of these input parameters are provided in the text below. Actual NJOY input for a few example problems is provided for further clarification. Complete input and output for another example problem are given in Ref. 12.

`NPEND, NGOUT` ... The user must supply either a PENDF tape on unit `NPEND` or a GENDF tape on unit `NGOUT`. If present, the `PENDF` tape should contain pointwise (resonance-reconstructed, but not multigrouped) data and is normally produced with the `RECONR` module. If the resonance region is of no interest, a simple copy of the ENDF tape will suffice for this purpose. The GENDF tape, if present, should contain multigroup cross sections and/or $\overline{\nu}$ values, produced by the GROUPR module, for all reactions for which multigroup covariances are needed. Group cross sections need not be in the same group structure as the requested output covariances, although if the input group structure is much coarser than the output structure, rather crude approximations will be made in deriving an effective set of fine-group cross sections and fluxes from the coarse input data. Certain types of covariance calculations related to fission data or the computation of cross-material covariances require the user to supply a GENDF tape on `NGOUT` (that is, `NPEND` must be zero).

`NIN, NOUT` ... Input and output covariance tapes in the user's group structure may either be both formatted or both binary. Although ERRORR lacks an explicit multimaterial loop, the same effect can be achieved by executing a series of ERRORR runs, with the output of one run becoming the input of the next. Only two unit numbers need be employed, with the data going back and forth between them until the multimaterial library is complete. To save time, binary files should be used for this purpose. MODER can be used to convert the final output tape from binary to formatted form, if desired.

`NSTAN` ... This tape is needed if covariances are requested for a reaction pair that is related by ratio measurements, as discussed in Section X.H. The ENDF subsection for such a pair will contain an NC-type sub-subsection with `LTY`=1, 2, or 3. The specific pairs in ENDF/B-V that require a standards tape are tabulated in Table 1 (Section X.H). For other evaluations, one can assume `NSTAN` is not needed. The code will stop with a clear error message if this assumption proves incorrect.

`IREAD` ... For Versions 5 and 6, the list of reactions for which covariances are produced is constructed in one of several ways, depending on the value of `IREAD`. If `IREAD=0`, which is the generally recommended choice, the reaction list is assumed to be identical to the list of sections contained in the ENDF/B covariance file (see `MFCOV` below). Although `IREAD=0` is the most convenient option for constructing the list of covariance reactions, it leads to a problem if some covariance reactions have thresholds above the highest group boundary of the user's structure. These reactions will have zero cross sections in all groups and thus will be omitted from

NGOUT. To avoid this difficulty, ERRORR automatically resets the user's highest group boundary to 20 MeV whenever IREAD=0. By judicious choice of weighting functions, one can minimize the effect of this resetting on the other cross sections and their covariances.

If IREAD=1, only the covariance reactions specifically named by the user will be included in the reaction list. For certain applications, this option can save considerable execution time. However, to take advantage of this option, the user must examine the ENDF evaluation visually to determine which reactions are derived from other reactions in each energy region. As discussed in Section X.C, this information is contained in NC-type sub-subsections with LTY=0. Incorrect results will be obtained if one requests processing for a given reaction without processing all of the reactions from which the given reaction is derived in the energy region spanned by the output group structure. The inclusion of those reactions may require, in turn, additional inclusions as well. In addition, the user must extract from the file (and enter into the input) the appropriate derivation coefficients and the energy ranges over which they apply. An example of the required input is presented below in the discussion of the parameters NMT, NEK, MTS, EK, and AKXY.

If IREAD=0 or 1, a complete set of covariance matrices is written. That is, covariance matrices are produced for every reaction-pair combination that can be formed from the given reaction list. For those reaction pairs where the evaluator has not specified the covariances, the output matrix contains only zeros.

In the evaluation containing cross-material covariances, subsections involving the other materials will be ignored if IREAD=0 or 1. These subsections can be selectively processed by specifying IREAD=2. If IREAD=2, the reaction list is initially constructed in the same way as for IREAD=0. This list is then supplemented with a list of extra reactions (MAT1_k, MT1_k) (where (MAT$1_k \neq$ MATD), specified by the user. The output in this case contains matrices for all of the (MATD, MT$_i$; MATD,,MT$_j$) combinations, as before, plus matrices for all (MATD, MT$_i$; MAT1_k, MT1_k) combinations. However, covariances among the extra reactions, for example (MAT1_k, MT1_k; MAT1_m,,MT1_m), are not computed. Input for an example problem that illustrates the use of IREAD=2 is given below, in the discussion of MFCOV. That discussion also includes an illustration (Table 2) of the set of MAT/MT combinations that are processed when IREAD=2.

MFCOV ... This parameter is used to specify whether covariances of fission $\overline{\nu}$ (MFCOV=31) or cross sections (MFCOV=33) are needed. If MFCOV=31, it is necessary to supply multigrouped cross sections and $\overline{\nu}$ values on a GENDF tape (that is, NPEND must be 0); the sample problem below shows the calculational sequence required. `MFCOV=32` is reserved for a planned future capability to compute uncertainties in self-shielded cross sections. If `MFCOV=33`, the contribution of the uncertainty in individual resonance parameters (File 32) is included in the calculated uncertainty in infinite-dilution group cross sections. Given below is the complete NJOY input for a calculation of a multigroup $\overline{\nu}$ covariance library for ^{238}U, including five cross-material reactions.

```
0
5
*MODER*/ MOUNT ENDF TAPES 515, 516, and 555 ON UNITS 20, 21, AND 22.
1 -23
*ENDF/B-V NUBAR COVARIANCE MATERIALS*/
20 1380
20 1381
21 1390
22 1395
22 1398
20 1399
0/
*MODER*/ COPY ENDF FOR USE AS A PENDF.
-23 -24
*GROUPR*/ PREPARE GENDF WITH MULTIGROUPED NUBARS.
-23 -24 0 25
1380 3 0 3 0 1 1 0
*BIG3 + 2 NUBAR*/
0.
1.E10
3 452 *TOTAL NUBAR*/
0/
1381
3 452 *TOTAL NUBAR*/
0/
1390
3 452 *TOTAL NUBAR*/
0/
1395
3 452*TOTAL NUBAR*/
0/
1398
3 452 *TOTAL NUBAR*/
3 455 *DELAYED NUBAR*/
3 456 *PROMPT NUBAR*/
0/
1399
3 452 *TOTAL NUBAR*/
0/
0/
*ERRORR*/ PREPARE MULTIGROUP NUBAR COVARIANCE LIBRARY.
-23 0 25 26/
1398 19 1 1
```

Table 2: Reaction Pairs in ^{238}U Library

	a	b	c	d	e	f	g	h	i
a = (1398,452)	X	X	X	X	X	X	X	X	X
b = (1398,455)		X	X	X	X	X	X	X	X
c = (1398,456)			X	X	X	X	X	X	X
d = (1380,452)				–	–	–	–	–	–
e = (1381,452)					–	–	–	–	–
f = (1390,452)						–	–	–	–
g = (1395,452)							–	–	–
h = (1398,452)								–	–
i = (1399,452)									–

```
2 31
1380 452
1381 452
1390 452
1395 452
1399 452
0/
1
1.E7 1.7E7
*STOP*
```

Note the use of the MODER module to prepare a special ENDF tape containing selected evaluations from other ENDF tapes. Because only high-energy $\overline{\nu}$ data are requested (10–17 MeV), it is unnecessary to use RECONR to prepare a PENDF tape for GROUPR. A copy of the ENDF tape is used instead.

Following the prescription given in the discussion of the `IREAD=2` option, with this particular input, covariance matrices will be produced for those reaction pairs marked with an X in Table 2. The remaining non-redundant possibilities (dashes) can be filled in with successive ERRORR runs with `MATD=1380`, `1381`, etc.

`NMT`, `NEK`, `MTS`, `EK`, `AKXY` ... For Version 5, if `IREAD=1`, the user specifies a subset of the evaluator's covariance reactions (that is, a subset of the sections of `MFCOV`), as the particular set of reactions for which processing is requested. These `NMT` desired reactions are entered in the array `MTS`. As mentioned in the discussion of `IREAD` above, one must also include in the `MTS` array all reactions from which the desired reactions are derived.

Another requirement of the IREAD=1 option is that the actual derivation coefficients [called AKXY in the code, but called $C_I(a,c)$ in the discussion in Section X.G] must be entered in the ERRORR input for NEK energy ranges spanning the output group structure. Adjacent ENDF derivation ranges may be merged into a single range if the derivation-coefficient matrix for the NMT explicitly requested reactions is the same in each of the adjacent ranges. The ordering of the $C_I(a,c)$ data is as follows: on one line of input the coefficients are specified for a fixed a-value and for all c-values ranging from 1 to NMT. One such line is given for each a-value. Finally, there is an outer loop over the NEK energy ranges. An example of the input that is required for READ=1 is given below for the case of ENDF/B-V carbon MAT1306. It will be necessary to examine File 33 of the evaluation (which is available on the ENDF/B-V standards file, Tape 511), in order to understand the details of this example.

```
0
5
*MODER*
20- 21
*MODER*/COPY ENDF FOR USE AS A PENDF.
-21 -22/
*ERRORR*
-21 -22 0 -23/
1306 3 1/
2 0 0
1 33
7 3
1 2 4 102 103 104 107
1.E-5 2E6 4.812E6 2E7
0 1 0 1 0 0 0
0 1 0 0 0 0 0
0 0 1 0 0 0 0
0 0 0 1 0 0 0
0 0 0 0 1 0 0
0 0 0 0 0 1 0
0 0 0 0 0 0 1
1 0 0 0 0 0 0
0 1 0 0 0 0 0
0 0 1 0 0 0 0
0 0 0 1 0 0 0
0 0 0 0 1 0 0
0 0 0 0 0 1 0
0 0 0 0 0 0 1
1 0 0 0 0 0 0
0 1 0 0 0 0 0
1 -1 0 -1 -1 -1 -1
0 0 0 1 0 0 0
0 0 0 0 1 0 0
0 0 0 0 0 1 0
0 0 0 0 0 0 1
```

```
*STOP*
```

Note that here, even if the user wanted to process only MT2 and MT4, for example, it is nevertheless necessary to include MT1, MT102, MT103, MT104, and MT107, because the IGN=3 group structure extends to 17.0 MeV, and above 4.812 MeV, MT4 is derived from the relation

$$\sigma_4 = \sigma_1 - \sigma_2 - \sigma_{102} - \sigma_{104} - \sigma_{107} \,. \tag{57}$$

See the corresponding $C_I(a,c)$ matrix in the input above (the last 7 lines before STOP).

MATB, MTB, MATC, MTC ... Card 11 provides a capability to remap all references to a given standards reaction (MATB,MTB) appearing in NC-type sub-subsections with LTY=1, 2, or 3 into references to a different reaction (MATC,MTC). (See the discussion of ratio measurements in Section X.H.) This facility is useful if the evaluation (MATB,MTB) is for some reason unavailable. Up to 5 such standards can be redefined. As explained in the note on the input instructions at the beginning of this section, Card 11 is also used [if MATB(1) and MTB(1) are negative] to process covariances between two distinct reactions, both measured relative to a common standards reaction. This was referred to as the LTY=4 case in Section X.H. A separate ERRORR run is required for each requested LTY=4 reaction pair.

This second use of Card 11 is illustrated in the sample NJOY input listed below, which is the input used to generate and plot the data shown in Fig. 2. The input to the COVR module contained in the sample is explained in the following chapter.

```
$ SETUP FOR PLOTTING FIG2 IN ERRORR MANUAL
$ MOUNT T562 ON TAPE30
$ MOUNT T563 ON TAPE40
$ MOUNT T560 ON TAPE50
 0
 5
 MODER
 1 -31
 *U235 FROM T562*/
 30 1395
 0/
 MODER
 1 -21
 *AM241 FROM T560 AND PU239 FROM T563*/
 50 1361/ AM241
 40 1399/ PU239
 0/
```

```
RECONR
-21 -22
*10 PERCENT PENDF FOR AM241 AND PU239*/
1361/
.1/
1399/
.1/
0/
GROUPR
-21 -22 0 -24
1361 3 0 2 0 1 1 0
*30 GROUP XSECS FOR AM241 AND PU239*/
0
1E10
3 1/
3 2/
3 4/
3 16/
3 17/
3 18/
3 102/
0/
1399
3 18/
3 102/
0/
0/
ERRORR
-21 0 -24 -25 0 -31
1361 3 1 1
0 33
0/
ERRORR
-21 0 -24 -28 -25 -31
1399 3 1 1
2 33
1395 18
0/
-1395 -18 1361 18
0/
COVR
-28/
0 0 0 8E4
1 1 0 0 2
1399 18 1361 18
STOP
```

L. ERRORR Output File Specification

The results from ERRORR are written to an output file on unit `NOUT`, provided that the input parameter `NOUT` is nonzero. This file contains the user's group structure, the multigroup cross sections, and either absolute (`IRELCO=0`) or relative (`IRELCO=1`) covariances. If `NOUT` is positive, then a formatted (card-image) file is written, and, if negative, a binary file is written. In either case, the output is written with the standard NJOY I/O utilities, and the result has an ENDF-like structure. As is the case for ENDF, PENDF, and GENDF files, ERRORR output files can be converted from binary to formatted form (and *vice versa*) by using the MODER module. The energy-group ordering of the data written to `NOUT` follows the ENDF convention. That is, low-energy groups precede high-energy groups.

A small, stand-alone retrieval program, which reads formatted ERRORR output files, reorders the energy groups to high-to-low order, and fills in the implicit zeros to make a full matrix, is listed in Table IV of Ref. 11. A much more powerful retrieval program, which produces libraries for sensitivity codes and publication-quality plots of the data, starting from either binary or formatted ERRORR output, is the COVR module of NJOY. This module is described in the following chapter of this report.

It is occasionally of interest to examine a formatted ERRORR output file visually. For this and other reasons, we describe below the detailed form of the formatted output file. To assist in the description, we give in Table 3 an example of such a file, which was produced during the processing of COVFILS-2 (Ref. 13).

The data in Table 3 are written in the form of standard, 80-column card-images consisting of 10 data fields. As in ENDF, the first 6 fields are 11 characters wide and are used for either floating-point numbers or integers. The seventh, eighth, ninth, and tenth fields are 4, 2, 3, and 5 characters wide, respectively, and are used for integers only. The four digits in Field 7 are the `MAT`, or material number, of the isotope or element; the two digits in Field 8 are the `MF`, or file number, which indicates the general type of data (for example, cross-section data *vs.* covariance data); the three digits in Field 9 are the `MT`, or section number, which indicates the particular nuclear reaction; and finally, the five digits in Field 10 are `NSEQ`, the card sequence number. As usual, sections are terminated by zeros in the `MT` field, files by zeros in the `MF` field, and materials by zeros in the `MAT` field.

Following an initial tape header record, the second card shown in Table 3 is the first data card for the material `MAT1326`, which is elemental iron. Note that on this card the number 2.6×10^4 appears in the first field and 55.365 in the second field. These are the "ZA" ($1000 \times Z - A$) and "AWR" (atomic weight relative to the neutron) numbers taken directly from the ENDF file. The fact that ZA is 26 000 (suggesting that $A = 0$) is a convention that means that the data are for the natural element Fe, rather than for a single isotope. The value of -11 appearing in Field 5 is a flag (read by the MODER module, for example) that identifies the present file format as the ERRORR output format.

Also note that `MF=1` and `MT=451` on cards `NSEQ=1` to `15`. This `MF-MT` combination is used in the ENDF format for descriptive Hollerith information, but it is used here to specify the boundaries of the multigroup structure used for the processed data to follow. On Card 2, note the number 74 in Field 3 and the number 75 in Field 5, which indicate, respectively, the number of energy groups and the number of energy-group boundaries in the multigroup set. The values of the group boundaries, given in eV from low to high energy, follow in Cards 3 through 15. Cards 16 and 17 are section and file terminators, respectively.

Multigroup cross-section data are given in barns on Cards 18 through 631. This file, denoted by `MF=3`, corresponds to the smooth cross-section file in ENDF. The MT-numbers (Field 9) can be identified with particular nuclear reactions by consulting Appendix B of Ref. 4. Note that cross sections for the lumped-partial reaction `MT=851` have been constructed by ERRORR according to the directions given in the ENDF file.

Table 3: Example of ERRORR Output Data File

```
                                                                     1 0  0    0
 2.600000+4 5.536500+1          0          0        -11          01326 1451    1
 0.000000+0 0.000000+0         74          0         75          01326 1451    2
 1.000000-5 7.602200-4 1.239500-2 4.275500-2 8.196800-2 1.523000-11326 1451    3
 4.139900-1 8.764200-1 1.125400+0 1.855400+0 3.927900+0 5.043500+01326 1451    4
 8.315300+0 1.760300+1 3.726700+1 7.889300+1 1.013000+2 1.670200+21326 1451    5
 3.535800+2 7.485200+2 1.584600+3 3.354600+3 7.101700+3 9.118800+31326 1451    6
 1.503400+4 2.478800+4 2.605800+4 2.808800+4 3.182800+4 4.086800+41326 1451    7
 5.247500+4 6.737900+4 8.651700+4 1.110900+5 1.426400+5 1.831600+51326 1451    8
 2.351800+5 3.019700+5 3.877400+5 4.393700+5 4.978700+5 5.641600+51326 1451    9
 6.392800+5 7.244000+5 8.208500+5 1.054000+6 1.194300+6 1.353400+61326 1451   10
 1.737700+6 1.969100+6 2.231300+6 2.528400+6 2.865000+6 3.246500+61326 1451   11
 3.678800+6 4.168600+6 4.723700+6 5.352600+6 6.065300+6 6.872900+61326 1451   12
 7.788000+6 8.825000+6 1.000000+7 1.100000+7 1.200000+7 1.300000+71326 1451   13
 1.350000+7 1.375000+7 1.394000+7 1.420000+7 1.442000+7 1.464000+71326 1451   14
 1.500000+7 1.600000+7 2.000000+7                                 1326 1451   15
                                                                  1326 1  0   16
                                                                  1326 0  0   17
 0.000000+0 0.000000+0          0          0         74          01326 3  1   18
 3.242538+1 1.638221+1 1.395614+1 1.310400+1 1.266828+1 1.222209+11326 3  1   19
 1.192867+1 1.180887+1 1.173992+1 1.164882+1 1.159180+1 1.155850+11326 3  1   20
 1.151292+1 1.146973+1 1.143331+1 1.140845+1 1.137811+1 1.103735+11326 3  1   21
 1.031032+1 9.276154+0 7.382612+0 7.137478+0 1.602539+1 4.178159+01326 3  1   22
 1.482726+0 1.406100+0 3.875233+1 3.832471+1 8.517735+0 5.325881+01326 3  1   23
 4.200487+0 6.723474+0 4.481126+0 3.610952+0 3.923129+0 4.868550+01326 3  1   24
 2.836503+0 3.245566+0 4.853495+0 3.640536+0 3.205600+0 2.250606+01326 3  1   25
 2.732808+0 3.895072+0 2.571093+0 2.501068+0 2.958182+0 2.985432+01326 3  1   26
```

```
2.899251+0 3.213480+0 3.189247+0 3.477117+0 3.389077+0 3.403654+01326 3  1   27
3.625322+0 3.668095+0 3.697471+0 3.674937+0 3.632669+0 3.545578+01326 3  1   28
3.383465+0 3.214864+0 3.053930+0 2.905813+0 2.743816+0 2.674006+01326 3  1   29
2.635890+0 2.613351+0 2.590513+0 2.567519+0 2.547020+0 2.517568+01326 3  1   30
2.457292+0 2.307503+0                                            1326 3  1   31
                                                                 1326 3  0   32
0.000000+0 0.000000+0          0          0         74          01326 3  2   33
1.140000+1 1.140000+1 1.139999+1 1.139998+1 1.139996+1 1.139991+11326 3  2   34
1.139978+1 1.139964+1 1.139947+1 1.139900+1 1.139839+1 1.139764+11326 3  2   35
1.139553+1 1.139053+1 1.137995+1 1.136763+1 1.134459+1 1.101228+11326 3  2   36
1.029462+1 9.055728+0 7.376526+0 7.127705+0 1.599799+1 4.168132+01326 3  2   37
1.450895+0 1.368534+0 3.867417+1 3.827977+1 8.473823+0 5.294164+01326 3  2   38
4.169383+0 6.691388+0 4.451224+0 3.586689+0 3.901454+0 4.844768+01326 3  2   39
2.815969+0 3.225118+0 4.830640+0 3.616074+0 3.180014+0 2.223638+01326 3  2   40
2.703083+0 3.863693+0 2.346491+0 2.057345+0 2.535809+0 2.262868+01326 3  2   41
2.127090+0 2.261804+0 2.256791+0 2.533315+0 2.231035+0 2.144008+01326 3  2   42
2.151420+0 2.170908+0 2.095557+0 2.088164+0 2.073116+0 2.006202+01326 3  2   43
1.857245+0 1.711327+0 1.565212+0 1.419054+0 1.283900+0 1.274210+01326 3  2   44
1.266290+0 1.253001+0 1.238749+0 1.224132+0 1.210283+0 1.196914+01326 3  2   45
1.165341+0 1.042323+0                                            1326 3  2   46
                                                                 1326 3  0   47
    .
    .
    .
    .
    .
    .
0.000000+0 0.000000+0          0          0         74          01326 3107  603
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  604
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  605
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  606
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  607
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  608
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  609
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  610
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3107  611
0.000000+0 0.000000+0 0.000000+0 0.000000+0 5.054213-6 3.154394-51326 3107  612
6.536392-5 1.636755-4 4.937945-4 1.599742-3 4.467725-3 9.026301-31326 3107  613
1.492042-2 2.174807-2 2.912657-2 3.467999-2 3.849531-2 3.982821-21326 3107  614
3.986411-2 3.988542-2 3.971171-2 3.918684-2 3.866013-2 3.800829-21326 3107  615
3.513214-2 1.922833-2                                            1326 3107  616
                                                                 1326 3  0  617
0.000000+0 0.000000+0          0          0         74          01326 3851  618
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3851  619
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3851  620
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+01326 3851  621
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 1.713016-41326 3851  622
2.605423-2 2.747897-2 2.715636-2 2.656936-2 2.500170-2 2.240780-21326 3851  623
2.044663-2 1.866612-2 1.650006-2 1.483479-2 1.452751-2 1.445474-21326 3851  624
1.484054-2 1.514701-2 1.823890-2 1.948106-2 2.054081-2 2.151007-21326 3851  625
2.239315-2 2.355651-2 2.568895-2 2.711755-2 2.775385-2 2.831557-21326 3851  626
2.892825-2 2.891470-2 2.891944-2 2.909114-2 2.816820-2 2.648783-21326 3851  627
2.379156-2 2.036489-2 1.658885-2 1.236790-2 8.719756-3 5.515926-31326 3851  628
```

```
2.789373-3 1.967219-3 1.199289-3 5.263406-4 1.809961-4 1.629883-41326 3851  629
1.542762-4 1.491088-4 1.438805-4 1.385182-4 1.332255-4 1.265700-41326 3851  630
1.111753-4 5.198675-5                                            1326 3851  631
                                                                 1326 3  0  632
                                                                 1326 0  0  633
2.600000+4 5.536500+1          0          0          0         41132633  1  634
0.000000+0 0.000000+0          0          1          0         74132633  1  635
0.000000+0 0.000000+0         17          1         17          1132633  1  636
4.771962-4 6.905149-4 7.654629-4 7.983731-4 8.169108-4 8.372624-4132633  1  637
8.514704-4 8.574701-4 8.609741-4 8.656539-4 8.686033-4 8.703185-4132633  1  638
8.707277-4 8.728724-4 8.748390-4 8.757964-4 7.461125-4           132633  1  639
0.000000+0 0.000000+0         17          1         17          2132633  1  640
6.905149-4 1.247608-3 1.443338-3 1.529285-3 1.577697-3 1.630846-3132633  1  641
1.667951-3 1.683619-3 1.692770-3 1.704992-3 1.712694-3 1.717174-3132633  1  642
1.722305-3 1.727680-3 1.731573-3 1.733468-3 1.476784-3           132633  1  643
0.000000+0 0.000000+0         17          1         17          3132633  1  644
7.654629-4 1.443338-3 1.681504-3 1.786085-3 1.844993-3 1.909666-3132633  1  645
1.954815-3 1.973881-3 1.985016-3 1.999887-3 2.009259-3 2.014710-3132633  1  646
2.021500-3 2.028010-3 2.032580-3 2.034804-3 1.733500-3           132633  1  647
0.000000+0 0.000000+0         17          1         17          4132633  1  648
7.983731-4 1.529285-3 1.786085-3 1.898848-3 1.962365-3 2.032098-3132633  1  649
2.080780-3 2.101337-3 2.113343-3 2.129378-3 2.139484-3 2.145360-3132633  1  650
2.152879-3 2.159888-3 2.164754-3 2.167123-3 1.846226-3           132633  1  651
    .
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    .
    .
    .
    .
0.000000+0 0.000000+0          0        102          0         74132633  1 1738
0.000000+0 0.000000+0         13          1         13          1132633  1 1739
2.593694-4 2.593694-4 2.593694-4 2.593694-4 2.593694-4 2.593694-4132633  1 1740
2.593694-4 2.593694-4 2.593694-4 2.593694-4 2.593694-4 2.593694-4132633  1 1741
7.341822-5                                                       132633  1 1742
0.000000+0 0.000000+0         13          1         13          2132633  1 1743
1.216493-4 1.216493-4 1.216493-4 1.216493-4 1.216493-4 1.216493-4132633  1 1744
1.216493-4 1.216493-4 1.216493-4 1.216493-4 1.216493-4 1.216493-4132633  1 1745
3.443457-5                                                       132633  1 1746
0.000000+0 0.000000+0         13          1         13          3132633  1 1747
7.326236-5 7.326236-5 7.326236-5 7.326236-5 7.326236-5 7.326236-5132633  1 1748
7.326236-5 7.326236-5 7.326236-5 7.326236-5 7.326236-5 7.326236-5132633  1 1749
2.073796-5                                                       132633  1 1750
0.000000+0 0.000000+0         13          1         13          4132633  1 1751
5.201525-5 5.201525-5 5.201525-5 5.201525-5 5.201525-5 5.201525-5132633  1 1752
5.201525-5 5.201525-5 5.201525-5 5.201525-5 5.201525-5 5.201525-5132633  1 1753
1.472366-5                                                       132633  1 1754
0.000000+0 0.000000+0         13          1         13          5132633  1 1755
4.004717-5 4.004717-5 4.004717-5 4.004717-5 4.004717-5 4.004717-5132633  1 1756
4.004717-5 4.004717-5 4.004717-5 4.004717-5 4.004717-5 4.004717-5132633  1 1757
1.133592-5                                                       132633  1 1758
0.000000+0 0.000000+0         13          1         13          6132633  1 1759
2.690806-5 2.690806-5 2.690806-5 2.690806-5 2.690806-5 2.690806-5132633  1 1760
2.690806-5 2.690806-5 2.690806-5 2.690806-5 2.690806-5 2.690806-5132633  1 1761
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7.616711-6                                                       132633  1 1762
0.000000+0 0.000000+0         13          1         13          7132633  1 1763
1.773523-5 1.773523-5 1.773523-5 1.773523-5 1.773523-5 1.773523-5132633  1 1764
1.773523-5 1.773523-5 1.773523-5 1.773523-5 1.773523-5 1.773523-5132633  1 1765
5.020211-6                                                       132633  1 1766
0.000000+0 0.000000+0         13          1         13          8132633  1 1767
1.386183-5 1.386183-5 1.386183-5 1.386183-5 1.386183-5 1.386183-5132633  1 1768
1.386183-5 1.386183-5 1.386183-5 1.386183-5 1.386183-5 1.386183-5132633  1 1769
3.923789-6                                                       132633  1 1770
0.000000+0 0.000000+0         13          1         13          9132633  1 1771
1.159959-5 1.159959-5 1.159959-5 1.159959-5 1.159959-5 1.159959-5132633  1 1772
1.159959-5 1.159959-5 1.159959-5 1.159959-5 1.159959-5 1.159959-5132633  1 1773
3.283431-6                                                       132633  1 1774
0.000000+0 0.000000+0         13          1         13         10132633  1 1775
8.578299-6 8.578299-6 8.578299-6 8.578299-6 8.578299-6 8.578299-6132633  1 1776
8.578299-6 8.578299-6 8.578299-6 8.578299-6 8.578299-6 8.578299-6132633  1 1777
2.428210-6                                                       132633  1 1778
0.000000+0 0.000000+0         13          1         13         11132633  1 1779
6.674139-6 6.674139-6 6.674139-6 6.674139-6 6.674139-6 6.674139-6132633  1 1780
6.674139-6 6.674139-6 6.674139-6 6.674139-6 6.674139-6 6.674139-6132633  1 1781
1.889210-6                                                       132633  1 1782
0.000000+0 0.000000+0         13          1         13         12132633  1 1783
5.566800-6 5.566800-6 5.566800-6 5.566800-6 5.566800-6 5.566800-6132633  1 1784
5.566800-6 5.566800-6 5.566800-6 5.566800-6 5.566800-6 5.566800-6132633  1 1785
1.575762-6                                                       132633  1 1786
0.000000+0 0.000000+0         17          1         17         13132633  1 1787
1.154480-6 1.154480-6 1.154480-6 1.154480-6 1.154480-6 1.154480-6132633  1 1788
1.154480-6 1.154480-6 1.154480-6 1.154480-6 1.154480-6 1.154480-6132633  1 1789
1.342892-5 1.827518-5 1.827518-5 1.827518-5 1.584766-5           132633  1 1790
0.000000+0 0.000000+0          5         13          5         14132633  1 1791
1.237530-5 1.726138-5 1.726138-5 1.726138-5 1.496853-5           132633  1 1792
0.000000+0 0.000000+0          5         13          5         15132633  1 1793
8.364854-6 1.166751-5 1.166751-5 1.166751-5 1.011770-5           132633  1 1794
0.000000+0 0.000000+0          5         13          5         16132633  1 1795
6.412509-6 8.944329-6 8.944329-6 8.944329-6 7.756243-6           132633  1 1796
0.000000+0 0.000000+0         27         13         27         17132633  1 1797
4.578647-6 6.386412-6 6.386412-6 6.386412-6 6.057870-6 3.913034-6132633  1 1798
3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6132633  1 1799
3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6132633  1 1800
3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6 3.913034-6132633  1 1801
3.913034-6 3.913034-6 7.376951-7                                 132633  1 1802
0.000000+0 0.000000+0         23         17         23         18132633  1 1803
3.017049-6 2.271340-5 2.271340-5 2.271340-5 2.271340-5 2.271340-5132633  1 1804
2.271340-5 2.271340-5 2.271340-5 2.271340-5 2.271340-5 2.271340-5132633  1 1805
2.271340-5 2.271340-5 2.271340-5 2.271340-5 2.271340-5 2.271340-5132633  1 1806
2.271340-5 2.271340-5 2.271340-5 2.271340-5 4.281989-6           132633  1 1807
0.000000+0 0.000000+0         23         17         23         19132633  1 1808
2.023187-6 1.523126-5 1.523126-5 1.523126-5 1.523126-5 1.523126-5132633  1 1809
1.523126-5 1.523126-5 1.523126-5 1.523126-5 1.523126-5 1.523126-5132633  1 1810
1.523126-5 1.523126-5 1.523126-5 1.523126-5 1.523126-5 1.523126-5132633  1 1811
1.523126-5 1.523126-5 1.523126-5 1.523126-5 2.871437-6           132633  1 1812
0.000000+0 0.000000+0         23         17         23         20132633  1 1813
3.156422-5 2.376265-4 2.376265-4 2.376265-4 2.376265-4 2.376265-4132633  1 1814
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 2.376265-4 2.376265-4 2.376265-4 2.376265-4 2.376265-4 2.376265-4132633  1 1815
 2.376265-4 2.376265-4 2.376265-4 2.376265-4 2.376265-4 2.376265-4132633  1 1816
 2.376265-4 2.376265-4 2.376265-4 2.376265-4 4.479796-5           132633  1 1817
      .
      .
      .
      .
      .
      .
 2.666295-6 2.007280-5 2.007280-5 2.007280-5 2.007280-5 2.007280-5132633  1 1899
 2.007280-5 2.007280-5 2.007280-5 2.007280-5 2.007280-5 2.007280-5132633  1 1900
 2.007280-5 2.007280-5 2.007280-5 2.007280-5 2.007280-5 2.007280-5132633  1 1901
 2.007280-5 2.007280-5 2.007280-5 2.007280-5 3.784176-6           132633  1 1902
 0.000000+0 0.000000+0         23         17         23         38132633  1 1903
 2.169670-6 1.633404-5 1.633404-5 1.633404-5 1.633404-5 1.633404-5132633  1 1904
 1.633404-5 1.633404-5 1.633404-5 1.633404-5 1.633404-5 1.633404-5132633  1 1905
 1.633404-5 1.633404-5 1.633404-5 1.633404-5 1.633404-5 1.633404-5132633  1 1906
 1.633404-5 1.633404-5 1.633404-5 1.633404-5 3.079335-6           132633  1 1907
 0.000000+0 0.000000+0         23         17         23         39132633  1 1908
 2.382007-7 1.793258-6 1.793258-6 1.793258-6 1.793258-6 1.793258-6132633  1 1909
 1.793258-6 1.793258-6 1.793258-6 1.793258-6 1.793258-6 1.793258-6132633  1 1910
 1.793258-6 1.793258-6 1.793258-6 1.793258-6 1.793258-6 1.793258-6132633  1 1911
 1.793258-6 1.793258-6 1.793258-6 1.793258-6 3.380696-7           132633  1 1912
 0.000000+0 0.000000+0          1         74          1         74132633  1 1913
 0.000000+0                                                       132633  1 1914
 0.000000+0 0.000000+0          0        103          0         74132633  1 1915
 0.000000+0 0.000000+0          1         74          1         74132633  1 1916
 0.000000+0                                                       132633  1 1917
 0.000000+0 0.000000+0          0        104          0         74132633  1 1918
 0.000000+0 0.000000+0          1         74          1         74132633  1 1919
 0.000000+0                                                       132633  1 1920
 0.000000+0 0.000000+0          0        105          0         74132633  1 1921
 0.000000+0 0.000000+0          1         74          1         74132633  1 1922
 0.000000+0                                                       132633  1 1923
 0.000000+0 0.000000+0          0        106          0         74132633  1 1924
 0.000000+0 0.000000+0          1         74          1         74132633  1 1925
 0.000000+0                                                       132633  1 1926
 0.000000+0 0.000000+0          0        107          0         74132633  1 1927
 0.000000+0 0.000000+0          1         74          1         74132633  1 1928
 0.000000+0                                                       132633  1 1929
 0.000000+0 0.000000+0          0        851          0         74132633  1 1930
 0.000000+0 0.000000+0          1         74          1         74132633  1 1931
 0.000000+0                                                       132633  1 1932
                                                                  132633  0 1933
 2.600000+4 5.536500+1          0          0          0         40132633  2 1934
 0.000000+0 0.000000+0          0          2          0         74132633  2 1935
 0.000000+0 0.000000+0         17          1         17          1132633  2 1936
 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1937
 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1938
 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.128462-3           132633  2 1939
 0.000000+0 0.000000+0         17          1         17          2132633  2 1940
 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1941
 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1942
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2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.128462-3            132633  2 1943
0.000000+0 0.000000+0         17          1         17           3132633  2 1944
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1945
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1946
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.128462-3            132633  2 1947
0.000000+0 0.000000+0         17          1         17           4132633  2 1948
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1949
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.500000-3132633  2 1950
2.500000-3 2.500000-3 2.500000-3 2.500000-3 2.128462-3            132633  2 1951
    .
    .
    .
    .
    .
```

The processed multigroup covariance data for MAT1326 begin with Card 634. The designation of MF=33 in Field 8 is the value of MFCOV, as discussed in Section X.K. Card 634 repeats the ZA and AWR numbers in Fields 1 and 2, and the number 41 in Field 6 indicates that covariance matrices follow for 41 reaction pairs. The number 1 in the MT field (Field 9) indicates that all 41 reaction-pairs have MT=1 as the first reaction.

The data for one such reaction pair begin at Card 1738. Field 4 of Card 1738 contains the number 102, so the second reaction here is MT1=102. In other words, the data to follow refer to the covariance matrix of the iron total cross section (MT=1) with the iron radiative capture reaction MT1=102. The occurence of the number 14 in Field 6 of Card 1791 indicates that the block of data starting there refers to Group 14 of MT=1, *i.e.*, the fourteenth row of the covariance matrix. The number 5 in Field 3 of Card 1791 indicates that there are 5 consecutive groups of MT1=102 for which covariances will be given explicitly. The first covariance applies to group 13 of MT1=102, as indicated by the number 13 in Field 4. Then, in referring to the entry in the fifth field of Card 1792, for example, one would say that the relative covariance of the iron total cross section in Group 14 (17.603-37.267 eV) with the iron radiative capture cross section in Group 17 (101.3–167.02 eV) is 1.496853×10^{-5}.

Any row of a covariance matrix, or any part of a row, that contains only zeros is omitted from the ERRORR output file. The only exception is that the last row (Group 74 here) is always given explicitly, even if it does contain only zeros. The occurrence of the last row terminates a given covariance matrix and signals that the next card will name a new reaction pair. These two conventions are applied simultaneously in Cards 1915–1917 to compactly represent the covariance matrix for a reaction pair (1, 103) having only zero covariances.

Although the output file in this example contained no cross-material covariances, the only difference in the file structure in the cross-material case is that `MAT1` is specified in the integer field just preceding `MT1`, for example, in Field 3 on Card 1738. The entry `MAT1=0` in that position is a flag to indicate that `MAT1=MAT=1326`.

M. Error Messages

`ERRORR***ILLEGAL IREAD=---`

Currently defined values are 0, 1, and 2.

`ERRORR***ONLY --- EK ENERGIES ALLOWED.`

The number of derived-cross-section energy-range boundaries is limited to 50.

`ERRORR***TOO MANY REACTION TYPES.`

This error occurs in runs with `IVERF=4` if the number of requested covariance reactions is more than 60. A possible solution is to use the `IREAD=1` option to select only the most needed reactions. This error also occurs in runs where internal group averaging is requested `(NGOUT=0)` if there are more than 200 sections in `MF=33`. An alternative is to run GROUP first, then ERRORR with `NGOUT.GT.0`.

`ERRORR***NOT CODED FOR MFCOV=---.`

Allowed values are 31 and 33.

`ERRORR***TOO MANY STANDARDS REDEFINED.`

Limit is 5. See input for `NSTAN.NE.0`.

`ERRORR***ILLEGAL MT GT 870.`

There is a fault in the evaluation.

`GRIDD***MT --- REFERENCED IN DERIVATION FORMULA FOR ENERGY RANGE....`

There is a fault in the evaluation or input.

`GRIDD***TOO MANY MT-NUMBERS IN NC-TYPE SUB-SUBSECTIONS WITH LTY=0`

Limit is 60.

`GRIDD***CANNOT CALCULATE COVARIANCES OF REACTION....`

This message is self-explanatory.

`GRIDD***COVARIANCES OF REACTION....`

There is a fault in the evaluation.

`GRIDD***TOO MANY REACTION TYPES.`

This error occurs if `IVERF=5` and if the requested number of covariance reactions is greater than 60. If cross-material covariances are not needed, then a possible solution is to use the `IREAD=1` option to select only the most needed reactions.

GRIDD***ILLEGAL MT1=0.

There is fault in the evaluation. Evaluator may have meant to indicate MT1=MT. If so, change the data value for MT1 on NENDF from 0 to MT and resubmit.

MERGE***STORAGE EXCEEDED.

Either the number of points in the x grid exceeds 150 or the number in the y grid exceeds 1000.

MERGE***Y(---)=--- LT Y(---)=---.

This problem should not occur.

GRIST***STANDARDS TAPE BAD.

There is a fault in the evaluation. Standards reactions must have at least one subsection; that is, they may not be components of a lumped reaction.

GRIST***ILLEGAL LB=0.

There is a fault in the evaluation. Absolute covariances are not permitted in the standards.

GRIST***ILLEGAL NI=0 IN THE STANDARD, MATSTD=---, MTSTD=---.

There is a fault in the evaluation. Standards reactions may not be derived from other reactions.

LMPMT***STORAGE EXCEEDED.

The number of component reactions of a lumped reaction is limited to 50.

COVCAL***STORAGE EXCEEDED IN LOC.

The number of NI-type sub-subsections in any subsection is limited to 30.

COVCAL***LB=--- WHEN LT=---.

There is a fault in the evaluation. LB-LT combination is not defined.

COVCAL***NOT CODED FOR LB=---.

Currently defined values are 0 through 6 and 8.

COVCAL***STORAGE EXCEEDED IN EGT.

At the time of COVCAL processing, the number of groups on NGOUT (equal to the number of union groups) is limited to 1000.

COVCAL***MFCOV MT FOUND NOT EQUAL TO INPUT MT.

There is a conflict between internal list of covariance reactions and the reactions encountered in the ENDF file. This problem should not occur.

COVCAL***STORAGE EXCEEDED IN A.

There is insufficient space in core to store the information from NI-type sub-sub-sections. Increase the size of /ESTORE/ and NAMAX.

COVCAL***ILLEGAL MT1=0.

See similar diagnostic in SUBROUTINE GRIDD above.

`COVCAL***DATA IN A(LOCI) ARE ILLEGAL.`

There is a fault in the evaluation. The ratio-to-standard data are bad. Either `LTY` is outside the legal ENDF range of 1–3 or the energies `EL, EH` are negative or out of order.

`COVCAL***MUST REQUEST MAT1=--- AND MT1=--- ON CARD 10.`

There is an input error in requesting covariances of X with Y when both are measured relative to Z. The standard Z must be specified on Card 10 and must appear as negative entries on Card 11.

`ROGOUT***MAT --- NOT FOUND.`

Cannot find `MAT` on multigroup library.

`RDGOUT***MF---, MT--- NOT FOUND.`

Cannot find requested group structure or cross sections on multigroup library.

`RDGOUT***BAD INDEX FOR B EQUIVALENT TO SIG(IG).`

This problem should not occur.

`COVOUT***UNABLE TO FIND IY OR IYP FROM MTS ARRAY.`

There is a conflict between the internal list of covariance reactions and the reactions encountered on the union-group covariance file produced in `COVCAL`. This problem should not occur.

`COVOUT***STORAGE EXCEEDED IN SUM.`

There is insufficient space in core to store the `NMT1*NGN` user-group cross sections. Increase the size of `/ESTORE/` and `NAMAX`.

`COVOUT***UNEXPECTEDLY, IX NE IY OR IXP NE IYP.`

This problem should not occur.

`SIGC***COVARIANCE REACTION MISSING FROM LUMPING TABLE.`

A covariance reaction in the 851–870 range cannot be found in the lumped reaction definition tables. This problem should not occur.

`RESPRP***ILLEGAL RESONANCE REPRESENTATION IN MF=32. LRF=---.`

There is a fault in the evaluation. Allowed values of `LRF` are 1 ane 2 (single- and multi-level Breit-Wigner representations).

`RESPRP***STORAGE EXCEEDED.`

There is insufficient space in array `ISCR` to store resonance-parameter covariances for the current L-value. Limit is 5006 words.

`RESPRP***BAD COVARIANCE DATA FOR RESONANCE PARAMETERS....`

There is a fault in the evaluation. Covariance matrix of the parameters has negative variances, infinite correlation coefficients, or correlation coefficients greater than 2.0. Data may be out of order.

`GRPAV---MF --- MT --- HAS THRESHOLD GT HIGHEST UNION ENERGY.`

Though not a fatal error, this message often precedes an abort in `COVCAL` caused by the absence of this reaction on `NGOUT`. If `IREAD=1`, then delete this reaction from the requested list of covariance reactions.

GRPAV***UNABLE TO FIND TEMP=---.

The program cannot locate requested material and temperature on NPEND.

GRPAV***CANNOT GROUP-AVERAGE MT=---. USE GROUPR FIRST....

The MFCOV=31 and NGOUT=0 options are not compatible.

GRPAV***NOT CODED FOR MULTIMATERIAL GROUP AVERAGING....

The IREAD=2 and NGOUT=0 options are not compatible.

COLAPS***DID NOT FIND EXPECTED MF1 MT451.

Multigroup libraries produced with the GROUPR modules always contain the group structure in MF=1, MT=451.

COLAPS***STORAGE EXCEEDED.

Number of groups in NGOUT library structure is limited to 2*NPAGE+50, which, for the standard value of NPAGE (306), gives a limit of 662 groups.

COLAPS***NGOUT GROUP STRUCTURE DOES NOT SPAN UNION GRID.

The supplied library must cover the entire energy range of the union grid, which is the same as the energy range of the user's grid.

COLAPS***NOT CODED FOR MULTIPLE SIGMA ZEROES OR LEGENDRE ORDERS.

Because of this restriction, existing "general-purpose" GENDF files may not be suitable for use as input to ERRORR, in which case a special GROUPR run, just to prepare the NGOUT file for ERRORR, will be required.

UNIONG***EXCEEDED STORAGE IN MFCOV ENERGY GRID.

Applies only if IVERF=4.

UNION***ENERGIES OUT OF ORDER. --- LT ---.

Applies only if IVERF=4.

UNIONG***EXCEEDED STORAGE IN UNION GRID.

Insufficient space in core to store the union grid. Increase /ESTORE/ and NAMAX.

EGNGPN***TOO MANY GROUPS.

User group structure is limited to 640 groups.

EGNGPN***READ-IN GROUP STRUCTURE IS OUT OF ORDER.

With the IGN=1 option, the supplied group structure must be in increasing order.

EGNGPN***ILLEGAL GROUP STRUCTURE REQUESTED.

Allowed values of IGN are 1–17 and 19.

EGNWTF***ILLEGAL WEIGHT FUNCTION REQUESTED.

Allowed values of IWT are 1–9.

EGTSIG***MT=0

In the NGOUT=0 option, a point cross section has been requested by GRPAV for an illegal MT number. In this context, the allowed values of MT are 1–150, 207, 251–253, and 600–799. MT numbers 600–699 are not defined in ENDF-5, but may be used on ENDF and PENDF files specially prepared as input to ERRORR, to allow processing of nonstandard reaction types.

N. Input/Output Units

The following logical units are used:

10 NGOUT in GRPAV and NTP in COLAPS. Contains the union group cross sections for all reactions with covariances. If the user input value of NGOUT is zero, point data are read from NPEND and written to NGOUT=-10 in GRPAV. If the input value NGOUT is not zero, coarse group multigroup data are read from the user's NGOUT in COLAPS and written to NTP=-10. When COLAPS is finished, NGOUT is reset to -10.

11 NSCR in COVCAL and COVOUT. Contains the union-group multigroup covariances for the directly evaluated reactions.

12 NSCR2 in COVOUT. This is a second copy of NSCR, which is read only for the "trivial" derivation case, ISD=1. Saves execution time by eliminating the calculation of many zero contributions.

13 NSCRG in the COVCAL and RDGOUT. This unit is used to extract a single MAT from a multimaterial NGOUT.

15 NSCR in LUMPTMT and LUMPXS. This unit is used if MT numbers in the 851–870 range (lumped reactions) are found in ENDF covariance file to keep a copy of the covariance file.

20–99 Users can choose any of these numbers for NENDF, NPEND, NGOUT, NOUT, NIN, and NSTAN.

Units 11 and 12 are normally binary, although they can be switched to formatted mode by changing the value of the variable IMODE in the main program to +1. Unit 13 has the same mode as NGOUT. The user can choose the modes for NENDF, NPEND, NGOUT, NOUT, NIN, and NSTAN, except that NOUT and NIN must have the same mode.

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