30. INTRODUCTION TO DATA COVARIANCE FILES

30.1. General Comments

The inclusion of uncertainty estimates is intrinsic to any evaluation of physical constants because the practical utility of a "constant" depends on whether the true magnitude of the quantity is sufficiently close to the quoted best value. The need is now accepted to include uncertainties in evaluated nuclear cross section files in order that the propagated uncertainties in nuclear analytic results can be estimated. The resulting files are called "covariance files" as shorthand for a more complete name such as "files of nuclear variance and covariance data." The priority for development of formats for and evaluation of covariance data is highest where the sensitivity of important calculated results to the quantities in the associated cross section file is high.

Until ENDF/B-IV, the only means available to evaluators for communicating the estimated uncertainties in the evaluated data was through publication of the documentation of the evaluations. During the preparation of ENDF/V-IV, a Data Covariance Subcommittee of CSEWG was formed to coordinate the efforts at standardizing statements made about the data uncertainties and correlations.

One of the important aspects of nuclear data and of cross sections in particular is that the various data tend to be correlated to an important degree through the measurement processes and the different corrections made to the observable quantities to obtain the microscopic cross sections. In many applications when one is interested in estimating the uncertainties in calculated results due to the cross sections, the correlations among the data play a crucial role.

In principle, the uncertainties in the results of a calculation due to the data uncertainties can be calculated, provided one is given all of the variances in and covariances among the data elements. In practice, in addition to the uncertainties due to the basic data, the results of calculations have uncertainties due to imperfections in the calculational models used. In some situations "modeling uncertainties" may dominate the uncertainties in computed results; in others they are negligible compared to the effects of microscopic data uncertainties. In principle improving the models may reduce “modeling uncertainties”, although sometimes at large cost. The data uncertainties may also be reduced, often at large cost, by performing better measurements, new kinds of measurements, or sometimes a more refined analysis of existing data.

One of the requirements of the uncertainty information is that it be easily processed to yield the (variances and) covariances for the multigroup or other "data" used directly in the calculations. For ENDF/B-IV, the principle of having the uncertainty information on the data file was adopted and a trial formalism was developed. This formalism has the virtue that the information is in such a form that it can be easily processed with minor modification to existing processing codes. Only a few evaluations of ENDF/B-IV were issued with data covariance information in this format. Since then, considerably more work has been done in trying to quantify data covariances within the ENDF formalism and using the information for purposes of sensitivity studies. These sensitivity studies have been made in three different areas where the data covariances play a crucial role: propagation of uncertainties to final calculated results, adjustment of data sets incorporating information from some integral measurements, and determination of data accuracies needed to meet targeted uncertainties in results. The formalism and formats for representing data covariances in ENDF/B-V were extended to cover all neutron cross section data in the files.

Formats and procedures exist in ENDF-6 for representing the data covariances in fission neutron multiplicity (File 1), resonance parameters (File 2), the neutron cross sections (Files 3 and 10), energy distributions (File 4) and angular distributions (File 5). There is also the capability to represent data covariances obtained from parameter covariances and sensitivities. The ability to represent cross section uncertainties is rather complete, while in the other cases there are restrictions. In some cases such as inelastic scattering one may employ the subterfuge of pseudo-discrete levels to treat a continuum using the formats and procedures of File 3 and 33.

Since covariance files will be incomplete, the absence of covariance data in a file in ENDF-6 formats does not imply that the uncertainty component of interest has been evaluated as zero. Evaluators should not unintentionally enter explicit zero covariance components into a file, since these would imply to a user that the uncertainty or correlation has been evaluated as negligibly small.

The dominant reason for the inclusion of covariance files in the ENDF system is to enable estimation of the nuclear data contributions to the uncertainties in calculated results for nuclear systems having broad (neutron) spectra. Therefore, in developing the ENDF formats the highest priority was given to attaining this goal. The ENDF covariance files are structured to enable processing them to any energy group structure. As is explained most fully in Chapter 33, except for LB=8 sub-subsections, the stored quantities are defined to yield the covariances between point cross sections. To simplify processing, the magnitudes of these components are constant between the points on the defined energy grid.

The files have a histogram appearance, but the quantities have a precise definition that can lead to incorrect inferences if the encoded values are used for other than the primary purpose of uncertainty propagation with broad particle energy spectra. For example, File 33 except for LB=8 sub-subsections literally implies that the cross sections at any two points within the same energy grid interval are perfectly correlated, and that the uncertainty is no larger for a cross section averaged over a tiny energy interval than if it were averaged over the whole interval between grid points. The new LB=8 format allows the evaluator to avoid this unrealistic implication. A broadly spaced energy grid was usually chosen in the past to achieve the primary purpose without attempting to provide greater covariance data detail than is warranted by the available information.

As indicated above, the main purpose of the covariance information in ENDF-6 formats is to permit the propagation of nuclear data uncertainties for applications with broad neutron spectra. Users of the file should interpret the files as they were designed. If modifications to the covariance data must be made by users to place the data on a finer grid without reconsideration of the uncertainties in the underlying data, those modifications should be designed so that the original evaluator's covariance data is recovered if the modified results are collapsed to the evaluator's energy grid.

Modifications of covariance files to a finer grid have been required in the past by users who employ the adjustment equations to update an existing evaluation by "adding" new data and their associated covariances. To minimize the extent to which such users will be tempted to make *ad hoc* changes to covariance files, covariance evaluators for reactions of particular importance should employ relatively fine energy meshes to reduce the difficulties to be encountered by future evaluator-users of the covariance files. Overlapping structures in energy and other techniques should be used to reduce the occurrence of large changes in correlation as one crosses any arbitrary energy boundary. The new file-30 format provides an alternate way to avoid the effects of artificial energy boundaries.

It is appropriate to define uncertainty quantities[1]. Each cross section or related quantity in an ENDF file represents a physical quantity that has a definite though unknown true magnitude. The knowledge of each such quantity X is summarized by its density function defined so that f(X) ΔX is the probability that the true numerical value of X lies in the range ΔX at X. The marginal density function f(X) is the average over all other independent variable Y, Z, ... of the overall multivariate density function for the cross section data base. The shape of a density function depends on the experiments that have been performed relevant to estimating the true values of the data elements. The density function has unit normalization for each variable.

The "expected value", <g(X)>, of any function g(X) is given by the average value of that function over the marginal density function. The simplest example is the expected value of the quantity itself:

$$< X >= \int X \; f(X)\, dX$$

In practice, one often uses the same symbol for a physical quantity, its expected value, and its value in a particular data set. In this Chapter, the last is written X = <X> + δX, where <δX>=0. In this language the cross section, *etc.*, quantities in ENDF-6 files are expected values.

The width of the density function reflects the scatter among experimental cross section results and/or the uncertainties ascribed to the values by the experimenters. That width is a property of the experiments, not of the cross section quantity, so one cannot in the usual sense "measure" nuclear covariance data. The width arises from the ambiguity with which each underlying experimental result defines the true value. These ambiguities are quantified as "errors" with modifiers like "systematic" or "statistical" to indicate the origin of the ambiguities and modifiers like "standard" or "relative" to indicate the normalization of the uncertainty quantities. Since both systematic errors and statistical counting errors broaden the density functions of evaluated quantities, evaluated uncertainty data must combine both types. The systematic uncertainties are harder to estimate, and are larger than statistical counting uncertainties in most modern nuclear experiments.

The ENDF-6 formats deal only with the expected values of quantities and the second-degree moments of the joint density function describing the evaluator's knowledge of the true value of the nuclear data vector. It is not necessary to assume that the density functions are normal in shape, or otherwise, unless one must estimate the probability that the true value lies within a certain range of the expected value. The ENDF-6 covariance quantities are not intended to represent, and cannot well represent, any known difference between and ENDF-6 formatted cross section and some more-recently realized "better" evaluation, or any cross-section imprecision induced by ENDF-6 procedures, or the widths of any physical distributions such as the fission neutron multiplicity distribution P(ν).

The following quantities are defined that relate to the second moments of the density function. Here <X> and <Y> are cross section or related quantities in a file using ENDF-6 formats. The quantity f(X,Y) is the full density function averaged over all variables other than X and Y. Recall that δX = X - <X>.

[1] The treatment below is paraphrased from R. Peelle, *Sensitivity and Uncertainty Analysis of Reactor Performance Parameters*, **Advances in Nuclear Science and Technology**, Vol. 14, pp 11, Lewins and Becker, Eds., Plenum Press, New York, 1982.

$\mathrm{Cov}(X,Y) = <\delta X\,\delta Y>$

$= \iint (X - <X>)(Y - <Y>)\,F(X,Y)\,dX\,dY$, the covariance between X and Y,

$\mathrm{Var}(X) = \mathrm{Cov}(X,X) = <\delta X^2>$, the standard error or uncertainty in <X>,

$s(X) = \left[\mathrm{Var}(X)\right]^{1/2}$, the variance of X,

$\rho(X<Y) = \mathrm{Cov}(X<Y) / \{s(X)\,s(Y)\}$, the correlation coefficient between X and Y.

The relative standard error, $s(X)/\langle X\rangle$, the relative variance $\mathrm{Var}(X)/<X>^2$, and the relative covariance, $\mathrm{Cov}(X,Y)/(<X><Y>)$, are often used.

Knowledge of the covariance is crucial to the joint application of the quantities X and Y; for example, the standard error in the sum X+Y can lie anywhere between *s(X)+s(Y)* and $|s(X) - s(Y)|$ depending upon the degree of correlation between X and Y. A nonzero covariance between two quantities can arise from a partial dependence of one upon the other or from a common dependence upon some third uncertain quantity.

30.1. FILE 30. DATA COVARIANCES OBTAINED FROM PARAMETER COVARIANCES AND SENSITIVITIES

30.1.1. General Description

File 30 is provided as a means of describing the covariances of tabulated cross sections, multiplicities, and energy-angle distributions that result from propagating the covariances of a set of underlying parameters (for example, the input parameters of a nuclear-model code) using an evaluator-supplied set of parameter covariances and sensitivities. Whenever nuclear data are evaluated primarily through the application of nuclear models, the covariances of the resulting data can be described very adequately, and compactly, by specifying the covariance matrix for the underlying nuclear parameters, along with a set of sensitivity coefficients giving the rate of change of each nuclear datum of interest with respect to each of the model parameters. Although motivated primarily by these applications of nuclear theory, use of File 30 is not restricted to any one particular evaluation methodology. It can be used to describe data covariances of any origin, so long as they can be formally separated into a set of parameters with specified covariances and a set of data sensitivities.

The need for a covariance format of this type became clear in connection with the R-matrix analysis of the ENDF/B-VI light-element standards. The key parameters here are the parameters of a few high-energy resonances in the relevant compound systems. Another area where this format is expected to find early application is in representing the covariances of cross sections and secondary-particle emission spectra and angular distributions due to neutron interactions in the 0.1-20 MeV range, when the data are obtained primarily from the optical model and statistical-pre-equilibrium theory. Relevant parameters here include the optical parameters, level-density prescription, pre-equilibrium matrix elements, and gamma-ray strength functions.

It is shown below that multi-group averages of parameter sensitivities are identical to the parameter sensitivities of the corresponding multi-group data. It is the latter that are actually needed in most applications. (See Section 30.1.4.) To take maximum advantage of this equivalence, sensitivity information is represented in File 30 in a format that is as close as possible to the format for the actual data, so that the sensitivities can be retrieved and integrated by processing codes with the least possible modification.

It should be emphasized that File 30 is ***not*** intended as a repository for complete "evaluations of parameters." In fact, to limit the bulk of the files and to minimize processing costs, evaluators are encouraged to reduce the number of parameters and the number of sensitivities per parameter to the minimum necessary to describe data uncertainties of practical importance. In defining the format for File 30, no attempt is made to prejudge the parameter definitions or types of nuclear theory that may be most appropriate or useful. Discussion of such points is obviously encouraged in the printed documentation, but the format itself is deliberately kept totally general. One advantage of this generality is that the results of a wide variety of evaluation methodologies can be described using a single format. As discussed in Section 30.1.3 below, this generality also facilitates various mathematical operations, such as diagonalizing the parameter covariance matrix.

30.1.1.1. Definitions

In the context of File 30 the word "sensitivity" is defined as the derivative of an evaluated quantity, call it σ, with respect to the logarithm of one of the parameters, α_i,

$$\sigma_i' \equiv \frac{\partial \sigma}{\partial \left(\ln \alpha_i\right)} = \alpha_i \frac{\partial \sigma}{\partial \alpha_i} \tag{30.1}$$

An advantage of employing such derivatives is that σ'_i is expressed in exactly the same units as σ, whether it be an actual cross section or a distribution (energy distribution, angle distribution, double-differential quantity, *etc*.). This means, among other things, that integrations over energy and angle can be performed with minimal changes in multi-group processing codes. The use of derivatives with respect to the logarithms of the parameters also meshes nicely with the use of relative parameter-covariance matrices, as shown below in Eq. (30.7).

As discussed in detail in Section 30.1.2.3, a ***sub-section*** of one section of File 30 is employed to store the sensitivities of the data in one ***section*** (called the **r*eferenced*** section) of a file elsewhere in the material of interest.

It should be emphasized that normally there will not be a direct, one-to-one correspondence between the energy or angular grid in a subsection of File 30 and that used in the referenced section. This follows from the fact that the derivatives in File 30 are not actually the derivatives of individual data values. Rather, the collection of data in one such subsection should form an adequate representation of the energy-and angle-dependence of the relevant derivative function, making effective use of the standard interpolation laws.

File 30 does not permit the representation of the uncertainty in independent variables (the floating-point numbers that define the energy and angle grids of an ENDF section). This would seriously complicate the calculation of the uncertainty in averaged quantities, as discussed below. Further, if σ is thought of as the output of a model calculation, quantities such as the incident energy or outgoing angle are specified by the model-code user and have no meaningful uncertainty.

In addition, File 30 may not be used to represent uncertainty of any integer, nor the uncertainty of stand-alone (untabulated) quantities that affect energy or angle grids, such as masses, Q-values, and the boundaries of energy ranges. Thus, it is understood that the data fields normally used to store probability information (cross sections, multiplicities, or normalized distributions) are used in File 30 to record sensitivity information, but that other quantities have standard (MF≠30) ENDF definitions.

30.1.1.2. Treatment of Various Data Types

Following the general guidelines stated above, subsections of File 30 describing cross-section (as opposed to multiplicity or distribution) sensitivities would have the same mechanical structure as sections of File 3. Of course, since sensitivities are derivatives, many more negative numbers would appear in the floating-point data fields than one normally expects to see File 3. One can treat $\bar{\nu}$ data in File 1 in the same way as cross sections.

Some interesting points arise with respect to distributions, for example tabulated data in File 4 for elastic scattering. If the derivatives of the normalized angular distribution $p(\theta)$ with respect to a given parameter are large, they should be described in a subsection with (MFSEN,MTSEN) = (4,2).

Note that since $p(\theta)$ is normalized to unity by definition, the angle integral of the sensitivities (equal to the parameter-derivative of the angle integral) should be zero. A second important aspect of the use of two separate functions to build the actual desired data is that, in order to build the corresponding sensitivities, the product rule is employed. For example, the differential elastic cross section $\gamma(\theta)$ (barns/steradian) at angle θ is formed as a product,

$$\gamma(\theta) \equiv d\sigma/d\Omega = \sigma p(\theta), \tag{30.2}$$

So that

$$\frac{\partial \gamma(\theta)}{\partial \alpha_i} = \sigma \frac{\partial p(\theta)}{\partial \alpha_i} + p(\theta)\frac{\partial \sigma}{\partial \alpha_i}. \tag{30.3}$$

Multiplying both sides of Eq. (30.3) by α_1, and recalling the notation of Eq. (30.1), one gets,

$$\gamma_i'(\theta) = \sigma p_i'(\theta) + \sigma_i' p(\theta). \tag{30.4}$$

Equation (30.4) shows, then, how the sensitivity $\gamma_i'(\theta)$ is constructed from the data in two different subsections (σ_i' and p_i') of File 30, plus data (σ and p) from Files 3 and 4, respectively. The generalizations needed to treat three or more separate factors are obvious.

Both to reduce the bulk and to reduce processing costs, evaluators should simply omit reference to sections in the main evaluation that exhibit little sensitivity to a given parameter. Such omissions will be treated as if zeroes had been entered explicitly. For example, if the angular distributions are omitted from File 30, then the first term on the right in Eq. (30.4) will be omitted.

Just as one is permitted to employ a Legendre representation of $p(\theta)$ in File 4, one is permitted in File 30 to use a Legendre expansion to represent $p_i'(\theta)$. In fact, if it reduces the size of the files, it is preferable to use Legendre moments for $p_i'(\theta)$, even if $p(\theta)$ itself is given in tabular form. As mentioned above $p_i'(\theta)$ must integrate to zero, so the magnitude of the implied zero-th Legendre moment of $p_i'(\theta)$ is zero, not unity. These considerations of File 4-type sensitivities can be extended in an obvious way to treat neutron spectra in file 5, isomer-ratios in File 9, photon-production multiplicities in File 12, fission-product yields, *etc.*

No fundamental new problems are introduced by considering double-differential data, as represented in File 6. In that case, p becomes a function $p(E',\theta)$ of both the final energy and angle of the outgoing particle. The only complication that this adds is that p'_i in Eq. (30.4), for example, is also doubly differential, $p'_i = p'_i(E',\theta)$. It is conceivable that p'_i for some parameter will exhibit more severe angle-energy correlations than $p(E',\theta)$ itself, so it is permitted to represent the emission sensitivities for a given reaction in File-6 format in File 30, even though the angle and energy distributions for that reaction are given separately in Files 4 and 5. In this case, the entry MFSEN=6 in the File-30 dictionary really points to both File 4 and File 5 in the main evaluation. Since the File-6 type matrix information will in general occupy more space than the approximate treatment in Files 4 and 5, this option should be exercised only on those parameters (*i.e.*, in those sections) where it is crucial.

30.1.1.3. Multi-grouped Sensitivities

Multi-group operations on the data in an evaluation can be summarized as the performance of certain weighted integrations over incident energy, secondary particle type, secondary energy, and secondary angle. Although these operations are very complicated, there is no commonality between variables (or limits) of integration and the parameters of concern in File 30. One can take advantage of this in calculating the derivatives of multigroup-averaged data with respect to the parameters. If we introduce g as a generic group-averaged quantity (such as a single Legendre moment of one element of a multigroup scattering matrix), which corresponds to a differential quantity γ, then

$$g = \int dE\, dE'\, d\Omega\, \gamma_i\left(E,E',\theta\right)\omega\left(E,E',\theta\right), \tag{30.5}$$

where ω is some weighting function. As discussed below, one frequently is interested in the uncertainty in such multi-group quantities, and to obtain this uncertainty, one will first need to calculate the derivative of g with respect to the parameter α_i.

$$g'_i = \frac{\partial g}{\partial(\ln\alpha_i)} = \alpha_i \int dE\, dE'\, d\Omega \frac{\partial\gamma\left(E,E',\theta\right)}{\partial\alpha_i}\omega\left(E,E',\theta\right),$$

or

$$g'_i = \int dE\, dE'\, d\Omega\ \gamma'_i\left(E,E',\theta\right)\omega\left(E,E',\theta\right), \tag{30.6}$$

Comparing Equations (30.5) and (30.6), we obtain the useful result that the sensitivity of a multigroup value to a given parameter is equal to the multigroup average of the (energy- and angle-dependent) parameter sensitivity. Thus an ENDF processing program that calculates multigroup cross sections, Equation (30.5), can be used, with few modifications, to calculate the parameter sensitivity of multigroup constants, Equation (30.6). As mentioned in the General Description above, this is the motivation for storing the sensitivities γ'_i in a format that is as close as possible to the format of the data γ.

30.1.2. Formats

File 30 is divided into sections identified by the value of MT. (In File 30, MT does not refer to a reaction type). Each section of File 30 begins with a HEAD record and ends with a SEND record.

30.1.2.1. Directory and Correspondence Table (MT=1)

The first section, MT=1, of File 30 consists of a "directory" that displays the contents and ordering of information in other sections of the file, plus an optional, cross-material "correspondence table," described below.

The following quantities are defined.

NP Total number of distinct parameters.

NDIR Number of CONT records in the MF=30 directory, including the internal data-block "marker" records described below, but excluding both the correspondence table and the SEND record.

NCTAB Number of CONT records in the correspondence table, excluding the SEND record.

MP_i Parameter index.

$MFSEN_i$, $MTSEN_i$ If non-zero, location of a section of data in the main body of the evaluation (the referenced data) that are sensitive to parameter MP_i.

MFSEN and MTSEN determine the formats to be used to represent the energy- and angle-dependence of the sensitivities. For example, if the referenced section describes a normalized angular distribution, MFSEN=4, then any of the formats described in Chapter 4 of this manual may be employed to describe the sensitivity of the distribution in (MFSEN,MTSEN) to parameter MP_i.

NC_i Number of records used to represent this sensitivity information. These NC records constitute a single subsection of a later section of File 30.

$LIBF_i$ Sublibrary number.

$MATF_i$ Material number.

MPF_i Parameter number.

A section with MT=1 has the following structure:

```
[MAT,30,1/  ZA,  AWR,   0,        0,     0,    NP] HEAD
[MAT,30,1/ 0.0,  0.0,   0,        0,  NDIR, NCTAB] CONT
[MAT,30,1/ 0.0,  0.0,  MP1,  MFSEN1, MTSEN1,   NC1] CONT
[MAT,30,1/ 0.0,  0.0,  MP2,  MFSEN2, MTSEN2,   NC2] CONT
           ------------------------------------
           ------------------------------------
[MAT,30, 1/ 0.0, 0.0, MPNDIR,MFSENNDIR,MTSENNDIR, NCNDIR] CONT
[MAT,30, 1/ 0.0, 0.0,   MP1,   LIBF1,   MATF1,  MPF1] CONT
[MAT,30, 1/ 0.0, 0.0,   MP2,   LIBF2,   MATF2,  MPF2] CONT
           ------------------------------------
           ------------------------------------
[MAT,30, 1/ 0.0, 0.0,MPNCTAB,LIBFNCTAB, MATFNCTAB,MPFNCTAB] CONT
[MAT,30, 1/ 0.0, 0.0,    0,       0,         0,       0] SEND
```

The directory serves as a guide for the processing codes and provides, in addition, a detailed, eye-readable list of the files and sections elsewhere in the current evaluation that are significantly sensitive to the parameters under consideration. As shown above, this information is presented in a format that is similar to the main index for this material in (MF,MT) = (1,451).

In general, a given parameter will affect the data in several different sections, so the same value of MP will appear in several consecutive entries in the dictionary. MP is higher in the ENDF hierarchy than MFSEN, which is in turn higher that MTSEN. Within the File-30 framework, then, MP can be considered an index to a "sub-material". The first value of MP_1 must be 1, the next new, non-zero value must be 2, and so on. Except for marker records, MP, MFSEN, and MTSEN must occur in normal ENDF ascending order.

Unlike the main directory in (MF,MT) = (1,451) the File-30 directory contains internal file-end and sub-material end "markers". That is, within the range of records describing a given parameter MP, and following the final reference to a given value of MFSEN, an explicit directory entry with MFSEN=0 is given in order to indicate the end of information concerning MFSEN-type sensitivities for parameter MP.

```
[MAT,30, 1/ 0.0, 0.0, MP,  0,  0,  0] CONT
```

Similarly, following the final reference to a given value of MP in the directory, a directory entry with MP=0 is given to indicate the end of information concerning the current parameter.

```
[MAT,30, 1/ 0.0, 0.0,  0,  0,  0,  0] CONT
```

It may occur that the evaluated data for two different materials are sensitive to the same parameter, or to a common set of parameters. Here "sensitive to the same parameter" means that the same numerical value of some particular quantity was employed in generating both evaluations. If, in addition, the numerical value thus employed has a substantial uncertainty, then this would imply substantial cross-material and/or cross-library data covariances. These covariances may be important in some applications, for example, in uncertainty analyses involving physical mixtures of the materials in question. In order to represent these cross-library or cross-material covariances, the evaluator may include a correspondence table in the first section of MF=30 to identify the common set. The covariances of these parameters must be given in both evaluations, and the covariances must be identical. However, since the parameter-numbering scheme need not be the same the different evaluation evaluations, the correspondence table is also used to specify the relationship of the numbers assigned to these parameters in the two evaluations.

The index parameter NCTAB indicates the number of CONT records appearing in the correspondence table of the current evaluation. NCTAB may be zero, in which case the table is omitted. If present, the table includes, in the format shown above, the sub-library number LIBF, the material number MATF, and the parameter number MPF of a parameter in some external, or "foreign" evaluation that is identical to parameter MP of the current evaluation. A value of LIBF=0 is entered if the foreign sub-library is the same as that of the current evaluation. The correspondence table should be ordered (in ascending order) first on MP, then on LIBF, then MATF, and then MPF. No internal "marker" records are included in the correspondence table.

30.1.2.2. Covariance Matrix (MT=2)

The second section of File 30, MT=2, contains the NP(NP+1)/2 unique, relative covariances RCOV(I,J) of the i^{th} parameter with the j^{th} parameter in the form of NP separate LIST records. This structure permits the inclusion of a large number of parameters without requiring excessive computer storage during routine data handling. There is one such LIST record for each MP value.

The structure of MT=2 is as follows:

```
[MAT,30, 2/   ZA,  AWR,  0,  0,    0, NP] HEAD
[MAT,30, 2/ PARM1, 0.0,  0,  0, NCS1,  1/ {RCOV(1,K, K=1,NCS1}]   LIST
[MAT,30, 2/ PARM2, 0.0,  0,  0, NCS2,  2/ {RCOV(2,1+K, K=2,NCS2}] LIST
[MAT,30, 2/ PARM3, 0.0,  0,  0, NCS3,  3/ {RCOV(3,2+K, K=3,NCS3}] LIST
          ---------------------------------------------
          ---------------------------------------------
[MAT,30, 2/ PARMNP, 0.0,  0,  0,   1,  NP/ {RCOV(NP,NP)}] LIST
[MAT,30, 2/    0.0, 0.0,  0,  0,   0,   0] SEND
```

Since the filing of the MPth row of covariance matrix begins with the diagonal element, RCOV(MP,MP), the number of matrix elements NCS_{MP} explicitly given in the list must be less than or equal to (NP-MP+1). If the number given is smaller than this, the remaining covariances in that row are taken to be zero. Evaluators can take maximum advantage of this zero-suppression feature by assigning consecutive MP-values to members of groups of strongly correlated parameters. The numerical value $PARM_{MP}$ of the MPth parameter (or optionally just a zero) is entered in the first floating-point field of the LIST.

30.1.2.3. Sensitivities (MT=11-999)

Sections MT≥11 contain the sensitivities. A single section in this range of MT-values is the collection of all sensitivities (or subsections) relevant to a given parameter MP. These section number is determined by the parameter index, using the relation MT=MP+10. While evaluators should employ the minimum number of parameters necessary, no particular limit is placed on MP, other than the obvious one that MT may not exceed 999. The structure of a section with MT≥11 is as follows:

```
[MAT,30,MT/  ZA, AWR,   0,   0,   0,  NL] HEAD   MT=MP+10
             <subsection for NSUB=1>
             <subsection for NSUB=2>
            ----------------------------
            ----------------------------
             <subsection for NSUB=NL>
[MAT,30, 0/ 0.0, 0.0,   0,   0,   0,   0] SEND
```

NL in the HEAD record is the number of subsections in the current section. In other words, NL is the number of referenced sections for the current parameter. The format of a subsection of a section with MT≥11 is, with very few exceptions, the same as the format of the referenced section in the main body of the evaluation. Certain minor "bookkeeping" changes are unavoidable; for example, the MF and MT positions of a data record will contain 30 and (MP+10), respectively, not MFSEN and MTSEN.

Of necessity, the subsections of a section of File 30 are simply abutted to one another without intervening SEND of FEND records. In a sense, the roles of the usual SEND and FEND records in defining data-type boundaries are taken over here by the contents of the File-30 directory. (See Section 30.1.2.1.) For example, by reading a copy of the directory in parallel with the reading of the subsections of a single File-30 "source section" with MT≥11, a processing code could create a new ENDF-formatted evaluation on a third file from the information encountered, with MFSEN and MTSEN written into the usual MF and MT positions, and with the required SEND, FEND, and MEND records inserted.

Each subsection of the source section must be constructed so that the sensitivity information in section (MFSEN,MTSEN) of a new evaluation created in this way will comply, in all mechanical details, with the correct, current ENDF formats, as described in the chapter of this manual devoted to data of the type (MFSEN,MTSEN). Of course, requirements of completeness (for example, the requirement that MT=2 must appear in File 4 if MT=2 appears in File 3) do not apply in this context, since the absence of such information simply indicates small sensitivities.

Because of the application of the product rule, as described in Section 30.1.1.2. above, each ***subsection*** of a section with MT≥11 leads in principle to a complete multigroup, multi-Legendre-table, "transfer" matrix in which the sensitivities corresponding to the referenced section are combined with regular data from the other sections of the evaluation. These NL matrices, when summed, give the net sensitivity of all multigroup data to parameter MP, as in Equation (30.4).

30.1.3. Additional Procedures

30.1.3.1. Relation of MP-values to Physical Parameters

Since the actual parameter definitions will vary from one evaluation to the next, it is clear that choices concerning:

a) the assignment of particular MP-values to different physical parameters, and

b) what physical parameters to omit altogether,

are left to the evaluator.

30.1.3.2. Parameter Values

Because many models are nonlinear, the actual numerical values of the parameters $PARM_n$ may be included in the file, in order to record the point in parameter space where the sensitivities were calculated. See the discussion of this item in Section 30.1.2.2. The value of $PARM_n$ has no effect on propagated data uncertainties, so the units of $PARM_n$ are given only in the printed documentation. At the evaluator's option, a zero may be entered in place of the actual parameter value.

30.1.3.3. Eigenvalue Representation

By use of eigenvalue methods[2], it is straightforward to find a linear transformation that diagonalizes a given covariance matrix. This is a useful method of locating blunders (indicated by the existence of negative eigenvalues) and redundancies (indicated by zero eigenvalues) and is recommended as a general procedure prior to submission of any covariance evaluation. Moreover, once having performed such a diagonalization of a parameter covariance matrix, one could report in MT=2 of File 30 only the eigenvalues of the matrix and, in MT=11 and above, sensitivities of the data to variations in the effectively-independent linear combinations of the parameters (as summarized in the eigenvectors). If it proves feasible in individual evaluation situations, and if it leads to a substantial reduction in the overall size of the file, evaluators are encouraged to employ this technique.

[2] For example, the SSIEV routine described in B.T. Smith, et. al., *Matrix Eigenvalue Routines - EISPACK Guide*, 1976.

30.1.3.4. Thinning of Sensitivity Information

The collection of sensitivities in one subsection should form an adequate representation of the energy-and angle-dependence of the relevant derivative function, making effective use of the standard interpolation laws. "Thinning" the sensitivity information (that is, removing intermediate grid points) is encouraged, in order to reduce the size of the file, but, as a general guide, such thinning should not induce changes greater than about 10% in the reconstructed covariances.

30.1.3.5. Cross-file Correlations

The information in File 30 is considered to describe sources of uncertainty that are independent of those described in Files 31-40. Thus, for a given set of multigroup cross sections, the multigroup covariance matrix obtained from File 30 should be added, in a matrix addition sense, to such a matrix derived from the other files. This is the only level on which File 30 "communicates" with the other files.

A complication that can occur with respect to cross-file correlations is that there may exist strong correlations (due to normalization procedures, for example) between certain low-energy cross sections that are evaluated directly from measurements and the parameters employed to calculate the evaluated data at higher energies. If the evaluator wishes to describe these correlations, the covariances for the low-energy normalization reaction (and those for other reactions strongly correlated to it) can be "moved" from File 33 to File 30. A possible method for accomplishing this is to consider the moved data to have been evaluated by multiplying a well-known reference cross section by an uncertain, energy-dependent, correction factor. The correction factor can be assumed to have been evaluated on some fixed, coarse energy grid, with linear interpolation applied between grid points. In this case the "parameters" would be the values of the correction factors at the coarse-grid points EG_i . The sensitivities [see Eq. (30.1)] of the "experimentally evaluated" cross sections σ to these new parameters would be a series of triangular "hat" functions, with peak values $\sigma(EG_i)$. (Alternative approaches exist.)

3.1.4. Multigroup Applications of Parameter Covariances

Given the relative covariances, $RCOV(\alpha_i,\alpha_j) \equiv Cov(\alpha_i,\alpha_j)/\alpha_i\alpha_j$, from (MF30, MT2), and the multigrouped sensitivities g'_{mi} from Eq. (30.6), it is straightforward to obtain the covariance between one multigroup datum g_m and another g_n. It is necessary to add the additional index to keep track of the multiplicity of data types, as well as the possible multiplicity of materials. (See discussion of the latter point at the end of Section 30.1.2.1.) Making the usual approximation that g_m is not an extremely nonlinear function of the parameters, we expand in a Taylor series and retain only the first term,

$$\begin{aligned} \mathrm{Cov}\left(g_m, g_n\right) &= \sum_{ij} \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j) \\ &= \sum_{ij} \alpha_i \alpha_j \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j) / \alpha_i \alpha_j \\ &= \sum_{ij} g'_{mi} g'_{nj} \mathrm{RCOV}(\alpha_i, \alpha_j) . \end{aligned} \tag{30.7}$$

Equation (30.7) gives the desired multigroup covariance matrix in terms of the multigrouped (logarithmic) sensitivities from Eq. (30.6) and data read directly from the second section of File 30.

In addition to providing a direct route to the calculation of the uncertainty of multigroup cross sections due to parameter uncertainties, data provided in File-30 format have the potential for additional kinds of application, not involving straightforward application of Equation (30.7). Since these issues relate to computing requirements, it is necessary to deal with specific examples. In situations presently foreseen, the number of nuclear parameters might be in the range of 10 to 100, so we take 50 as typical. On the other hand, it is easy to imagine neutronics applications where the number of individual multigroup constants exceeds 10000. For example, if there are 3 high-threshold neutron-emitting reactions for a given material, the number of individual cross section items might be 3 reactions × 10 "source" groups × 80 "sink" groups × 4 Legendre tables = 9600. In such cases, the data covariance matrix $\mathrm{Cov}(g_m,g_n)$ becomes prohibitively large (10^8 items), while the sensitivity matrix g'_{mi} (containing 500000 items) and parameter covariance matrix $\mathrm{RCOV}(\alpha_i,\alpha_j)$ (with 2500 items) remain fairly manageable. Since, according to Equation (30.7), all covariance information content is already contained in the latter two items, it seems likely that multigroup libraries for high-energy neutronics applications will store these items separately, rather than in the expanded product form.

Further efficiencies are possible if the ultimate aim is to calculate the uncertainties in a set of predicted integral quantities (dose, radiation damage, fuel-breeding ratio, *etc.*), which can be denoted by a column vector, y. A typical number of such quantities might also be around 50. The covariance matrix D(y) for the integral quantities is related (again in the first-order approximation) to the cross section covariance matrix D(g), with elements given by Equation (30.7), by the familiar propagation of errors relation,

$$D(y) = S\ D(g)\ S^T \tag{30.8}$$

where S is the 50 × 10000 sensitivity matrix relating the integral quantities y to the multigroup cross sections g. S can be obtained from standard neutronics analyses. If we introduce a 10000 × 50 matrix R, having elements g'_{mi}, Equation (30.7) can be re-written in matrix form,

$$D(g) = R\,D(\alpha)R^T$$

Equation (30.8) can then becomes

$$D(y) = S\left[R\,D(\alpha)\,R^T\right]S^T = T\,D(\alpha)\,T^T \tag{30.9}$$

The product matrix $T = S\ R$, which contains the direct sensitivity of the integral data to the nuclear-model parameters, is very compact, having about the same size as the covariance matrix $D(\alpha)$. Note that in evaluating the matrix products in Equation (30.9) one actually never need calculate the full 10000 × 10000 cross section covariance matrix.

In cases where the evaluator chooses to use File 33 for certain data and File 30 for others, there is no logical problem with adding together integral covariances $D_{33}(y)$ based on conventional sensitivity and uncertainty analysis (*i.e.*, based on Files 3 and 33 only) with analogous data $D_{30}(y)$ obtained from File 30, using Equation (30.9), because the data covariances due to the parameter covariances are, by definition, independent of those described in the other covariance files.