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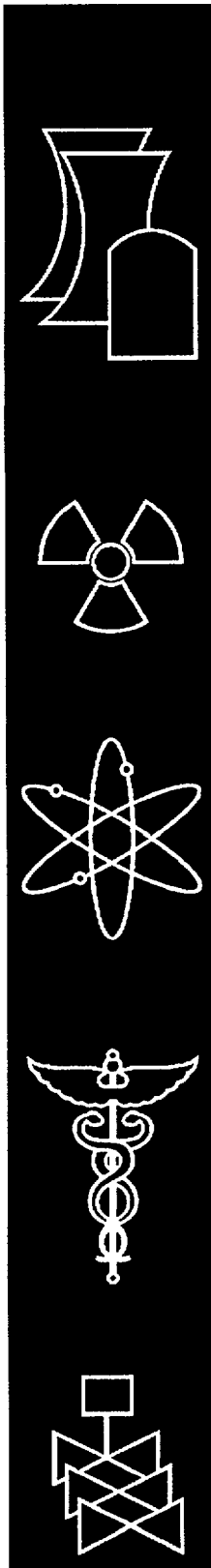

PUFF-III: A Code for Processing ENDF Uncertainty Data Into Multigroup Covariance Matrices

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Office of Nuclear Regulatory Research
Washington, DC 20555-0001

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ABSTRACT

PUFF-III is an extension of the previous PUFF-II code that was developed in the 1970s and early 1980s. The PUFF codes process the Evaluated Nuclear Data File (ENDF) covariance data and generate multigroup covariance matrices on a user-specified energy grid structure. Unlike its predecessor, PUFF-III can process the new ENDF/B-VI data formats. In particular, PUFF-III has the capability to process the spontaneous fission covariances for fission neutron multiplicity. With regard to the covariance data in File 33 of the ENDF system, PUFF-III has the capability to process short-range variance formats, as well as the lumped reaction covariance data formats that were introduced in ENDF/B-V. In addition to the new ENDF formats, a new directory feature is now available that allows the user to obtain a detailed directory of the uncertainty information in the data files without visually inspecting the ENDF data. Following the correlation matrix calculation, PUFF-III also evaluates the eigenvalues of each correlation matrix and tests each matrix for positive definiteness. Additional new features are discussed in the manual. PUFF-III has been developed for implementation in the AMPX code system, and several modifications were incorporated to improve memory allocation tasks and input/output (I/O) operations. Consequently, the resulting code has a structure that is similar to other modules in the AMPX code system. With the release of PUFF-III, a new and improved covariance processing code is available to process ENDF covariance formats through Version VI.

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1 INTRODUCTION

1.1 Background

Since the release of Version IV of the Evaluated Nuclear Data File (ENDF), standards and formats have been in place to permit the communication of estimated uncertainties in the evaluated cross-section data. By including the uncertainty or covariance information, the analyst can propagate cross-section data uncertainties through sensitivity studies to the final calculated quantities of interest in nuclear applications. The covariance data files provide the estimated uncertainty for the individual data as well as any correlations that may exist. The following list provides a description of the ENDF covariance information and the corresponding file number location within the ENDF system:

File	Covariance information
31	Average number of neutrons per fission
32	Resonance parameters
33	Neutron cross sections
34	Angular distributions of secondary particles
35	Energy distributions of secondary particles
40	Production of radioactive nuclei

Prior to using the covariance information in applications, a processing code must be used to convert the energy-dependent covariance information in the ENDF library to a multigroup form. At the Oak Ridge National Laboratory (ORNL), PUFF has been used to process ENDF uncertainty information and to generate the desired multigroup correlation matrix for the evaluation of interest. The initial version of PUFF[1] is limited to processing ENDF/B-IV formats; however, only a limited number of ENDF/B-IV evaluations have covariance information.

With the release of ENDF/B-V, many new formats and procedures were introduced for representing covariance data. The ENDF/B-V uncertainty formats permit the representation of explicit covariance relationships between different reactions as well as different materials. In addition, the capability exists for the representation of uncertainties that are based on derived mathematical relationships. For example, the total cross section is a redundant reaction that can be obtained by summing the respective partial cross sections. Consequently, the evaluator may specify that the linear relationship (i.e., equation defining summation of partial reactions) must be used to determine the components of the covariance matrix over a specified energy range. Although the linear relationship defines an explicit covariance matrix, the relationship also defines other implicit covariance matrices. The processing code must be able to determine the appropriate covariance matrix based on the linear relationship. PUFF-II was developed to process the ENDF/B-V formats as well as the older ENDF/B-IV data.[2]

Subsequent to the release of ENDF/B-V, several new formats were developed and implemented in ENDF/B-VI.[3] Within the ENDF/B-VI file system, formats exist for the representation of covariances for fission neutron multiplicity, or $\bar{\nu}$; resonance parameters; neutron cross sections, as well as energy and angular distributions of secondary particles. PUFF-III has the capability to process the covariance information for fission neutron multiplicity and neutron cross-section data. In addition, PUFF-III has the capability to process some of the resonance parameter uncertainty formats; however, all of the ENDF/B-VI resonance parameter uncertainty formats are not currently in use. Consequently, PUFF-III does not process the resonance parameter formats that are not in use because the data are unavailable for testing. The resonance parameter uncertainty formats that can be treated by PUFF-III are discussed in Sect. 1.2. Currently, PUFF-III cannot process the covariance information for the energy and angular distributions of secondary particles. The processing capabilities and limitations of PUFF-III are provided in Sect. 1.2.

1.2 Purpose and Scope

Since PUFF-II can only process ENDF formats through version V, a new version of PUFF (i.e., PUFF-III) has been developed to process the latest ENDF covariance data formats through ENDF/B-VI. PUFF-III was developed based on the original coding in PUFF-II. Consequently, all of the user input/output options (I/O) and existing formats are maintained in PUFF-III.

Previously, PUFF has existed as a stand-alone program. The objective of this work is to bring PUFF into the AMPX code system as part of the upgrade to process ENDF/B-VI cross-section formats. In order to accomplish this objective, several modifications were incorporated to improve memory allocation tasks and I/O operations. For example, some of the "hard-wired" array limits were replaced by problem-dependent limits. Moreover, the "front-end" of the code was restructured without impacting the current user input format.

Although many new covariance formats exist in the current ENDF/B-VI file system, all of the formats are not currently in use. In particular, several new formats are provided for processing resonance parameter uncertainties. Data are now provided for cross-resonance covariances between different resonance parameters. Moreover, for the General Resolved Resonance formats (i.e., LCOMP = 1),* covariance formats are available for the Reich-Moore and Adler-Adler formalisms in addition to the single- and multi-level Breit Wigner formalisms (SLBW and MLBW, respectively). Despite the new resonance parameter uncertainty formats, all of the (covariance) ENDF/B-VI isotopes currently use SLBW or MLBW uncertainty formats with no cross-resonance covariances. Since the new resonance parameter uncertainty formats (i.e., covariances between different resonances, Reich-Moore and Adler-Adler uncertainty formats) were not in use at the time of development, PUFF-III only processes the Compatible Resolved Resonance format (i.e., LCOMP = 0) which is only applicable for the Breit Wigner formalisms. With regard to unresolved-resonance data, the ENDF formats also have provisions for unresolved-resonance parameter uncertainty information; however, at the time of development, no ENDF/B-VI evaluation provided uncertainty data for the unresolved-resonance parameters. Consequently, PUFF-III does not process the unresolved-resonance uncertainty formats.

Regarding the additional ENDF/B-VI uncertainty-data formats, PUFF-III does not process the covariance information in Files 34 and 35 (i.e., uncertainty data for the angular and energy distributions of secondary particles, respectively). Furthermore, PUFF-III does not process the covariance information in File 40 (i.e., uncertainty data for the production of radioactive nuclei). At the time of development, no ENDF/B-VI evaluation provided covariances for the angular distribution of secondary particles. With regard to File 35 and File 40 data, ^{252}Cf is the only evaluation with covariance information for the energy distribution of secondary particles, and ^{93}Nb is the only evaluation with covariance information for the production of radioactive nuclei. These new formats will be addressed in a future version of PUFF.

1.3 New Features

As part of the upgrade, PUFF-III has the capability to process the spontaneous fission covariances for fission neutron multiplicity, or $\bar{\nu}$. With regard to neutron cross-section covariances, PUFF-III has the capability to process

*"General Resolved Resonance format" is an ENDF term used to identify a specific type of resonance parameter uncertainty data in File 32.[3] This uncertainty information is provided if the compatibility flag (LCOMP) is set equal to 1.

short-range variance formats for the covariance information that is provided in File 33. Following the release of PUFF-II, lumped reaction covariance data formats were introduced into ENDF/B-V; however, PUFF-II cannot process this covariance information. Consequently, PUFF-III has been updated to process the lumped reaction covariance information that is available in ENDF/B-V and -VI.

Several new enhancements have been incorporated into PUFF-III. In the previous version of PUFF, the user must visually inspect the ENDF uncertainty file and identify the covariance matrices for calculation. To reduce the amount of user interaction with the ENDF uncertainty files, two new options are available in PUFF-III: (1) a directory option that instructs the code to print a directory of all possible covariance matrices for a selected nuclide; (2) the capability to process all possible File 31 and 33 covariances with a single input option, thereby reducing the amount of user input for a particular problem. Because of the wide use of the 44-group ENDF/B-V library in the SCALE[4] system, PUFF-III has an input option to select the 44-group structure for the generation of correlation matrices. PUFF-III also has the capability to examine the neutron cross-section uncertainty file and determine the necessary cross-section information for the problem. If covariance data are specified for a redundant reaction (i.e., reaction that is obtained by summing the appropriate partial reactions) and the requisite partial cross sections are available, PUFF-III can compute the desired redundant cross sections for use in the covariance calculation.

Previous versions of PUFF provided the calculated correlation matrices based on the input ENDF uncertainty information. Unfortunately, PUFF did not provide an assessment of the calculated correlation matrices. If the uncertainty information provided in the ENDF file(s) is not "positive definite," the processing code will generate correlation matrices that are not positive definite. A correlation matrix that is either positive definite or positive semi-definite is suitable for use in applications. In an effort to assess the calculated results, PUFF-III determines the eigenvalues (ϕ_i) for each calculated correlation matrix and identifies the matrix with one of the following categories:

1.	positive definite	All $\phi_i > 0$
2.	positive semi-definite	All $\phi_i \geq 0$
3.	indefinite	$\phi_i \leq 0$ and $\phi_i \geq 0$
4.	negative semi-definite	All $\phi_i \leq 0$
5.	negative definite	All $\phi_i < 0$

1.4 Corrections for Historical Problems

In 1983, investigations revealed that PUFF-II does not correctly calculate the implicitly defined cross-reaction-covariance matrices for ENDF/B-V aluminum.[5] For example, the PUFF-II calculation for the cross correlation between elastic scattering (MT = 2) and inelastic scattering (MT = 4) revealed no positive correlation over the entire energy range. Based on the ENDF/B-V covariance data for aluminum and hand calculations, positive correlations for some off-diagonal elements do exist. The problem was subsequently traced to subroutine CROSS in PUFF-II. In particular, PUFF-II does not determine the correct linear relationship for calculating off-diagonal elements in the implicitly defined covariance matrices. To correct the problem, subroutine CROSS in PUFF-III has been rewritten to determine the appropriate linear relationship for the covariance calculation based on the evaluator-defined energy grid. As a result, the historical problems with PUFF-II have been corrected, and PUFF-III is a powerful tool that has the capability to generate correlation matrices for nuclear applications.

2 THEORY

2.1 Statistical Uncertainty

Prior to describing the details of processing the ENDF covariance information, the variables of interest must be discussed. Cross-section values are determined from experimental measurements that have a certain amount of uncertainty. In the ENDF file system, the value provided for each cross section represents an estimate or expectation value $\langle x \rangle$ of the true cross-section value x. Moreover, there is a probability that the true value of x lies in the range Δx about x. If $f(x)$ is defined as the density function that is an average over all other independent variables of the multivariate density function for the cross-section data, the probability that x lies in the range Δx about x can be approximated as $f(x)\Delta x$. The estimate of the probability improves as Δx becomes smaller about x. In the limit as Δx approaches the differential dx, the probability can be defined as $f(x)dx$. Therefore, the expected value $\langle x \rangle$ is an average over the probability distribution and is defined by the following equation:

$$\langle x \rangle = \int x f(x) dx \ , \tag{2.1}$$

where

$$\int f(x) dx = 1 \ .$$

The density function $f(x)$ is a property of the experiments and reflects the variation or scatter associated with the measured experimental data. The variation or amount of error associated with the experimental measurements can be classified as either systematic or stochastic in nature. The evaluated uncertainty data are composed of both types of errors. Typically, the stochastic errors are due to statistical counting uncertainties in the measurements. The systematic errors (e.g., operator error) are usually harder to estimate and may dominate the uncertainty in the measurement process. The difference between the true value of x and the estimate is the deviation, and the following equation can be used to define the deviation of the expected value from the true value:

$$\delta x = x - \langle x \rangle. \tag{2.2}$$

Prior to establishing the definition of the second moment of the density function, the estimated value of an additional cross-section quantity y must be defined. If y is the true cross-section value and $\langle y \rangle$ is the expected value of y, the expectation value can be defined using Eq. (2.1):

$$\langle y \rangle = \int y f(y) dy \ , \tag{2.3}$$

where

$$\int f(y) dy = 1 \ .$$

Using a similar definition for $f(x)$, $f(y)$ is defined as the density function that is an average over all other independent variables of the multivariate density function for the cross-section data. Likewise, the difference between the true value of y and the expected value is provided by the following equation:

$$\delta y = y - \langle y \rangle \ . \tag{2.4}$$

Equation (2.1) represents the first moment of the density function and is the cross-section quantity that is tabulated in the ENDF files. Prior to the release of ENDF/B-IV, only the first moments or expectation values were provided in the data files. Following the release of ENDF/B-IV and extending through the release of ENDF/B-VI, the second moments are tabulated for some of the evaluated cross-section data. The second moments, or covariance data, provide information about the individual data uncertainty, as well as the correlations among other evaluated quantities.

Considering both x and y, the quantity $f(x,y)$ can be defined as the density function averaged over all independent variables except x and y. The second moment of the density function $f(x,y)$ is defined as the covariance of x with y. The covariance can be defined as follows:

$$COV(x,y) = \langle \delta x \delta y \rangle = \iint (x - \langle x \rangle)(y - \langle y \rangle) \, f(x,y) dx dy \ . \tag{2.5}$$

The covariance of x with itself is known as the variance. Moreover, the variance is the average of the squared deviations over the probability distribution and is given by the following equation:

$$VAR(x) = \langle \delta x^2 \rangle = \int (x - \langle x \rangle)^2 f(x) dx \ . \tag{2.6}$$

The standard deviation, or uncertainty, in x is obtained by taking the square root of the variance:

$$s(x) = [VAR(x)]^{1/2} = [\langle \delta x^2 \rangle]^{1/2} \ . \tag{2.7}$$

Using the definition for the covariance and standard deviation, the correlation between x and y is defined with the following equation:

$$\rho(x,y) = \frac{COV(x,y)}{s(x)s(y)} \ . \tag{2.8}$$

The value of the correlation coefficient will always be greater than or equal to -1 and less than or equal to $+1$. If the correlation coefficient equals $+1$, there is a direct correlation between x and y. Conversely, if $\rho(x,y)$ equals -1, x and y have a direct inverse correlation. A correlation coefficient of zero indicates that there is no correlation between x and y.

The preceding equations define absolute quantities; however, the uncertainty information can be defined relative to the estimated quantities of interest. In particular, the relative covariance is obtained by dividing the absolute covariance by the product of $\langle x \rangle$ and $\langle y \rangle$:

$$RCOV(x,y) = \frac{COV(x,y)}{\langle x\rangle\langle y\rangle} . \quad (2.9)$$

Following the same procedure, the relative variance is obtained by dividing the variance by the square of the expected value:

$$RVAR(x) = \frac{VAR(x)}{\langle x\rangle^2} . \quad (2.10)$$

Likewise, the relative standard deviation is obtained by taking the square root of the relative variance:

$$rs(x) = \sqrt{\frac{VAR(x)}{\langle x\rangle^2}} = \frac{s(x)}{\langle x\rangle} . \quad (2.11)$$

Equations (2.1) through (2.11) are the basis for the uncertainty information provided in the ENDF file system. These equations will be used in the subsequent sections to describe the processing of ENDF/B-VI covariance data.

2.2 Energy-Dependent Uncertainty Data

ENDF Files 31 and 33 provide the covariance information for the average number of neutrons per fission (i.e., $\bar{\upsilon}(E)$) and the energy-dependent cross sections, respectively. The formats of Files 31 and 33 are equivalent; therefore, the discussion in this section is devoted to processing the energy dependent covariance data in ENDF Files 31 and 33. In Sect. 2.2.1, an overview of the ENDF formats is provided for both files and is based on the descriptions provided in Ref. 3. The overview does not describe the intimate details of the ENDF format; rather, the discussion highlights the information that is essential for understanding the processing methods in PUFF-III. The specific formatting rules for the energy-dependent covariance data are described in greater detail in Ref. 3.

2.2.1 ENDF/B-VI Uncertainty Formats

The cross-section covariances in File 33 are intended to characterize the variances of the cross sections within a specified energy range, as well as the correlations between cross sections of several adjacent energy ranges. In addition, the covariance data are intended to represent the long-range correlations between cross sections over many energy ranges. In the resolved-resonance region, the covariance data of the partial cross sections are characterized by long-range and short-range components. Moreover, the File 33 covariance data represent the correlations between cross sections that are attributed to the interaction of resonances over many energy ranges (i.e., long-range components). A component of the covariance data for the partial cross sections may be attributed to the interaction of resonances in the neighborhood of an individual resonance (i.e., short-range components). As a result, there may be a rapid variation of the covariance information over an individual resonance. The short-range components of the covariance data due to the resonances are provided in File 32. In order to obtain the complete covariance information in the resonance region, the covariance data due to the long-range components in File 33

must be combined with the short-range components from File 32. The processing of File 32 data and the combination with File 33 covariance data are discussed further in Sect. 2.3.2.

In File 33, the evaluator specifies components of the covariance matrix for certain energy intervals using a set of grid points. The magnitudes of these components are constant between points on the evaluator-specified energy grid. As a result, the data have a histogram appearance, but the data are not considered to be multigroup covariances which would imply a covariance of one multigroup-averaged quantity with another group-averaged quantity. In reality, the data represent the covariance between a cross section at an energy within one interval to another energy point in another interval. In particular, the evaluator specifies a set of data and corresponding equations that are used to calculate the covariance between cross section x_i at energy E_i and cross section y_j at energy E_j. Due to the ENDF covariance file structure, the covariance data are processed to a user-defined energy group structure. Because the ENDF data represent covariances between point energy data, PUFF-III processes the point covariance data into multigroup covariances.

Unless noted otherwise, the following discussion applies to both Files 31 and 33. If File 33 is specified in the text, the discussion also applies to the data formats in File 31. For a specific material evaluation, File 33 is divided into sections according to the MT number or reaction identifier. Each section for the MAT and MT describes the uncertainty information for the specific reaction. Moreover, each section may be divided into several subsections, and each individual subsection is used to describe a single covariance matrix. Within each subsection, there may be several sub-subsections, and each sub-subsection is used to define a component of the covariance matrix identified in the subsection. The complete covariance matrix for a subsection is obtained by summing the components from each sub-subsection.

The sub-subsections are categorized as either an "NC-type" or "NI-type." The NI sub-subsections explicitly define the components of the covariance matrix provided in the subsection. In contrast, The NC sub-subsections indicate that the contribution to the covariance matrix for a specified energy range may be obtained through a linear combination of other covariance matrices from different sections with the same MAT number in File 33. In addition, the NC sub-subsections may indicate that the contribution to the covariance matrix in a specified energy range is based on the covariance data of a standard cross section that has a different MAT number from the material of interest. Essentially, the NC sub-subsection points the analyst to a different section in File 33 or to a File 33 of a different material in order to obtain the covariance information. Note that each NC sub-subsection points to a specific energy range of a specific section that must be provided in terms of NI sub-subsections. In other words, the NC sub-subsection cannot point to another NC sub-subsection. Although the NC sub-subsection introduces additional complexities for the covariance processing code, these sub-subsections reduce the amount of redundant covariance data that would otherwise be present on the ENDF tape. Initially, the details of the NI sub-subsections are presented with a subsequent description of the four different NC sub-subsections.

2.2.1.1 NI Sub-subsections

Within each NI sub-subsection for a given reaction pair, an LB flag is used to identify the type of components (i.e., either absolute or relative) for the contribution to the covariance matrix. Associated with each LB flag is an equation and corresponding data table(s) that must be used to construct the contribution to the covariance matrix. Each data table defines a function that has a histogram appearance over the energy range of interest. One or at most two data tables may be provided for a NI sub-subsection, and each table is composed of NP pairs of energy and functional values (e.g., $\{E_k,F_k\}; k = 1,\text{NP}$). As noted previously, the data table defines a histogram function $f(E)$ that has a value F_k between energies E_k and E_{k+1} for $E_{k+1} > E_k$:

$$f(E) = F_k \; ; \; E_k \le E < E_{k+1} \; . \tag{2.12}$$

For LB = 0, the contribution to the covariance matrix is based on absolute components that are correlated within each interval defined by the single data table $\{E_k,F_k\}$. The expression for the LB = 0 covariance contribution is provided in Table 2.1. In Eqs. (2.15) through (2.21) that are presented in Table 2.1, the dimensionless operator P is defined as the product of the dimensionless operator S as follows:

$$P_{j,m,n,\ldots}^{i,k,l,\ldots} = S_i^k \, S_i^l \ldots S_j^m \, S_j^n \ldots , \tag{2.13}$$

where

$$S_i^k = 1; \; if \; E_k \le E_i < E_{k+1} ,$$

and

$$S_i^k = 0; \; if \; E_i \; is \; outside \; the \; interval \; [E_k, E_{k+1}] .$$

For LB values 1 through 6, contributions to the covariance matrix are based on relative components. Table 2.1 also provides the corresponding covariance equations for LB values between 1 and 6. The contribution based on LB = 1 describes the relative components that are correlated within each E_k interval. For LB = 2, the contribution to the covariance matrix is based on relative components that are correlated over all E_k intervals, as noted by the double summation in Eq. (2.17). The NI sub-subsections as defined by LB = 3 and 4 have two data tables, $\{E_k,F_k\}$ and $\{E_\ell ,F_\ell\}$, that define two different histogram functions. The contribution based on LB = 3 describes the relative components that are correlated over the E_k and E_ℓ intervals. For LB = 4, the equation is slightly more complex relative to LB = 3. In particular, LB = 4 describes the contribution based on the relative components that are correlated over all E_ℓ intervals within each E_k interval, as noted by the triple summation in Eq. (2.19).

The LB = 3 sub-subsections can be used to define a sub-subsection; however, the LB = 3 sub-subsection only permits the construction of each sub-subsection one row or column at a time. Consequently, one sub-subsection must be used for each row or column, and the same energy mesh is repeated in the corresponding data table of each sub-subsection. To alleviate possible inefficiencies in the data files, the LB = 5 and 6 representations are available. For LB = 5, a single energy grid $\{E_k\}$ is provided with the associated ***square matrix*** of fractional components $\{F_{kk'}\}$ that can be used to construct the sub-subsection. The square matrix has the following functional representation:

$$f(E_i, E_j) = F_{k,k'} \; ; \;\; E_k \le E_i < E_{k+1} \; and \; E_{k'} \le E_j < E_{k'+1} . \tag{2.14}$$

The covariance contribution from the LB = 5 sub-subsection is provided by Eq. (2.20) in Table 2.1. The LB = 5 sub-subsection defines the row and column components simultaneously. Note that the covariance matrix between two reactions or materials may have different energy grids for the rows and columns. If two different grids are required to describe the covariance matrix, the LB = 5 sub-subsection is not suitable for defining the contribution. Therefore, the LB = 6 format is available for defining a ***rectangular matrix***. The LB = 6 representation is similar to the LB = 5 format; however, two energy grids (i.e., $\{E_k\}$ and $\{E_\ell\}$) are provided with a corresponding rectangular matrix of fractional components $\{F_{k\ell}\}$. The covariance contribution from the LB = 6 sub-subsection is provided in Eq. (2.21) in Table 2.1.

Table 2.1 Summary of covariance equations for NI sub-subsections (point covariance)

LB	Equation	
0[a]	$COV\ (x_i,y_j) = \sum_k P_{j;k}^{i;k} F_{xy;k}$	(2.15)
1[a]	$COV\ (x_i,y_j) = \sum_k P_{j;k}^{i;k} F_{xy;k}\ x_i\ y_j$	(2.16)
2	$COV\ (x_i,y_j) = \sum_{k,k'} P_{j;k}^{i;k'} F_{xy;k}\ F_{xy;k'}\ x_i\ y_j$	(2.17)
3	$COV\ (x_i,y_j) = \sum_{k,\ell} P_{j;\ell}^{i;k} F_{x;k}\ F_{y;\ell}\ x_i\ y_j$	(2.18)
4	$COV\ (x_i,y_j) = \sum_{K,k,k'} P_{j;k,k'}^{i;k,\ell}\ F_k\ F_{xy;\ell}\ F_{xy;\ell'}\ x_i\ y_j$	(2.19)
5	$COV\ (x_i,y_j) = \sum_{k,k'} P_{j;k'}^{i;k}\ F_{xy;k,k'}\ x_i\ y_j$	(2.20)
6	$COV\ (x_i,y_j) = \sum_{k,\ell} P_{j;\ell}^{i;k}\ F_{xy;k,\ell}\ x_i\ y_j$	(2.21)
8[a,b]	$COV\ (x_I,x_I) = VAR\ (x_I) = F_k \dfrac{\Delta E_k}{\Delta E_I}\ ;\ E_k \le E_I < E_{I+1} \le E_{k+1}$	(2.22)

[a]These equations define a diagonal matrix.
[b]$\Delta E_k = E_{k+1} - E_k$ and $\Delta E_I = E_{I+1} - E_I$.

The final NI sub-subsection is denoted with LB = 8.** The LB = 8 representation, which is vastly different from the other NI sub-subsections, provides an absolute variance component in the group-averaged cross sections, as opposed to the variance in pointwise cross sections. The evaluator may use the LB = 8 format to account for statistical fluctuations induced in the group-averaged cross sections by the underlying resonances. Moreover, no off-diagonal contributions are made from the LB = 8 sub-subsection. The equation for the LB = 8 sub-subsection is provided in Eq. (2.22). The short-range variance representation has a single table of energies and constants $\{E_k,F_k\}$. For the group-averaged cross sections for energy group I with width ΔE_I, the values of F_k define an absolute contribution to the variance averaged over the energy interval ΔE_I that includes a portion of the interval defined by the E_k grid.

2.2.1.2 NC Sub-subsections

As noted previously, the NC sub-subsections describe the contribution to the covariance matrix based on information provided in another subsection on the ENDF file. Four types of NC sub-subsections are identified with an LTY = 0, 1, 2 or 3 flag. The LTY = 0 flag is typically used for sub-subsection components for derived redundant cross sections (e.g., MT = 1, 3, 4, etc.). For an evaluator-specified energy range, the LTY = 0 flag indicates that the cross-section quantities were obtained as a linear combination of other measured cross sections with the same material identifier but a different reaction identifier. The LTY = 0 sub-subsection defines the energy range where the cross sections were derived in terms of the other evaluated cross sections. In addition, the NC sub-subsection also defines the linear relationship that is used to construct the derived redundant cross section in the specified energy range. For an energy range between E_k and E_{k+1}, the linear relationship for the derived redundant cross section has the following form:

$$\sigma_{MT}^{MAT}(E) = \sum_{i=1}^{NCI} C_i \, \sigma_{MT_i}^{MAT}(E) \ , \tag{2.23}$$

where

NCI = total number of evaluated cross sections,
C_i = coefficient for combining evaluated cross sections,
$\sigma_{MT_i}^{MAT}(E)$ = evaluated cross section.

By specifying an LTY = 0 flag, the evaluator specifies that the covariance matrix for the derived redundant cross section is obtained by combining the covariance matrix components using the same linear relationship. As a result, the LTY = 0 sub-subsection defines a linear relationship to be used to construct a single covariance matrix from NI sub-subsections of a different subsection within the same material evaluation.

As a consequence of the LTY = 0 format, the linear relationship also implies that additional covariance matrices may exist and are not defined explicitly in the subsections of the material of interest. The possibility of implicitly defined covariance matrices contributes to the complexity of processing the NC sub-subsections, and the processing code must determine the implied contribution to other covariance matrices from the LTY = 0 sub-subsection. An example of this concept is provided in the sample problems of Appendix B.

**Note: The ENDF/B-VI formats do not provide an LB = 7 representation.

The remaining NC sub-subsections are used to define the covariance matrices of cross sections that are derived from ratio measurements to standard cross sections in the energy range (E_k,E_{k+1}). In other words, a derived cross section is related to a standard cross section by a ratio $R(E)$ that is determined experimentally. The derived cross section can be defined as the product of the ratio and the standard cross section:

$$\sigma_i(E) = R(E)\sigma_{std}(E) \; ; \quad E_k \le E < E_{k+1} \; , \tag{2.24}$$

where

$R(E)$ = ratio of derived cross section to the standard,
$\sigma_{std}(E)$ = standard cross section.

For example, the ^{241}Pu fission cross section has been obtained in the past through ratio measurements to the ^{235}U fission cross section. Consequently, the covariance data for the evaluated cross section are dependent on the covariance information for the standard cross section. Since the determination of $R(E)$ and $\sigma_{std}(E)$ is almost always performed independently, the uncertainty in $R(E)$ is not correlated with the uncertainty in the standard cross-section measurement. Based on the ratio measurement and Eq. (2.24), the following relative covariance relationships can be defined:[3]

$$RVAR[\sigma_i(E)] = RVAR[R(E)] + RVAR[\sigma_{std}(E)] \; ; \; E_k \le E < E_{k+1} \tag{2.25}$$

$$RCOV[\sigma_i(E),\sigma_i(E')] = RCOV[R(E),R(E')] + RCOV[\sigma_{std}(E),\sigma_{std}(E')] \; ; \quad E_k \le E < E_{k+1}, \; E_k \le E' < E_{k+1} \tag{2.26}$$

$$RCOV[\sigma_i(E),\sigma_{std}(E')] = RCOV[\sigma_{std}(E),\sigma_{std}(E')] \; ; \; E_k \le E < E_{k+1} \tag{2.27}$$

If cross-section MT_i for material MAT is derived over the interval (E_k,E_{k+1}) based on ratio measurements to a standard cross-section MATS with reaction MT_{std}, there will be three corresponding NC sub-subsections in the ENDF covariance files. For the material of interest, LTY = 1 is used to define the self covariance for MT_i (i.e., <MAT,MT_i;MAT,MT_i>. The LTY = 1 sub-subsection in MAT indicates that the contribution to the covariance matrix over (E_k,E_{k+1}) is obtained from the NI sub-subsection in MATS for the same energy interval. In addition to the LTY = 1 sub-subsection, an LTY = 2 sub-subsection must also be given in the MAT subsection. The LTY = 2 sub-subsection defines the covariance between the derived cross section and the standard cross section (i.e., <MAT,MT_i;MATS,MT_{std}>). With regard to the standard cross-section File 33, an LTY = 3 sub-subsection must be specified in the MT_{std} subsection to indicate the correlation between the standard cross section and the derived cross section (i.e., <MATS,MT_{std};MAT,MT_i>).

2.2.2 Processing Energy-Dependent Data into Multigroup Formats

2.2.2.1 NI Sub-subsections

Before the point covariance equations in Table 2.1 can be used in a multigroup application, the equations must be converted to multigroup form. Equation (2.5) expresses the covariance between the continuous-energy cross sections x and y. The cross-section $x(E)$ can be averaged over an energy group I using the following equation:

$$x_I = \frac{\int_I \phi(E)x(E)dE}{\int_I \phi(E)dE}, \tag{2.28}$$

where

x_I = group-averaged cross section for energy group I,
$x(E)$ = cross-section x at energy E,
$\phi(E)$ = flux at energy E.

Using Eq. (2.28) and letting $x_0 = \langle x \rangle$ and $y_0 = \langle y \rangle$, Eq. (2.5) can be defined in a multigroup format:

$$COV(x_I,y_J) = \langle \delta x_I \delta y_J \rangle = \iint (x_I - x_{0,I})(y_J - y_{0,J})\, f(x_I,y_J)dx_I dy_J . \tag{2.29}$$

Before Eq. (2.29) can be expressed in terms of point covariances, the expression for dx must be determined by taking the derivative of x_I with respect to x. Using Eq. (2.28) and taking the partial derivative with respect to x leads to the following expressions:

$$\frac{\partial x_I}{\partial x} = \frac{\partial}{\partial x}\left[\frac{\int_I \phi(E)x(E)dE}{\int_I \phi(E)dE}\right], \tag{2.30}$$

$$\frac{\partial x_I}{\partial x} = \frac{1}{\int_I \phi(E)dE}\frac{\partial}{\partial x}\left[\int_I \phi(E)x(E)dE\right]. \tag{2.31}$$

Both integrals in Eq. (2.31) are definite, and the limits of integration range from I to $I + 1$. Taking the partial of the integral with respect to x yields the following result:

$$\frac{\partial}{\partial x}\left[\int_I^{I+1}\phi(E)x(E)dE\right] = \phi(E_{I+1})x(E_{I+1})\frac{\partial E_{I+1}}{\partial x} - \phi(E_I)x(E_I)\frac{\partial E_I}{\partial x} + \int_I^{I+1}\phi(E)\frac{\partial x}{\partial x}\,dE\ . \tag{2.32}$$

In Eq. (2.32), the partial of E_{I+1} and E_I with respect to x is zero. Therefore, the partial of x_I with respect to x becomes

$$\frac{\partial x_I}{\partial x} = \frac{\int_I\phi(E)dE}{\int_I\phi(E)dE} = 1\ . \tag{2.33}$$

Note that the partial of y_J with respect to y also equals 1. Using the result from Eq. (2.33) and the multigroup cross-section definition, Eq. (2.29) can be expressed in the following form:

$$COV(x_I,y_J) = \int\int\left[\frac{\int_I\phi(E)x(E)dE}{\int_I\phi(E)dE} - \frac{\int_I\phi(E)x_0(E)dE}{\int_I\phi(E)dE}\right]\times \left[\frac{\int_J\phi(E')y(E')dE'}{\int_J\phi(E')dE'} - \frac{\int_J\phi(E')y_0(E')dE'}{\int_J\phi(E')dE'}\right]f(x,y)dxdy\ . \tag{2.34}$$

Equation (2.34) expresses the multigroup covariances in terms of the continuous-energy parameters; however, the expression can be simplified to obtain the following expression:

$$COV(x_I,y_J) = \frac{1}{\phi_I\,\phi_J}\int\int\left[\int_I\phi(E)[\,x(E) - x_0(E)\,]dE\right]\times \left[\int_J\phi(E')[\,y(E') - y_0(E')\,]dE'\right]f(x,y)dxdy\ , \tag{2.35}$$

where

$$\phi_I = \int_I\phi(E)dE\ ,$$

and

$$\phi_J = \int_J \phi(E')dE'.$$

By rearranging the integrals in Eq. (2.35), the multigroup covariance equation can be expressed in the following form:

$$COV(x_I,y_J) = \frac{1}{\phi_I \phi_J} \int_I \int_J \phi(E)\phi(E') \left[\iiint [x - x_0][y - y_0] f(x,y)dxdy \right] dEdE' . \quad (2.36)$$

Based on the definition of the covariance of $x(E)$ with $y(E)$, Eq. (2.36) can be expressed in terms of the point covariances:

$$COV(x_I,y_J) = \frac{1}{\phi_I \phi_J} \int_I \int_J \phi(E)\ \phi(E')\ COV(x,y)\ dEdE' . \quad (2.37)$$

Equation (2.37) can be used to derive the multigroup equations for the NI sub-subsections. The derivation of the multigroup expression for LB = 0 is presented in the subsequent discussion. The same procedure can be used to derive the multigroup equations for the remaining NI sub-subsections.

The expressions in Table 2.1 define the covariance between cross sections x and y at discrete values i and j, respectively. In order to use Eq. (2.37), the energy region is assumed to be divided into infinitesimal intervals so that $x(E)$ can be approximated by the discrete value x_i (i.e., x evaluated at energy E_i). Therefore, the flux at discrete energies i and j can be defined with the following expressions:

$$\phi_i = \int_i \phi(E)dE , \quad (2.38)$$

and

$$\phi_j = \int_j \phi(E')dE'. \quad (2.39)$$

Using the definitions for ϕ_i and ϕ_j, the integrals in Eq. (2.37) can be converted to discrete sums:

$$COV(x_I,y_J) = \frac{1}{\phi_I \phi_J} \sum_{i \in I} \sum_{j \in J} \phi_i \phi_j COV(x_i,y_j) . \quad (2.40)$$

Substituting the discrete covariance equation for LB = 0 (i.e., Eq. (2.15)) into Eq. (2.40), the multigroup expression for LB = 0 has the following form:

$$COV(x_I,y_J) = \frac{1}{\phi_I \phi_J} \sum_{i \in I} \sum_{j \in J} \phi_i \phi_j \sum_k P_{j,k}^{i,k} F_{xy,k} . \quad (2.41)$$

Using the definition for the dimensionless operator P, the LB = 0 multigroup covariance equation can be expressed as follows:

$$COV(x_I,y_J) = \frac{1}{\phi_I \phi_J} \sum_k \sum_{i \in I} \sum_{j \in J} S_i^k S_j^k \phi_i \phi_j F_{xy,k} . \quad (2.42)$$

In order to simplify Eq. (2.42), the multigroup fluxes for the k^{th} interval can be defined as follows:

$$\phi_{I,k} = \sum_{i \in I} S_i^k \phi_i , \quad (2.43)$$

and

$$\phi_{J,k} = \sum_{j \in J} S_j^k \phi_j . \quad (2.44)$$

Using the definitions from Eqs. (2.43) and (2.44), the multigroup covariance equation for LB = 0 becomes

$$COV(x_I,y_J) = \frac{\sum_{k \in I,J} F_{xy,k} \phi_{I,k} \phi_{J,k}}{\phi_I \phi_J} . \quad (2.45)$$

The multigroup equations for the remaining NI sub-subsections can be derived following the same procedure. The multigroup equations for LB = 0 through 8 are presented in Table 2.2.

Table 2.2 Summary of multigroup covariance equations for NI sub-subsections

LB	Equation	
0[a]	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J} \sum_{k\,\epsilon I,J} F_{xy;k}\,\phi_{I,k}\phi_{J,k}$.	(2.45)
1[a]	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J} \sum_{k\,\epsilon I,J} F_{xy;k}\,\phi_{I,k}\,x_{I,k}\,\phi_{J,k}\,y_{J,k}$.	(2.46)
2	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J}\left[\sum_{k\,\epsilon I} F_{xy;k}\,\phi_{I,k}\,x_{I,k}\right]\left[\sum_{k'\epsilon J} F_{xy,k'}\,\phi_{J,k'}\,y_{J,k'}\right]$.	(2.47)
3	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J}\left[\sum_{k\,\epsilon I} F_{x,k}\,\phi_{I,k}\,x_{I,k}\right]\left[\sum_{\ell\,\epsilon J} F_{y,\ell}\,\phi_{J,\ell}\,y_{J,\ell}\right]$.	(2.48)
4	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J} \sum_{k\,\epsilon I,J} F_k\left[\sum_{\ell\,\epsilon I} F_{xy;\ell}\,\phi_{I,\ell}\,x_{I,\ell}\right]\left[\sum_{\ell'\,\epsilon J} F_{xy,\ell'}\,\phi_{J,\ell'}\,y_{J,\ell'}\right]$.	(2.49)
5	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J} \sum_{k\,\epsilon I} \sum_{k'\,\epsilon J} F_{xy;k,k'}\,\phi_{I,k}\,x_{I,k}\,\phi_{J,k'}\,y_{J,k'}$.	(2.50)
6	$COV\,(x_I,y_J) = \frac{1}{\phi_I\,\phi_J} \sum_{k\,\epsilon I} \sum_{\ell\,\epsilon J} F_{xy;k,\ell}\,\phi_{I,k}\,x_{I,k}\,\phi_{J,\ell}\,y_{J,\ell}$.	(2.51)
8[a,b]	$COV\,(x_I,x_I) = VAR\,(x_I) = F_k\,\frac{\Delta E_k}{\Delta E_I}\;;\; E_k \le E_I < E_{I+1} \le E_{k+1}$	(2.52)

[a]These equations define a diagonal matrix.
[b]$\Delta E_k = E_{k+1} - E_k$ and $\Delta E_I = E_{I+1} - E_I$.

2.2.2.2 NC Sub-subsections

The NC sub-subsections are used to define the components of the covariance matrix for derived redundant cross sections (LTY = 0). In addition, the NC sub-subsections are used to define covariance matrices of cross sections that are derived from ratio measurements (1 ≤ LTY ≤ 3). The multigroup NI sub-subsection equations from Sect. 2.2.2.1 are used to construct the covariance matrix components defined by the NC sub-subsections.

Equation (2.23), which defines the linear relationship for a derived redundant cross section over the energy range from E_k to E_{k+1}, can be expressed in terms of multigroup parameters:

$$x_I = \sum_{m=1}^{NCI} C_{mI}\, y_{mI} \ , \tag{2.53}$$

where

I	=	energy group I,
m	=	index for the evaluated cross section,
NCI	=	total number of evaluated cross sections,
C_{mI}	=	coefficient for combining evaluated cross sections at energy group I,
y_{mI}	=	m^{th} evaluated cross section at energy group I.

For energy group I, the deviation of the expected cross-section value, x_{0I}, from the true value x_I is defined as δx_I:

$$\delta x_I = x_I - x_{0I} \ . \tag{2.54}$$

Likewise, a similar expression for the deviation can be defined for the evaluated cross-section values:

$$\delta y_{mI} = y_{mI} - y_{m0I} \ . \tag{2.55}$$

Using the definition in Eq. (2.53), the covariance for the derived redundant cross section, x_I, can be defined as follows:

$$COV(x_I, x_J) = < \delta x_I \, \delta x_J > = \sum_{m=1}^{NCI} \sum_{m'=1}^{NCI} C_{mI}\, C_{m'J} < \delta y_{mI} \, \delta y_{m'J} > \ , \tag{2.56}$$

where

$$\delta x_I = \sum_{m=1}^{NCI} C_{mI}\, \delta y_{mI} \ , \tag{2.57}$$

and

$$\delta x_J = \sum_{m'=1}^{NCI} C_{m'J}\, \delta y_{m'J} \ . \tag{2.58}$$

Equation (2.56) defines a component of the covariance matrix for a specific energy range between E_k and E_{k+1}. Note that several NC sub-subsections may be provided in a subsection, and each NC sub-subsection is ordered

according to the lower-energy boundary of the sub-subsection. For a derived redundant cross section, there may be several different energy ranges that are defined with different linear relationships. Consequently, a different form of Eq. (2.56) could be defined for each energy range. Moreover, each covariance equation will be explicitly defined for the different energy ranges; however, there could be implicitly defined linear relationships for off-diagonal energy ranges that must be derived from the explicitly defined equations.

As an example, consider a cross-section x that is derived over the energy ranges $\{E_k, E_{k+1}\}$ and $\{E_{k+1}, E_{k+2}\}$, where $E_k < E_{k+1} < E_{k+2}$. For simplicity, assume that energy groups 1 and 2 correspond to the energy ranges $\{E_k, E_{k+1}\}$ and $\{E_{k+1}, E_{k+2}\}$, respectively. Furthermore, x is equal to $y_{a1} - y_{c1}$ for all energies between E_k and E_{k+1}, and x is equal to $y_{a2} - y_{b2}$ for all energies between E_{k+1} and E_{k+2}. In addition, assume that cross covariances are zero (i.e., $COV(y_{mI}, y_{m'J}) = 0$ for $m \neq m'$). The parameters for the example are summarized in Table 2.3.

Table 2.3 Summary of parameters for example calculation of $COV(x_I, x_J)$ for LTY = 0 NC sub-subsection

Group	Equation	Constants
1	$x_1 = y_{a1} - y_{c1}$	$C_{11} = 1, C_{21} = -1$
2	$x_2 = y_{a2} - y_{b2}$	$C_{12} = 1, C_{22} = -1$

Based on Eq. (2.56), the covariance matrix for the two-group example can be determined as follows:

$$\begin{aligned} < \delta x_I \, \delta x_J > &= \sum_{m=1}^{2} \sum_{m'=1}^{2} C_{mI} \, C_{m'J} < \delta y_{mI} \, \delta y_{m'J} > \\ &= \sum_{m=1}^{2} C_{mI} \left\{ C_{1J} < \delta y_{mI} \, \delta y_{1J} > + C_{2J} < \delta y_{mI} \, \delta y_{2J} > \right\} \\ &= C_{1I} \, C_{1J} < \delta y_{1I} \, \delta y_{1J} > + C_{1I} \, C_{2J} < \delta y_{1I} \, \delta y_{2J} > \\ &\quad + C_{2I} \, C_{1J} < \delta y_{2I} \, \delta y_{1J} > + C_{2I} \, C_{2J} < \delta y_{2I} \, \delta y_{2J} > \; . \end{aligned} \tag{2.59}$$

Because the $COV(y_{mI}, y_{m'J}) = 0$ for $m \neq m'$, Eq. (2.59) can be reduced to the following form:

$$< \delta x_I \, \delta x_J > = C_{1I} \, C_{1J} < \delta y_{1I} \, \delta y_{1J} > + C_{2I} \, C_{2J} < \delta y_{2I} \, \delta y_{2J} > . \tag{2.60}$$

The contribution to the diagonal element of the covariance matrix for energy group 1 is given by the following equation:

$$<\delta x_1 \, \delta x_1> = <\delta y_{11} \, \delta y_{11}> + <\delta y_{21} \, \delta y_{21}> . \tag{2.61}$$

For energy group 1 in Table 2.3, $x_1 = y_{a1} - y_{c1}$. Therefore, the first y reaction corresponds to y_{a1}, and the second y reaction corresponds to y_{c1} (i.e., $y_{21} = y_{c1}$). The diagonal element of the covariance matrix for energy group 1 becomes:

$$<\delta x_1\ \delta x_1> = <\delta y_{a1}\ \delta y_{a1}> + <\delta y_{c1}\ \delta y_{c1}> . \quad (2.62)$$

For energy group 2, the contribution to the diagonal element is given by the following equation:

$$\begin{aligned} <\delta x_2\ \delta x_2> &= <\delta y_{12}\ \delta y_{12}> + <\delta y_{22}\ \delta y_{22}> \\ &= <\delta y_{a2}\ \delta y_{a2}> + <\delta y_{b2}\ \delta y_{b2}> . \end{aligned} \quad (2.63)$$

For the off-diagonal elements, the contribution may or may not be zero. Therefore, the processing code must evaluate the possible correlations between the derived energy range and the off-diagonal energy ranges. Because the diagonal elements are both correlated to $<\delta y_{a\,I},\ \delta y_{a\,J}>$, there may be a nonzero correlation in the off-diagonal elements as a function of $<\delta y_{a\,I},\ \delta y_{a\,J}>$. With regard to the covariance between energy groups 1 and 2, Eq. (2.60) can be expressed as follows:

$$< \delta x_1\ \delta x_2 > = C_{11}\ C_{12} < \delta y_{11}\ \delta y_{12} > + C_{21}\ C_{22} < \delta y_{21}\ \delta y_{22} > . \quad (2.64)$$

As noted for Eq. (2.61), y_{21} corresponds to y_{c1}. In addition for energy group 2, y_{22} corresponds to y_{b2}. Since the cross covariances are zero, the second quantity in Eq. (2.64) vanishes because $< \delta y_{c1}\ \delta y_{b2} >$ is zero. The covariance between energy groups 1 and 2 is expressed as follows:

$$< \delta x_1\ \delta x_2 > = < \delta y_{11}\ \delta y_{12} > = < \delta y_{a1}\ \delta y_{a2} > . \quad (2.65)$$

Likewise, the covariance between energy groups 2 and 1 is obtained as follows:

$$< \delta x_2\ \delta x_1 > = < \delta y_{12}\ \delta y_{11} > = < \delta y_{a2}\ \delta y_{a1} > \quad (2.66)$$

The covariance matrix for $<\delta x_I\ \delta x_J>$ is summarized in Table 2.4. This simple example demonstrates that the processing code must determine the implicitly defined linear relationships for the off-diagonal elements based on the explicitly defined linear relationships.

Table 2.4 Example $COV(x_i, x_j)$ calculation for LTY = 0 NC sub-subsection

	1	2
1	$<\delta y_{a1}\ \delta y_{a1}> + <\delta y_{c1}\ \delta y_{c1}>$	$<\delta y_{a1}\ \delta y_{a2}>$
2	$<\delta y_{a2}\ \delta y_{a1}>$	$<\delta y_{a2}\ \delta y_{a2}> + <\delta y_{b2}\ \delta y_{b2}>$

In addition, to the covariance matrix in Eq. (2.56), the derived redundant cross section may also be correlated to the different evaluated cross sections denoted as y_m. Based on Eq. (2.53), there are additional *NCI* implicitly defined covariance matrices that define correlations between the derived redundant cross section, x, and the *NCI*-evaluated cross sections. The covariance between the derived redundant cross section and each evaluated cross section is obtained with the following expression:

$$COV(x_I, y_{mJ}) = < \delta x_I \, \delta y_{mJ} > = \sum_{m'=1}^{NCI} C_{m'I} < \delta y_{m'I} \, \delta y_{mJ} > . \quad (2.67)$$

Equation (2.67) becomes increasingly complex if y_{mJ} is also derived from an expression similar to Eq. (2.53) over a specific energy range. Note that the derived energy range for the $COV(y_{mI}, y_{mJ})$ cannot be the same as the derived energy range specified for the $COV(x_I, x_J)$ that is determined from the $COV(y_{mI}, y_{mJ})$. In other words, if the $COV(x_I, x_J)$ is derived from the $COV(y_{mI}, y_{mJ})$ over the interval from E_k to E_{k+1}, the $COV(y_{mI}, y_{mJ})$ cannot be derived from some $COV(y_{nI}, y_{nJ})$ over the same energy range. However, the $COV(y_{mI}, y_{mJ})$ can be derived from the $COV(y_{nI}, y_{nJ})$ over some interval outside of $\{E_k, E_{k+1}\}$ (e.g., E_{k+1} to E_{k+2}). The following discussion illustrates the calculation of the implicitly defined covariance matrix between the derived redundant cross section, x, and the evaluated cross section, y_m, that is also derived as function of y_n over a different energy range.

Continuing with the previous example, x is derived over the energy ranges $\{E_k, E_{k+1}\}$ and $\{E_{k+1}, E_{k+2}\}$, where $E_k < E_{k+1} < E_{k+2}$. Furthermore, x is equal to $y_{a1} - y_{c1}$ for all energies between E_k and E_{k+1}, and x is equal to $y_{a2} - y_{b2}$ for all energies between E_{k+1} and E_{k+2}. In addition, y_{b1} is equal to $y_{a1} - y_{d1}$ for all energies between E_k and E_{k+1}. As in the previous example, the cross covariances are assumed to be zero (i.e., $<\delta y_{mI} \, \delta y_{m'J}> = 0$ for $m \neq m'$). The parameters for the second example are summarized in Table 2.5.

Table 2.5 Summary of parameters for example calculation of $COV(x_I, y_{mJ})$ for LTY = 0 NC sub-subsection

Group	Equation	Constants
1	$x_1 = y_{a1} - y_{c1}$ $y_{b1} = y_{a1} - y_{d1}$	$C_{11} = 1, C_{21} = -1$ $K_{11} = 1, K_{21} = -1$
2	$x_2 = y_{a2} - y_{b2}$	$C_{12} = 1, C_{22} = -1$

Because x is derived from y_{aJ}, y_{cJ} and y_{bJ}, three implicitly defined covariance matrices must be considered: $<\delta x_I \, \delta y_{aJ}>$, $<\delta x_I \, \delta y_{cJ}>$ and $<\delta x_I \, \delta y_{bJ}>$. For the second example, the covariance between x and y_{bJ} is presented in detail. Equation (2.67) for the covariance between x and y_{bJ} is given by the following expression:

$$COV(x_I, y_{bJ}) = < \delta x_I \, \delta y_{bJ} > = \sum_{m'=1}^{2} C_{m'I} < \delta y_{m'I} \, \delta y_{bJ} > . \quad (2.68)$$

Equation (2.68) may have a different form, depending on the values of I and J. With regard to the covariance between energy groups 1 and 1, Eq. (2.68) can be expressed as follows:

$$< \delta x_1 \, \delta y_{b1} > = \sum_{m'=1}^{2} C_{m'1} < \delta y_{m'1} \, \delta y_{b1} > . \quad (2.69)$$

As noted in Table 2.4 for energy group 1, y_{b1} is obtained by subtracting y_{d1} from y_{a1}. As a result, δy_{b1} can be expressed in the following form:

$$\delta y_{b1} = \sum_{n=1}^{2} K_{n1}\, \delta y_{n1} = \delta y_{11} - \delta y_{21} = \delta y_{a1} - \delta y_{d1} \,. \tag{2.70}$$

Based on Eq. (2.70), the covariance between x and y_b for energy group 1 can be expressed as follows:

$$< \delta x_1\, \delta y_{b1} > = \sum_{m'=1}^{2} \sum_{n=1}^{2} C_{m'1}\, K_{n1} < \delta y_{m'1}\, \delta y_{n1} > \,. \tag{2.71}$$

Expanding Eq. (2.71) leads to the diagonal element of the covariance matrix corresponding to the first energy group:

$$\begin{aligned} < \delta x_1\, \delta y_{b1} > &= \sum_{m'=1}^{2} C_{m'1} \left\{ K_{11} < \delta y_{m'1}\, \delta y_{11} > + K_{21} < \delta y_{m'1}\, \delta y_{21} > \right\} \\ &= \sum_{m'=1}^{2} C_{m'1} \left\{ < \delta y_{m'1}\, \delta y_{a1} > + (-1) < \delta y_{m'1}\, \delta y_{d1} > \right\} \\ &= C_{11} < \delta y_{11}\, \delta y_{a1} > - C_{11} < \delta y_{11}\, \delta y_{d1} > \\ &\quad + C_{21} < \delta y_{21}\, \delta y_{a1} > - C_{21} < \delta y_{21}\, \delta y_{d1} > \\ &= < \delta y_{a1}\, \delta y_{a1} > - < \delta y_{a1}\, \delta y_{d1} > \\ &\quad + < \delta y_{c1}\, \delta y_{a1} > - < \delta y_{c1}\, \delta y_{d1} > \,. \end{aligned} \tag{2.72}$$

Assuming that the cross covariances are zero, the covariance between x and y_b for energy group 1 reduces to the following:

$$< \delta x_1\, \delta y_{b1} > = <\delta y_{a1}\, \delta y_{a1}> \,. \tag{2.73}$$

Because y_b is a function of y_a and y_d in the first energy group, the covariance between x in group 2 and y_b in group 1 is obtained using an equation that is similar to Eq. (2.71):

$$< \delta x_2\, \delta y_{b1} > = \sum_{m'=1}^{2} \sum_{n=1}^{2} C_{m'2}\, K_{n1} < \delta y_{m'2}\, \delta y_{n1} > \,. \tag{2.74}$$

Expanding Eq. (2.74) leads to the following covariance element:

$$
\begin{aligned}
< \delta x_2 \; \delta y_{b1} > &= \sum_{m'=1}^{2} C_{m'2} \left\{ K_{11} < \delta y_{m'2} \; \delta y_{11} > + K_{21} < \delta y_{m'2} \; \delta y_{21} > \right\} \\
&= \sum_{m'=1}^{2} C_{m'2} \left\{ < \delta y_{m'2} \; \delta y_{a1} > + (-1) < \delta y_{m'2} \; \delta y_{d1} > \right\} \\
&= C_{12} < \delta y_{12} \; \delta y_{a1} > - C_{12} < \delta y_{12} \; \delta y_{d1} > \\
&\quad + C_{22} < \delta y_{22} \; \delta y_{a1} > - C_{22} < \delta y_{22} \; \delta y_{d1} > \\
&= < \delta y_{a2} \; \delta y_{a1} > - < \delta y_{a2} \; \delta y_{d1} > \\
&\quad + < \delta y_{b2} \; \delta y_{a1} > - < \delta y_{b2} \; \delta y_{d1} > .
\end{aligned}
\tag{2.75}
$$

If the cross covariances are zero, the covariance element from Eq. (2.75) reduces to the following:

$$
< \delta x_2 \; \delta y_{b1} > = <\delta y_{a2} \; \delta y_{a1}> . \tag{2.76}
$$

For the remaining two elements of the covariance matrix, Eq. (2.68) can be used to calculate the contribution for $<\delta x_1 \; \delta y_{b2}>$ and $<\delta x_2 \; \delta y_{b2}>$. The remaining two elements are obtained with the following equations:

$$
\begin{aligned}
< \delta x_1 \; \delta y_{b2} > &= C_{11}<\delta y_{11} \; \delta y_{b2}> + C_{21}<\delta y_{21} \; \delta y_{b2}> \\
&= <\delta y_{a1} \; \delta y_{b2}> - <\delta y_{c1} \; \delta y_{b2}> = 0,
\end{aligned}
\tag{2.77}
$$

and

$$
\begin{aligned}
< \delta x_2 \; \delta y_{b2} > &= C_{12}<\delta y_{12} \; \delta y_{b2}> + C_{22}<\delta y_{22} \; \delta y_{b2}> \\
&= <\delta y_{a2} \; \delta y_{b2}> - <\delta y_{b2} \; \delta y_{b2}> \\
&= - <\delta y_{b2} \; \delta y_{b2}>.
\end{aligned}
\tag{2.78}
$$

The covariance matrix for $<\delta x_I \; \delta y_{bJ}>$ is summarized in Table 2.6. These examples demonstrate that the processing code must determine the implicitly defined covariance matrices that are defined in the LTY = 0 sub-subsections. In addition, the code must determine the appropriate linear relationship for the energy ranges of interest.

Table 2.6 Example $COV(x_I, y_{bJ})$ calculation for LTY = 0 NC sub-subsection

	1	2
1	$<\delta y_{a1}\ \delta y_{a1}>$	0
2	$<\delta y_{a2}\ \delta y_{a1}>$	$-<\delta y_{b2}\ \delta y_{b2}>$

In the preceding examples, the energy-group boundaries coincide with the energy boundaries that are defined for the LTY = 0 NC sub-subsections. Since the linear relationship for each NC sub-subsection is applicable for a specified energy range, the multigroup covariances must be processed on an energy grid that contains the energy points defined by the NC sub-subsections as well as the user-specified energy grid. PUFF-III uses different energy grids to process the multigroup covariance information. A complete description of the different energy grids in PUFF-III is provided in Sect. 2.2.2.3.

In addition to the covariances for derived redundant cross sections, PUFF-III must process covariances of cross sections that are derived from ratio measurements to standard cross sections (i.e., $1 \le LTY \le 3$). Sect. 2.2.1.2 describes the continuous-energy format of the cross-section covariances that are derived from ratio measurements. Equation (2.24), which defines the derived cross section in terms of the standard cross section over the energy range E_k to E_{k+1} can be expressed in terms of multigroup parameters:

$$x_I = R_I\ y_I\ , \tag{2.79}$$

where

R_I = ratio of the derived cross section to the standard for the I^{th} energy group,
y_I = standard cross-section value for energy group I.

The deviation of x_I can also be defined in terms of multigroup parameters:

$$\delta x_I = \delta R_I\ y_I + R_I\ \delta y_I\ . \tag{2.80}$$

Using Eq. (2.80), the multigroup covariance of x can be expressed as follows:

$$<\delta x_I\ \delta x_J> = <\delta R_I\ \delta R_J>y_I\ y_J + 2R_I\ y_J<\delta R_I\ \delta y_J> + R_I\ R_J<\delta y_I\ \delta y_J>. \tag{2.81}$$

As noted in Sect. 2.2.1.2, the determination of the ratio and the standard cross section is always performed independently. Consequently, the uncertainty in R_I is assumed to be uncorrelated with the uncertainty in y_I, and $<\delta R_I\ \delta y_J>$ in Eq. (2.81) is assumed to be zero. The multigroup covariance of x can be simplified as follows:

$$<\delta x_I\ \delta x_J> = <\delta R_I\ \delta R_J>y_I\ y_J + R_I\ R_J<\delta y_I\ \delta y_J>\ . \tag{2.82}$$

As an alternative expression, Eq. (2.82) can be divided by the quantity $(y_I y_J R_I R_J)$ on both sides of the equation:

$$\frac{\langle \delta x_I \, \delta x_J \rangle}{(R_I \, y_I)(R_J \, y_J)} = \frac{\langle \delta R_I \, \delta R_J \rangle}{R_I \, R_J} + \frac{\langle \delta y_I \, \delta y_J \rangle}{y_I \, y_J} \, . \tag{2.83}$$

Based on the definition of the relative covariance in Eq. (2.9), the terms in Eq. (2.83) are provided in terms of the relative covariance:

$$RCOV(x_I, x_J) = RCOV(R_I, R_J) + RCOV(y_I, y_J) \, . \tag{2.84}$$

Since the derived cross-section x is a function of the standard cross-section y, Eq. (2.79) also implies that a correlation between x and y exists. The deviation of the standard cross-section value from the true value y_{0I} is denoted as $\delta y_I = y_I - y_{0I}$. The covariance between x and y is obtained by multiplying both sides of Eq. (2.80) by the deviation in y, taking the expectation value of both sides and dividing by $(R_I y_I)$:

$$\frac{\langle \delta x_I \, \delta y_J \rangle}{R_I \, y_I} = \frac{\langle \delta R_I \, \delta y_J \rangle}{R_I} + \frac{\langle \delta y_I \, \delta y_J \rangle}{y_I} \, . \tag{2.85}$$

Because R_I is not correlated with the standard cross section, the covariance between R_I and y_J is zero. In order to express the relative covariance between x_I and y_J, the right-hand side of Eq. (2.85) must be multiplied by y_J/y_J:

$$\begin{aligned} \frac{\langle \delta x_I \, \delta y_J \rangle}{R_I \, y_I} &= \frac{\langle \delta y_I \, \delta y_J \rangle}{y_I} \cdot \frac{y_J}{y_J} \\ \frac{\langle \delta x_I \, \delta y_J \rangle}{R_I \, y_I \, y_J} &= \frac{\langle \delta y_I \, \delta y_J \rangle}{y_I \, y_J} , \end{aligned} \tag{2.86}$$

or

$$RCOV(x_I, y_J) = RCOV(y_I, y_J) \, . \tag{2.87}$$

Equations (2.84) and (2.87) are the basic equations for processing multigroup covariance matrices for cross sections that are derived from ratio measurements to a standard cross-section value.

Although the covariance equations for the derived cross sections are rather simple, there is an unapparent difficulty associated with the calculation of covariance matrices for cross sections that are derived from ratio measurements. The uncertainty information for the ratio (i.e., $\langle \delta R_I \, \delta R_J \rangle$) is provided in the NI sub-subsection of the cross-section x. Based on Eq. (2.84), the relative covariance in x must be determined by summing the relative covariance matrix for the ratio with the relative covariance matrix of the standard. In order to obtain the covariance matrix on the user-specified energy grid, Eq. (2.84) implies that the covariance matrix for the ratio and the standard cross section must be collapsed to the user grid and summed to provide the relative covariance in x. Before the covariance matrix for the ratio can be collapsed to the user grid, the processing code must compute the covariance matrix for x, which cannot be completed without the contribution from the uncertainty in the ratio. Therefore, Eq. (2.84) must be computed on a fine grid structure that includes the user grid structure and the grid structure of the uncertainty data. Once the relative covariance matrix for x is computed on the fine grid structure, the relative covariance matrix can

be collapsed to the user grid. As noted previously, PUFF-III uses different energy grids to process the multigroup covariance information. A complete description of the different energy grids is provided in Sect. 2.2.2.3.

2.2.2.3 Energy Grid Structure

The multigroup equations for calculating covariance matrices from the NI and NC sub-subsections are presented in Sects. 2.2.2.1 and 2.2.2.2, respectively. Since covariance matrices are computed by combining submatrix components that are defined in the various sub-subsections, the multigroup matrix operations dictate that the different submatrices have the same group structure. However, the grid structure for the uncertainty data may not coincide with the grid structure of the multigroup cross-section data. In addition, the grid structure that is specified by the user may not coincide with the uncertainty data or the multigroup cross-section data. Based on the various grid structures, the covariance analysis must process the covariance data with a union energy mesh that includes the energy points from the different grid structures . Ultimately, the multigroup covariance matrices are calculated using the union group structure and collapsed to the user-specified group structure.

PUFF-III considers five possible energy grid structures while processing the ENDF covariance information. A brief description of each energy grid is provided in Table 2.7. Figure 2.1 illustrates the relation between the different grid structures. All covariance calculations are performed using a multigroup structure that is defined by the supergrid (i.e., supergroup). Before the cross sections and the flux can be used in the calculations, the cross sections and flux must be defined in the supergroup structure. Initially, the weighting function (i.e., flux) is read as input from the user or constructed as $1/E$ or $1/(E\Sigma_0)$. The weighting function may also be constructed as $1/E$ times a user-specified function, $G(E)$, (i.e., $1/E\ G(E)$). The flux is constructed on the same grid structure as the multigroup cross sections. An energy weighting procedure is used in PUFF-III to collapse or expand the multigroup cross sections to the supergrid structure. The supergroup cross-section values are obtained with the following expression:

$$\bar{\sigma}_{sI} = \frac{\sum_{g}^{NG} \sigma_g \phi_g \left[\frac{E_{sI} - E_g}{E_{g+1} - E_g}\right]}{\sum_{g}^{NG} \phi_g \left[\frac{E_{sI} - E_g}{E_{g+1} - E_g}\right]}, \tag{2.88}$$

where

I	=	supergroup index,
NG	=	number of cross-section energy groups,
σ_g	=	multigroup cross section for group g,
ϕ_g	=	multigroup flux for group g,
E_{sI}	=	lower energy boundary for supergroup I,
E_g, E_{g+1}	=	energy boundaries for energy group g.

A similar energy-weighting procedure is also used to collapse or expand the multigroup flux to the supergrid structure. Once the cross sections and flux are converted to the supergrid structure, the covariance calculations are performed using the supergrid parameters, and the multigroup covariance matrices are generated using the super-user group structure by determining the contribution to each super-user group from the finer supergroup structure. As the calculation proceeds, the covariance matrices are stored in the super-user group structure. Since the super-user grid structure has the energy boundaries from all the NC sub-subsections, the linear summing operations for the submatrices can be performed as needed. The final covariance matrices are obtained by collapsing the super-user group matrices to the user group structure.

Table 2.7 Different energy grid structures considered in PUFF-III

Grid	Grid Title	Description
1	Cross section	Multigroup cross-section energy grid provided as user input or from an AMPX master library
2	User	Final multigroup structure provided as user input for the calculated covariance matrices
3	Uncertainty	Energy grid values provided by evaluator in the ENDF uncertainty file(s)
4	Supergrid	Union of the user grid and the uncertainty energy grid
5	Super-user	Union of the user grid and the energy grid values for the NC sub-subsections in the uncertainty data

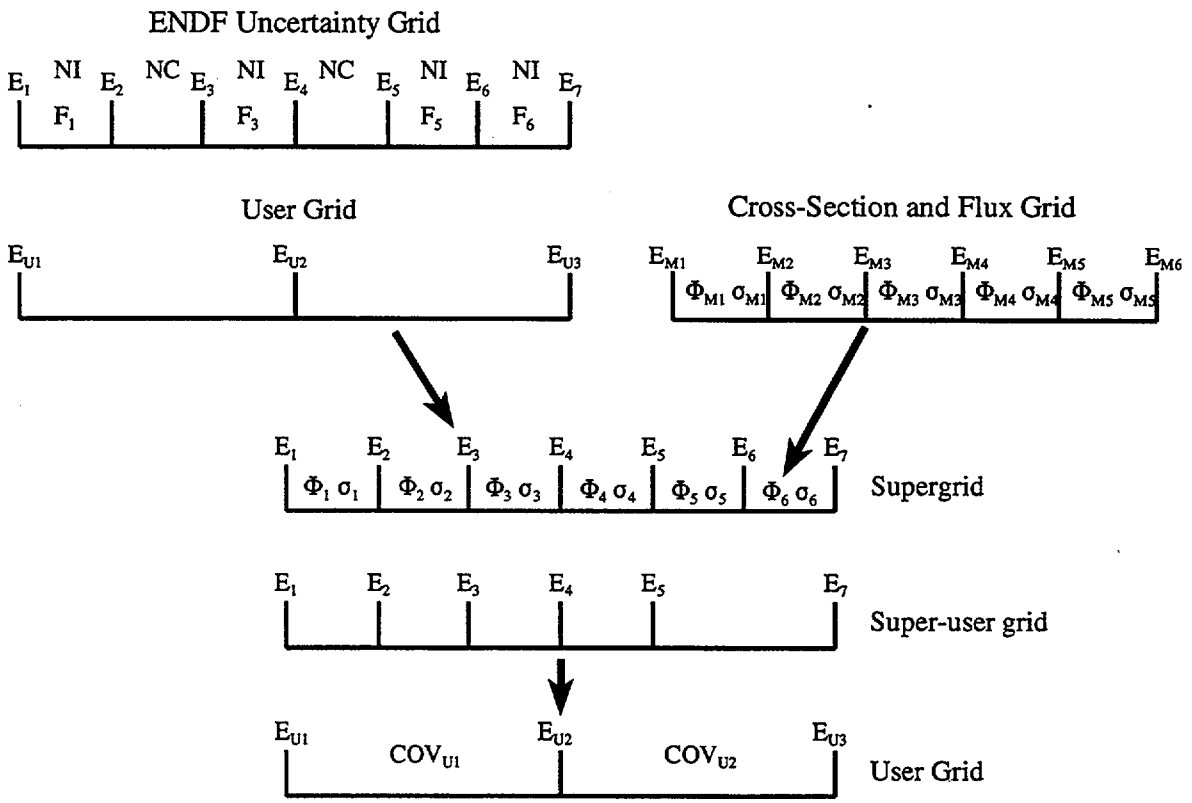

Figure 2.1 Energy grid structures used to process covariance data

2.3 Resonance Parameter Uncertainty Data

ENDF File 32 provides the variances and covariances of the resonance parameters of File 2. The resonance-parameter uncertainty data provide a representation of the cross-section covariance variation due to the rapid variation associated with the individual resonances. Moreover, the File 32 information is used to represent the short-range components that affect the cross-section covariances in the neighborhood of each individual resonance. Ultimately, the final cross-section covariance data should include the effects of the resonance parameter uncertainty information from File 32 as well as the point cross-section uncertainty data from File 33. The following discussion provides an overview of the ENDF File 32 formats; however, the discussion is not intended to be an exhaustive presentation of the ENDF formats. As with the energy-dependent uncertainty data, the overview highlights the information that is needed to understand the processing methods in PUFF-III. The specific formatting rules for the resonance parameter uncertainty data are provided in Ref. 3.

2.3.1 ENDF/B-VI Uncertainty Formats

The ENDF/B-VI resolved resonance parameter uncertainty formats have been greatly enhanced relative to the earlier ENDF/B-V formats. The newer formats permit the representation of cross resonance covariances between parameters of different resonances. For the General Resolved Resonance formats (i.e., LCOMP = 1), covariance data can be provided for the Reich-Moore and Adler-Adler formats in addition to the single and multi-level Breit Wigner formats (SLBW and MLBW, respectively). Outside the resolved-resonance region, the ENDF/B-VI formats also permit the representation of the unresolved-resonance covariance data. Despite the new resonance-parameter covariance formats, all of the ENDF/B-VI evaluations at the time of publication for this document use the SLBW or MLBW formats with the Compatible Resolved Resonance format (i.e., LCOMP = 0), which does not permit the representation of covariance information between parameters of different resonances. In addition, no covariance information is available for the unresolved-resonance region at the time of publication of this document. Consequently, PUFF-III only processes the Compatible Resolved Resonance uncertainty formats in the resolved-energy range, and the following discussion is limited to the current processing capability in PUFF-III.

The File 32 Compatible Resolved Resonance uncertainty format is similar to the ENDF/B-V format; however, in ENDF/B-VI, the resonance spin covariances are zero. The Compatible Resolved Resonance formats are only applicable for the SLBW and MLBW representations in the resolved-resonance region. The format of the File 32 resonance-parameter uncertainty section parallels the format of the File 2 resonance parameter data. In particular, an ENDF LIST record is used to describe the covariance information for NRS resonances corresponding to a specific ℓ-value (i.e., angular momentum). Within the LIST record, there are 18 parameters that are provided to describe the covariance information for each resonance. Consequently, a total of 18*NRS parameters are provided for the resonances corresponding to a specific ℓ-value (i.e., ℓ = 0,1,2, ... etc.). Note that covariance data may not be provided for every resonance in File 2. Covariance information is only provided for the appropriate resonances as determined by the evaluator. A similar LIST record is provided for each additional ℓ-value that is defined by the evaluator. As noted above, eighteen parameters are provided to describe the covariance information for each resonance; however, the eighteenth resonance parameter is always zero. As a result, the following seventeen parameters are defined for each available resonance:

ER	=	the resonance energy, [eV];
J	=	the resonance spin;
Γ_t	=	the total resonance width;
Γ_n	=	the resonance neutron width;

Γ_γ	=	the resonance gamma width;
Γ_f	=	the resonance fission width;
DE^2	=	the variance of the resonance energy, [eV^2];
DN^2	=	the variance of the neutron width, Γ_n, [eV^2];
$DNDG$	=	the covariance between the neutron width, Γ_n, and the gamma width, Γ_γ, [eV^2];
DG^2	=	the variance of the gamma width, Γ_γ, [eV^2];
$DNDF$	=	the covariance of the neutron width, Γ_n, and the fission width, Γ_f, [eV^2];
$DGDF$	=	the covariance of the gamma width, Γ_γ, and the fission width, Γ_f, [eV^2];
DF^2	=	the variance of the fission width, Γ_f, [eV^2];
$DJDN$	=	the null covariance between the resonance spin, J, and the neutron width, Γ_n;
$DJDG$	=	the null covariance between the resonance spin, J, and the gamma width, Γ_γ;
$DJDF$	=	the null covariance between the resonance spin, J, and the fission width, Γ_f;
DJ^2	=	the null variance of the resonance spin, J.

2.3.2 Processing Resonance Parameter Data into Multigroup Formats

As noted in Sect. 2.3.1, File 32 provides the covariance information for the available resonance parameters. Since the uncertainty information is expressed in terms of the resonance parameters, the covariance information cannot be combined directly with the cross-section covariance data from File 33. Therefore, the processing code must calculate the contribution to the cross-section covariance matrix, and combine the contribution with the cross-section covariances from File 33. The approach used in PUFF-III is to calculate cross-section sensitivities and fold the sensitivities with the resonance parameter covariances to obtain the cross-section covariance contribution from the resonance parameter uncertainty data. The following discussion provides a detailed overview of the calculation of the cross-section covariances due to the resonance parameter uncertainties.

In order to process the resonance parameter uncertainties, various assumptions are used in the analysis scheme. The different assumptions can be summarized as follows:

1. Uncertainties due to resonance self shielding are not considered.
2. The resonances are widely spaced, as dictated by the Breit-Wigner representation.
3. Each resonance is assumed to be completely within an energy group k.

These assumptions provide the basis for the cross-section covariance calculation due to the resonance parameter uncertainties.

Consider a partial cross section, σ_i, where i denotes either fission or capture. Using the single-level Breit-Wigner representation, the partial cross section can be expressed in the following format:

$$\sigma_i = \frac{\pi g}{k^2} \frac{\Gamma_n \Gamma_i}{(E - E_r)^2 + \frac{\Gamma_t^2}{4}}, \tag{2.89}$$

where

g = statistical spin factor;
k = the neutron wave number;
Γ_n = the neutron width;
Γ_i = the capture or fission width (i.e., $i = \gamma$ or f, respectively);
Γ_t = the total width;
E = energy;
E_r = resonance energy.

The total resonance width is defined as the sum of the neutron width, the fission width and the gamma width:

$$\Gamma_t = \Gamma_n + \Gamma_f + \Gamma_\gamma \ . \tag{2.90}$$

The statistical spin, g, is defined in terms of the resonance spin and the spin of the target nucleus:

$$g = \frac{2J + 1}{2(2I + 1)} \ , \tag{2.91}$$

where

J = resonance spin,
I = spin of the target nucleus.

In addition, the neutron wave number is defined in the center-of-mass system as follows:

$$k = 2.196771 \times 10^{-3} \frac{AWRI}{AWRI+1} \sqrt{E_r} \ , \tag{2.92}$$

where

$AWRI$ = the ratio of the isotope mass to the mass of the neutron.

The average cross section in the energy group from E_k to E_{k+1} can be obtained by integrating over a flat flux distribution:

$$\bar{\sigma}_i = \frac{\int_{E_k}^{E_{k+1}} \sigma(E)\, dE}{E_{k+1} - E_k} \ . \tag{2.93}$$

In the SLBW approximation, the energy limits are extended to -∞ and +∞ ; hence, by integrating Eq. (2.89) with respect to E from -∞ to ∞, an expression is obtained for the resonance area:

$$A_i = \int_{-\infty}^{\infty} \sigma(E)\,dE = \frac{2g\pi^2}{k^2}\,\frac{\Gamma_n\,\Gamma_i}{\Gamma_t}\,. \tag{2.94}$$

In the preceding integration, a flat weighting spectrum was used to obtain the cross-section area as defined by Eq. (2.94). Sensitivities are obtained by taking the partial of the cross-section area with respect to each resonance parameter. As an example, the sensitivity of the capture cross section with respect to the capture width is obtained by taking the partial of Eq. (2.94) (i.e., $i = \gamma$) with respect to Γ_γ:

$$\frac{\partial A_\gamma}{\partial \Gamma_\gamma} = \frac{2g\pi^2}{k^2}\,\frac{\partial}{\partial \Gamma_\gamma}\left[\frac{\Gamma_n\,\Gamma_\gamma}{\Gamma_t}\right]. \tag{2.95}$$

$$\frac{\partial A_\gamma}{\partial \Gamma_\gamma} = \frac{2g\pi^2\Gamma_n}{k^2}\,\frac{\partial}{\partial \Gamma_\gamma}\left[\frac{\Gamma_\gamma}{\Gamma_t}\right]. \tag{2.96}$$

$$\frac{\partial A_\gamma}{\partial \Gamma_\gamma} = \frac{2g\pi^2\Gamma_n}{k^2}\left[\frac{\Gamma_t - \Gamma_\gamma}{\Gamma_t^2}\right] = \frac{2g\pi^2}{k^2}\frac{\Gamma_n}{\Gamma_t}\left[1 - \frac{\Gamma_\gamma}{\Gamma_t}\right]. \tag{2.97}$$

The remaining sensitivities, which are calculated in a similar fashion, are provided in Table 2.8.

Table 2.8 Flat weighted cross-section sensitivities with respect to resonance parameters

Capture cross-section sensitivities	Fission cross-section sensitivities
$\frac{\partial A_\gamma}{\partial \Gamma_\gamma} = \frac{2g\pi^2}{k^2}\frac{\Gamma_n}{\Gamma_t}\left[1 - \frac{\Gamma_\gamma}{\Gamma_t}\right]$. (2.97)	$\frac{\partial A_f}{\partial \Gamma_\gamma} = \frac{-2g\pi^2}{k^2}\frac{\Gamma_n\Gamma_f}{\Gamma_t^2}$. (2.102)
$\frac{\partial A_\gamma}{\partial \Gamma_n} = \frac{2g\pi^2}{k^2}\frac{\Gamma_\gamma}{\Gamma_t}\left[1 - \frac{\Gamma_n}{\Gamma_t}\right]$. (2.98)	$\frac{\partial A_f}{\partial \Gamma_n} = \frac{2g\pi^2}{k^2}\frac{\Gamma_f}{\Gamma_t}\left[1 - \frac{\Gamma_n}{\Gamma_t}\right]$. (2.103)
$\frac{\partial A_\gamma}{\partial \Gamma_f} = \frac{-2g\pi^2}{k^2}\frac{\Gamma_n\Gamma_\gamma}{\Gamma_t^2}$. (2.99)	$\frac{\partial A_f}{\partial \Gamma_f} = \frac{2g\pi^2}{k^2}\frac{\Gamma_n}{\Gamma_t}\left[1 - \frac{\Gamma_f}{\Gamma_t}\right]$. (2.104)
$\frac{\partial A_\gamma}{\partial J} = \frac{2\pi^2}{k^2(2I+1)}\frac{\Gamma_n\Gamma_\gamma}{\Gamma_t}$. (2.100)	$\frac{\partial A_f}{\partial J} = \frac{2\pi^2}{k^2(2I+1)}\frac{\Gamma_n\Gamma_f}{\Gamma_t}$. (2.105)
$\frac{\partial A_\gamma}{\partial E_r} = -2g\pi^2\frac{\Gamma_n\Gamma_\gamma}{\Gamma_t}\left[\frac{1}{\beta^2 E_r^2}\right]$; $\beta = 2.196771 \times 10^{-3}\frac{AWRI}{AWRI + 1}$ (2.101)	$\frac{\partial A_f}{\partial E_r} = -2g\pi^2\frac{\Gamma_n\Gamma_f}{\Gamma_t}\left[\frac{1}{\beta^2 E_r^2}\right]$; $\beta = 2.196771 \times 10^{-3}\frac{AWRI}{AWRI + 1}$ (2.106)

For each resonance in File 32, PUFF-III constructs the resonance parameter covariance matrix in the following form:

$$D = \begin{bmatrix} <\delta\Gamma_n\ \delta\Gamma_n> & <\delta\Gamma_n\ \delta\Gamma_\gamma> & <\delta\Gamma_n\ \delta\Gamma_f> & <\delta J\ \delta\Gamma_n> & 0 \\ 0 & <\delta\Gamma_\gamma\ \delta\Gamma_\gamma> & <\delta\Gamma_\gamma\ \delta\Gamma_f> & <\delta J\ \delta\Gamma_\gamma> & 0 \\ 0 & 0 & <\delta\Gamma_f\ \delta\Gamma_f> & <\delta J\ \delta\Gamma_f> & 0 \\ 0 & 0 & 0 & <\delta J\ \delta J> & 0 \\ 0 & 0 & 0 & 0 & <\delta E_r\ \delta E_r> \end{bmatrix}. \quad (2.107)$$

Using Eqs. (2.90) through (2.99), the cross-section sensitivities with respect to the resonance parameters are calculated, and the sensitivity matrix is constructed as follows:

$$H = \begin{bmatrix} \frac{\partial A_\gamma}{\partial \Gamma_n} & \frac{\partial A_\gamma}{\partial \Gamma_\gamma} & \frac{\partial A_\gamma}{\partial \Gamma_f} & \frac{\partial A_\gamma}{\partial J} & \frac{\partial A_\gamma}{\partial E_r} \\ \frac{\partial A_f}{\partial \Gamma_n} & \frac{\partial A_f}{\partial \Gamma_\gamma} & \frac{\partial A_f}{\partial \Gamma_f} & \frac{\partial A_f}{\partial J} & \frac{\partial A_f}{\partial E_r} \end{bmatrix}. \quad (2.108)$$

The covariance matrix of the group-averaged cross sections is formed by folding the sensitivity matrix, H, with the covariance matrix, D:

$$H(\ DH^T\ ) = \begin{bmatrix} <\ \delta A_\gamma\ \delta A_\gamma\ > & <\delta A_\gamma\ \delta A_f\ > \\ <\ \delta A_f\ \delta A_\gamma\ > & <\ \delta A_f\ \delta A_f\ > \end{bmatrix} \quad (2.109)$$

The matrix defined by Eq. (2.109) must be divided by the square of the energy group width (i.e., $(E_{k+1} - E_k)^2$) to obtain the cross-section covariances due to the resolved-resonance parameters. The final matrix provides the contribution to the capture and fission covariance matrix, which corresponds to the uncertainty data for resonance E_r. In addition, Eq. (2.109) provides the cross-reaction covariance between the capture and fission cross sections due to the resonance parameter uncertainties. As noted in Sect. 2.3.1, resonance parameter covariances can be provided for each resonance and corresponding ℓ-state (i.e., angular momentum). For an energy group k, Eq. (2.109) provides the resonance parameter uncertainty contribution from a resonance E_r. To obtain the complete contribution to energy group k from all resonance parameters for a given isotope, a summation must be performed over each resonance and subsequent ℓ-state(s) using the matrix defined in Eq. (2.109). If more than one isotope is present, the atom abundance is used to weight the contribution from each isotope.

As noted previously, the cross-section area, A_i, was obtained by integrating the SLBW representation of the cross-section value against a constant or flat weighting function. An additional cross-section weighting option is

available for the resonance parameter uncertainties and is documented in Ref. 2. In the $1/E$ weighting approach, the average cross section is expressed in the following form:

$$\bar{\sigma}_i = \frac{\int_{E_k}^{E_{k+1}} \sigma_i(E)\,\frac{dE}{E}}{\int_{E_k}^{E_{k+1}} \frac{dE}{E}} \; ; \; i = \gamma \text{ or } f \, . \tag{2.110}$$

In Eq. (2.110), the "true" cross-section, σ_i, is approximated by the quantity $A_i/2\Gamma_i$. By using this approximation, the resonance has a width of $2\Gamma_i$. With the approximation, the integral in Eq. (2.110) can be evaluated, and the average cross section for group k can be approximated as follows:

$$\bar{\sigma}_i \approx \frac{A_i}{2\Gamma_i} \frac{\ln\left[\frac{E_r + E_i}{E_r - E_i}\right]}{\ln\left[\frac{E_{k+1}}{E_k}\right]} \; ; \; i = \gamma \text{ or } f \, . \tag{2.111}$$

Using the same procedure as in the flat-weighting case, the sensitivities are obtained by taking the partial of the cross-section area with respect to each resonance parameter. The sensitivities for the $1/E$ weighting case are provided in Tables 2.9 and 2.10. Using Eqs. (2.112) through (2.121), the sensitivity matrix, H, is constructed, and the cross-section covariance matrix is formed by folding the sensitivity matrix with the covariance matrix, D. Once the sensitivity matrix is constructed, the procedure to construct the cross-section covariance matrix from the resonance parameter uncertainty data is the same as the constant-weighting approach.

Since the cross-section covariance matrices due to the resonance parameter uncertainties must be combined with the cross-section covariance matrices from File 33, the cross-section covariance matrices generated from File 32 are produced on the super-user grid, or supergrid, as appropriate. The subsequent covariance matrices are combined with the covariance matrices from File 33, and the final matrices are collapsed to the desired user grid structure.

Table 2.9 $1/E$ weighted capture cross-section sensitivities

Sensitivity equation	
$\frac{\partial A_\gamma}{\partial \Gamma_\gamma} = \frac{1}{2a}\left\{ \frac{1}{\Gamma_\gamma}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right) \frac{2g\pi^2\Gamma_n}{k^2} \frac{(\Gamma_t - \Gamma_\gamma)}{\Gamma_t^2} - \frac{A_\gamma}{\Gamma_\gamma^2}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right) + \frac{2E_r A_\gamma}{\Gamma_\gamma(E_r + \Gamma_\gamma)(E_r - \Gamma_\gamma)} \right\}$	(2.112)
$\frac{\partial A_\gamma}{\partial \Gamma_n} = \frac{g\pi^2}{a\,k^2\Gamma_t}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right)\left[1 - \frac{\Gamma_n}{\Gamma_t}\right].$	(2.113)
$\frac{\partial A_\gamma}{\partial \Gamma_f} = \frac{-g\,\pi^2\,\Gamma_n}{a\,k^2\,\Gamma_t^2}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right).$	(2.114)
$\frac{\partial A_\gamma}{\partial J} = \frac{\pi^2\,\Gamma_n}{a\,k^2\,(2I + 1)\Gamma_t}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right).$	(2.115)
$\frac{\partial A_\gamma}{\partial E_r} = \frac{-g\,\pi^2\,\Gamma_n}{a\,\Gamma_t}\ln\left(\frac{E_r + \Gamma_\gamma}{E_r - \Gamma_\gamma}\right)\left(\frac{1}{\beta^2 E_r^2}\right) - \frac{2g\pi^2}{ak^2}\frac{\Gamma_n\Gamma_\gamma}{\Gamma_t}\left[\frac{1}{(E_r + \Gamma_\gamma)(E_r - \Gamma_\gamma)}\right].$	(2.116)
Note: $a = \ln\left(\frac{E_{k+1}}{E_k}\right)$.	

Table 2.10 1/*E* weighted fission cross-section sensitivities

Sensitivity equation
$\frac{\partial A_f}{\partial \Gamma_\gamma} = \frac{-g\pi^2}{a\,k^2}\,\frac{\Gamma_n}{\Gamma_t^2}\,\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right).$ (2.117)
$\frac{\partial A_f}{\partial \Gamma_n} = \frac{g\pi^2}{a\,k^2\Gamma_t}\,\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right)\left[1 - \frac{\Gamma_n}{\Gamma_t}\right].$ (2.118)
$\frac{\partial A_f}{\partial \Gamma_f} = \frac{1}{2a}\left\{\frac{1}{\Gamma_f}\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right)\frac{2g\pi^2}{k^2}\,\frac{\Gamma_n}{\Gamma_t}\left(1 - \frac{\Gamma_f}{\Gamma_t}\right) - \frac{A_f}{\Gamma_f^2}\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right) + \frac{2E_r A_f}{\Gamma_f\,(E_r + \Gamma_f)(E_r - \Gamma_f)}\right\}$ (2.119)
$\frac{\partial A_f}{\partial J} = \frac{\pi^2\,\Gamma_n}{a\,k^2\,(2I+1)\Gamma_t}\,\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right).$ (2.120)
$\frac{\partial A_f}{\partial E_r} = \frac{-g\,\pi^2\,\Gamma_n}{a\,\Gamma_t}\,\ln\left(\frac{E_r + \Gamma_f}{E_r - \Gamma_f}\right)\left(\frac{1}{\beta^2 E_r^2}\right) - \frac{A_f}{a\,(E_r + \Gamma_f)(E_r - \Gamma_f)}.$ (2.121)

Note: $a = \ln\left(\frac{E_{k+1}}{E_k}\right)$.

3 LOGICAL PROGRAM FLOW

The following sections outline the logical program flow of PUFF-III. Because of the number of subroutines involved in the program, the logical flow description is divided into separate sections. Consequently, an overall flow diagram for the program is not provided. Each section describes a portion of the program flow with an abbreviated flow diagram. In the subsequent flow diagrams, the PUFF-III subroutines are shown with the names enclosed by boxes, and the AMPX library routines are depicted without boxes. A brief description of each subroutine is provided with the accompanying flowchart. In each abbreviated flow chart, a PUFF-III subroutine box may also have an arrow indicating additional information. The additional flow logic associated with each arrow is described in greater detail in another section.

3.1 Program Initiation

Figure 3.1 provides a flow diagram for the initiation of PUFF-III.

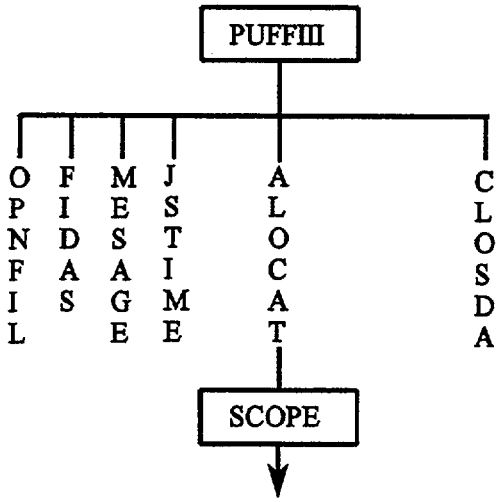

Figure 3.1 Flowchart for program initiation

The function of this portion of the code is to perform the initialization tasks for the program execution. In particular, the program reads the first data block of the input file, determines the type of problem to execute and the amount of core needed for the problem. Subsequently, PUFF-III calls the library routine ALOCAT, which allocates the requested storage space for the problem and calls the controlling subroutine SCOPE.

PUFF-III: The main program that opens the user input file and reads the first block of data for the problem. In addition, PUFF-III calls MESAGE to print the banner page and initiates the timing routine JSTIME for the problem. Subsequently, SCOPE is called after the required storage space is obtained by ALOCAT. After the program execution is complete, CLOSDA is used to close the direct-access files.

OPNFIL: Library routine that initializes the input and output logical units.

FIDAS: Library routine that reads the FIDO input structure.

MESAGE: Library routine that prints the banner page on the logical output device.

JSTIME: Library routine that provides the initial time of the program execution. JSTIME is also called after program execution is complete to determine the total CPU time.

ALOCAT: Assembly language program that is called with three arguments. The first argument is a subroutine name, and the second argument is the maximum number of words of storage to be allocated. ALOCAT calls subroutine SCOPE with two arguments, an array name and the corresponding array length. The third argument is prefixed by an asterisk and specifies the statement number to return to if there is insufficient space to execute the problem.

SCOPE: Controlling subroutine for PUFF-III. SCOPE, which is called by ALOCAT, controls the overall flow of PUFF-III and is described in more detail in Sect. 3.2.

CLOSDA: Library routine that closes each direct-access file upon normal completion of the problem.

3.2 Overall Program Flow

SCOPE is designed to direct the primary flow of PUFF-III (Figure 3.2). Moreover, SCOPE reads the remaining user input data, sets up the problem, calls the appropriate subroutine (i.e., DANNY) to process the ENDF covariance data and prints the correlation matrices in the COVERX format.

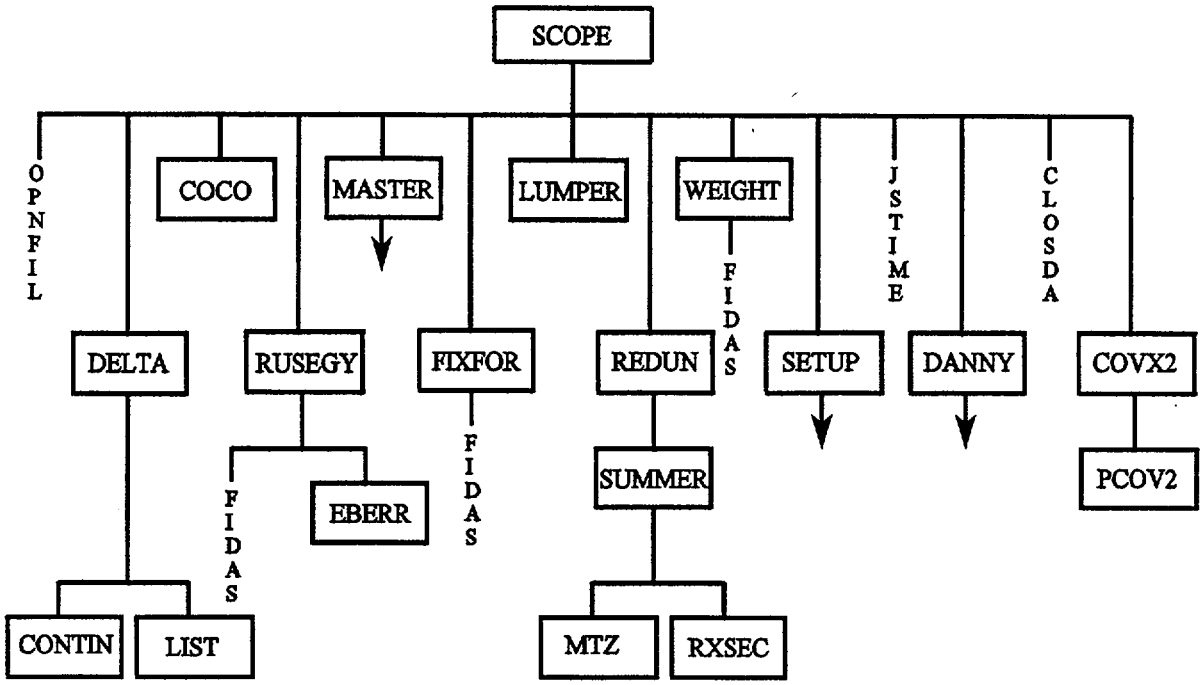

Figure 3.2 Flowchart of overall program flow

SCOPE: Reads the user input data and prints the appropriate information on the logical output device. Subsequently, SCOPE calls the appropriate routines to read the ENDF uncertainty information and store the necessary information on a scratch device for retrieval. Various routines are then called to construct the different energy grids, as well as read the cross-section data and weighting spectrum. Once the problem is set up, DANNY is called to calculate the multigroup covariances from the ENDF uncertainty data. Upon completion, the correlation matrices are stored and control of the program is returned to PUFF-III. A summary of the subroutines called by SCOPE is provided in Table 3.1, and a complete description of each subroutine in Table 3.1 is provided in the following discussion.

OPNFIL: Library routine used to open ENDF uncertainty files, cross-section files, etc.

Table 3.1 Summary of subroutines called by SCOPE

Subroutine	Function	Condition
OPNFIL	Open files specified by the user	Always
DELTA	Read ENDF uncertainty data	Always
COCO	Construct directory of covariance data	Always
RUSEGY	Read user grid and construct super- and super-user grids	Always
MASTER	Read AMPX master library	If AMPX library is provided
FIXFOR	Read cross-sections input by user	If AMPX library is not provided
LUMPER	Construct cross sections for lumped reaction covariances	If lumped reaction covariances are on ENDF uncertainty file
REDUN	Calculate redundant cross sections from partials	If redundant cross sections are needed, but the cross sections are not provided
WEIGHT	Read or generate weighting spectrum	Always
SETUP	Put cross sections and flux on supergrid	Always
JSTIME	Timing	Always
DANNY	Calculate multigroup covariance matrices	Always
CLOSDA	Close direct-access devices	Always
COVX2	Print correlation matrices in COVERX format	Always

DELTA: Subroutine that reads the ENDF uncertainty information on IO32 as well as the standard uncertainty information on I19. DELTA calls subroutines CONTIN and LIST to read the control and list records, respectively. The ENDF data are stored on a binary scratch device for later retrieval.

CONTIN: Subroutine that reads a single ENDF control record.

LIST: Subroutine that reads the ENDF list records.

COCO: Subroutine that reads the ENDF uncertainty information and determines the explicitly as well as implicitly defined covariance matrices. A complete directory of the possible covariance matrices is printed on the logical output device.

RUSEGY: Subroutine that reads the user-defined energy grid. If the user grid is specified in the input file, RUSEGY uses FIDAS to read the grid specified in the FIDO format. If one of the library user grids is selected, RUSEGY constructs the appropriate energy grid. Based on the user grid and ENDF uncertainty data, RUSEGY constructs the supergrid and super-user grid. Subroutine EBERR is used to add points to an existing grid without duplicating points.

FIDAS: Library routine that reads the FIDO input structure.

EBERR: Subroutine that combines two vectors into a single vector.

MASTER: Subroutine that reads an AMPX master library and stores the required cross-section data on a scratch device for later retrieval.

FIXFOR: Subroutine that reads cross-section information specified by the user. FIXFOR uses FIDAS to read the user-defined cross sections in the FIDO format.

FIDAS: Library routine that reads the FIDO input structure.

LUMPER: Subroutine that sums the partial reaction for the lumped reaction covariance matrices.

REDUN: Subroutine that sums the partial reactions for the redundant reactions. REDUN is used only if covariance information is provided for a redundant reaction, but the required cross-section information is not available. All partial cross sections must be available for the redundant reaction to be calculated. REDUN calls SUMMER to construct the redundant reaction. Subroutine MTZ is called by SUMMER to determine the appropriate reactions needed for the redundant reaction, and subroutine RXSEC is called by SUMMER to read the partial reaction cross sections from the scratch device.

SUMMER: Subroutine that calculates the redundant cross sections from the partial reactions.

MTZ: Subroutine that is used to determine the partial reactions for a redundant reaction.

RXSEC: Subroutine that reads the partial cross-section data from the scratch device.

WEIGHT: Subroutine that determines the weighting function for the subsequent covariance calculations. If a user-defined weighting function is provided, FIDAS is used to read the input function in a FIDO format. If a library weighting function is specified (e.g., 1/E), the function is constructed from the cross-section energy grid.

FIDAS: Library routine that reads data in the FIDO format.

SETUP: Subroutine that collapses or expands the flux and cross sections to the supergrid structure.

JSTIME: Library routine used for timing the covariance calculation. JSTIME is called before and after the covariance calculation (i.e., before and after DANNY).

DANNY: Subroutine that guides the program through the generation of multigroup covariance matrices. A complete description of DANNY is provided in Sect. 3.4.

CLOSDA: Library routine that is used to close the direct-access units.

COVX2: Subroutine that prints the calculated correlation matrices in the COVERX format on unit NO28. Subroutine PCOV2 is called to print the correlation matrices in the COVERX format.

PCOV2: Subroutine used to format the correlation matrices in the COVERX format.

3.3 Problem Setup

The purpose of this section is to set up the problem (Figure 3.3) for execution. The cross sections are read and stored for later retrieval. Subsequently, the weighting spectrum is constructed on the supergrid for the problem. Using the weighting spectrum, the cross sections are collapsed or expanded to the supergrid structure.

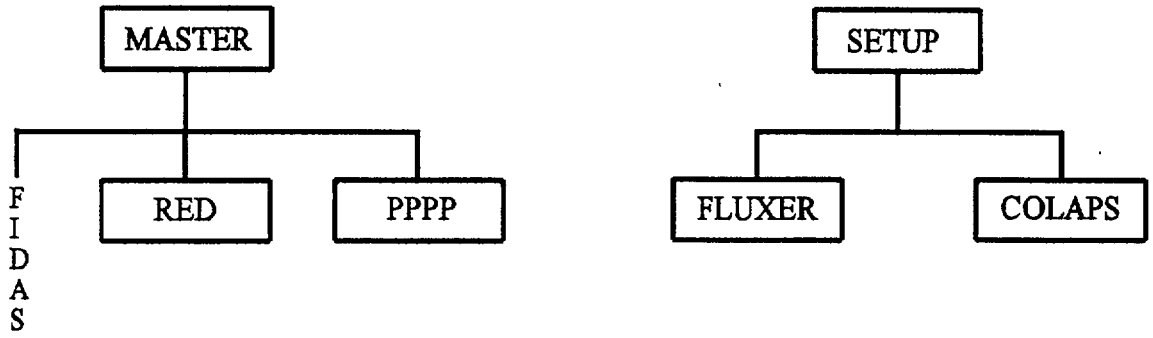

Figure 3.3 Program flow for problem setup

MASTER: Subroutine that reads an AMPX master cross-section library. Subroutine RED is used to read the multigroup energy structure, and PPPP is used to write the cross-section data on a scratch device for later retrieval.

- RED: Subroutine that reads the energy grid structure on the AMPX master library.
- PPPP: Subroutine that writes the cross-section data on a scratch device.

SETUP: Subroutine that generates the weighting spectrum on the supergrid and collapses or expands the cross sections to the supergrid.

- FLUXER: Subroutine that collapses or expands the weighting spectrum to the supergrid.
- COLAPS: Subroutine that collapses or expands the multigroup cross sections to the supergrid.

3.4 Covariance Calculation

This portion of the program performs the calculation of multigroup covariance matrices (Figure 3.4) based on the ENDF uncertainty information.

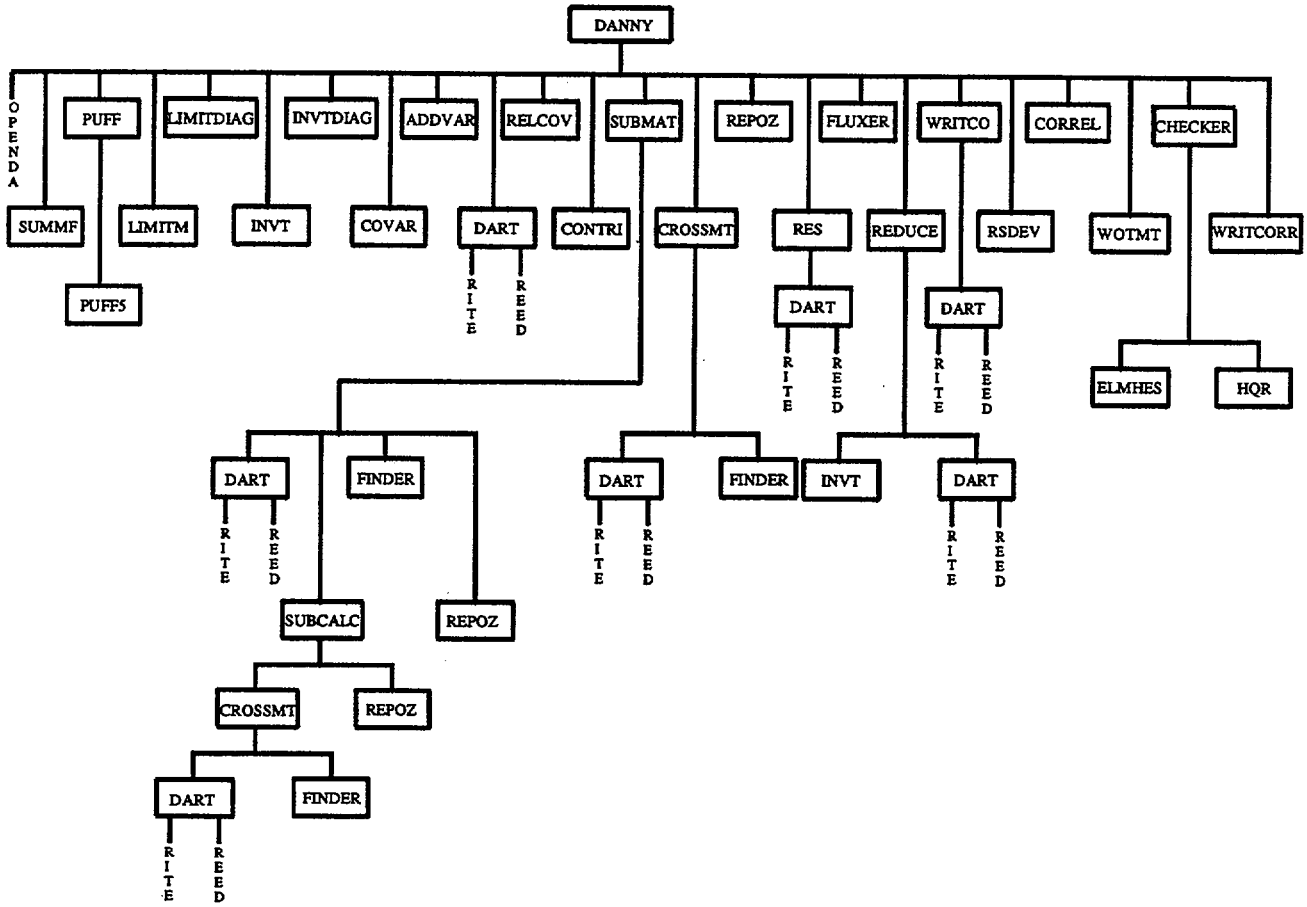

Figure 3.4 Program flow for covariance matrix calculation

OPENDA: Library routine that opens the direct-access binary files.

SUMMF: Subroutine that calculates the flux on the super-user grid and collapses the multigroup cross sections from the super-user grid to the user grid.

PUFF: Subroutine that calculates the contribution to the covariance matrix from an NI sub-subsection using the appropriate equations that are specified in Sect. 2.2.2.1.

PUFF5: Subroutine called by PUFF to process the LB = 5 and 6 NI sub-subsections to obtain the contribution to the covariance matrix.

LIMITM: Subroutine that extracts the desired component of the standard covariance matrix based on the energy range specified in the NC subsection of the derived covariance file.

LIMITDIAG: Subroutine that extracts the desired component of the diagonal following the LB = 8 calculation. The portion of the diagonal matrix is added to the covariance matrix by subroutine ADDVAR.

INVT: Subroutine that performs different matrix inversion operations.

INVTDIAG: Subroutine that inverts a vector.

COVAR: Subroutine that converts a relative covariance matrix to an absolute covariance matrix.

ADDVAR: Subroutine that adds the diagonal component from an LB = 8 calculation to the covariance matrix.

DART: Subroutine that writes and reads covariance matrices to and from direct-access files.

- RITE: Library routine that writes data on a direct-access device.
- REED: Library routine that reads data from a direct-access device.

RELCOV: Subroutine that converts an absolute covariance matrix to a relative covariance matrix.

CONTRI: Subroutine that calculates a derived redundant covariance matrix based on the linear relationship specified by the LTY = 0 flag of the NC sub-subsection.

SUBMAT: Subroutine that calculates all explicitly and implicitly defined cross-reaction covariance matrices (i.e., COV(x_i, y_j)) that are defined by the LTY = 0 sub-subsection. In addition, SUBMAT calculates all off-diagonal components for COV(x_i, x_j) that may be correlated with other energy ranges through the use of the LTY = 0 NC sub-subsection.

- DART: Subroutine that writes and reads covariance matrices to and from direct-access files.
  - RITE: Library routine that writes data on a direct-access device.
  - REED: Library routine that reads data from a direct-access device.
- SUBCALC: Subroutine that determines the derived redundant linear relationship (explicit and implicit) for an energy range and calculates the corresponding component of the cross-reaction covariance matrix.
  - CROSSMT: Subroutine that calculates the cross-reaction covariance matrix. When called by SUBCALC, CROSSMT is used to calculate the implicitly defined covariance matrices.
- FINDER: Subroutine that reads the requested uncertainty information from scratch device IO33.

REPOZ: Subroutine that moves to a specific location in the scratch device containing the ENDF uncertainty data (i.e., IO33).

CROSSMT: Subroutine that calculates the cross-reaction covariance matrix. When called by DANNY, CROSSMT is used to calculate the covariance matrices that are defined by the linear relationship of the LTY = 0 sub-subsections.

REPOZ: Subroutine that moves to a specific location in the scratch device containing the ENDF uncertainty data (i.e., IO33).

RES: Subroutine that calculates the cross-reaction covariance matrices based on the resonance parameter uncertainties.

FLUXER: Subroutine that collapses the weighting spectrum to the super-user grid.

REDUCE: Subroutine that collapses the covariance matrices from the super-user grid to the user grid.

WRITCO: Subroutine that writes the absolute covariance matrices on ICOV (binary) using the following format:

MAT1,MAT2,MT1,MT2, ((COV(i,j),i = 1, NG), j = 1,NG)

RSDEV: Subroutine that calculates the relative standard deviation.

CORREL: Subroutine that calculates the correlation matrices for printing to the logical output device (i.e., correlations range between - 1000 and 1000 instead of - 1 and 1).

WOTMT: Subroutine that formats and prints the correlation matrices for output on the logical output device.

CHECKER: Subroutine that evaluates the calculated correlation matrices and categorizes each matrix based on the calculated eigenvalues.

ELMHES: Subroutine that reduces the correlation matrix to the Hessenberg form.[6]

HQR: Subroutine that calculates the eigenvalues of the matrix.[6]

WRITCORR: Subroutine that writes the correlation matrices on ICORR (binary) using the following format:

MAT1,MAT2,MT1,MT2, ((CORR(i,j),i = 1, NG), j = 1,NG)

4 INPUT DATA GUIDE

PUFF-III uses the FIDO input method, which is described in Appendix C, for specifying the input data for a problem. The following section provides a detailed description of the PUFF-III input options.

4.1 FIDO Input Structure

Block 1.

-1$ Core Allocation [1]

1. LENGTH - Number of words to allocate **(500000)**

0$ Directory Flag [1]

1. LDIR - Unit number for ENDF uncertainty file **(0)**
   Note: Use only if a directory of the ENDF uncertainty file is desired and no calculations are to be performed.

1$ Integer Parameters [18]

1. NO28 - Unit for COVERX formatted output { -/+ = Binary/BCD} **(0)**
2. ISS - Unit number for standard deviations in user group structure from standard cross-section file in binary format **(0)**
   Note: Only used if processing LTY=1 NC sub-subsection, and the standard cross-section uncertainties must be processed apriori.
   Normally on unit I16 after processing standard uncertainty file.
3. I19 - Unit number for standard material ENDF uncertainty file in BCD format **(0)**
   Note: Only used if processing LTY=1 or 2 NC sub-subsections.
   I19 cannot equal IO32,
4. IO11 - Unit number for AMPX master library if IXSOP = 1 **(0)**
5. IO32 - Unit number for ENDF uncertainty file in BCD format **(0)**
6. MATUSE - MAT number of material to process
7. IUSER - Number of user groups for covariance calculation
   - >0: user input in 2* array
   - -2: 240 group CSEWG
   - -3: 99 group GAM2
   - -4: 620 group SAND2
   - -5: 30 group LASL
   - -6: 68 group GAMI
   - -7: 171 group VITAMIN-C
   - -8: 26 group ORNL-5517
   - -9: 100 group GE
   - -10: 6 group ORNL-5318
   - -11: Unavailable
   - -12: 44 group AMPX

8. IXS - Number of groups of input cross sections
   -2 through -10 or -12: same as IUSER
   -11: Read number of groups from AMPX master library
   Note: IXSOP must be 1.
9. IWT - Weighting function
   1: $1/E$
   2: $1/(E\Sigma_t)$
   3: $(1/E)$*INPUT (INPUT placed in 5* array)
   4: INPUT (placed in 5* array)
10. IXSOP - Cross-Section Input
   0: User input in 4* array
   1: AMPX master library
11. JOPT1 - File 31 and 33 Processing Options
   0: Process File 33
   1: Process File 31
   2: Process File 31 and 33
12. JOPT2 - File 32 Processing Options
   0: Do not process
   1: Process File 32
13. JOPT3 - Not used
14. NOX - Not used
15. NOCVX - Not used
16. NMT - Number of MAT-MT Reaction Pairs to Process
   -1: Process all reaction pairs on ENDF tape
   >0: Number of reaction pairs to be entered in Block 4
17. NDM1 - Not used
18. NDM2 - Not used

T Terminate Block 1.

Block 2.

2* User Energy Grid if IUSER > 0 [IUSER+1]

1.	E (eV) for group 1
2.	E (eV) for group 2
.	
.	
IUSER	E (eV) for group IUSER
IUSER+1	Lower energy bound (eV) for group IUSER

T Terminate Block 2.

Block 3.

3* Cross-Section Energy Grid if IXS > 0 [IXS+1]

1.	*E* (eV) for input cross-section group 1
2.	*E* (eV) for input cross-section group 2
.	
.	
IXS.	*E* (eV) for input cross-section group IXS
IXS+1	Lower energy bound (eV) for group IXS

T Terminate Block 3.

Block 4.

4* MAT-MT Reaction Information if NMT > 0 [NMT*2]

1.	MAT number for 1st reaction pair
2.	MAT number for 2nd reaction pair
.	
.	
NMT.	MAT number for NMTth reaction pair
NMT+1.	MT number corresponding to 1st MAT number
NMT+2.	MT number corresponding to 2nd MAT number
.	
.	
NMT*2.	MT number corresponding to NMTth MAT number

Note: If IXSOP ≠ 0, terminate 4* array with T.

User Input Multigroup Cross-Section Values if IXSOP = 0 [NMT*IXS]

1.	Cross section for energy group 1 corresponding to 1st MAT-MT
2.	Cross section for energy group 2 corresponding to 1st MAT-MT
.	
.	
IXS	Cross section for energy group IXS corresponding to 1st MAT-MT
IXS+1	Cross section for energy group 1 corresponding to 2nd MAT-MT
IXS+2	Cross section for energy group 2 corresponding to 2nd MAT-MT
.	
.	
IXS+IXS	Cross section for energy group IXS corresponding to 2nd MAT-MT
.	
.	
(NMT-1)*IXS+1	Cross section for energy group 1 corresponding to NMTth MAT-MT
(NMT-1)*IXS+2	Cross section for energy group 2 corresponding to NMTth MAT-MT
.	
.	
NMT*IXS	Cross section for energy group IXS corresponding to NMTth MAT-MT

T Terminate Block 4.

Block 5.

5* User Defined Weighting Function if IWT ≥ 3 [IXS]

1. Weight function value for energy group 1
2. Weight function value for energy group 2
.
.
IXS Weight function value for energy group IXS

T Terminate Block 5.

COVERX Title Card (Character*72)

4.2 Logical Unit Parameters

Table 4.1 File parameters for logical units

Var.	Unit No.	Type	Description
IO5	5	BCD	FIDO formatted input file
IO6	6	BCD	Formatted output file
NO28	User defined	BCD or Binary	COVERX-formatted output file
ISS	User defined	Binary	Standard deviation for standard material(s)
I19	User defined	BCD	ENDF uncertainty file for standard material
IO11	User defined	Binary	AMPX master library
IO32	User defined	BCD	ENDF uncertainty file for MATUSE
I18	18	Binary	Scratch
IOUT	21	Binary	Scratch
IO12	19	Binary	Scratch
I57	20	Direct access Binary	Scratch
IO33	22	Binary	Scratch
ISR	17	Binary	Scratch
I15	15	Direct access Binary	Scratch
I16	16	Binary	Scratch
ILUM	23	Binary	Scratch
ICOV	24	Binary	Scratch
ICORR	25	Binary	Scratch

5 DESCRIPTION OF OUTPUT

The following section provides a brief description of the PUFF-III output. An entire output file is not provided in this section. However, portions of the output are printed and discussed.

5.1 Header Page

A sample header page is provided in Figure 5.1. The program title is printed in the first line of block letters. Within the second line of block letters, the problem identification is provided. The third line provides the date the job was executed in terms of the month, day and year. The last line provides the time of execution in an hour, minute and second format. Note that the time printout is in terms of a 24-hour clock, with midnight denoted as 2400 hours. The header page is printed by subroutine MESAGE, which is discussed in Sect. 3.

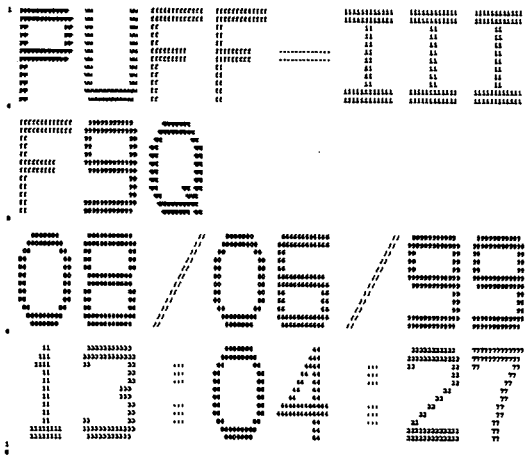

Figure 5.1 Example header page output

5.2 Program Verification Information

Following the header page, the program verification information is provided for quality-assurance purposes. An example of the program-verification information is provided in Figure 5.2. The information includes the code name, the creation date of the load module, library that contains the load module, the computer code name from the configuration control table and the revision number. In addition, the job name, date, and time of execution are printed.

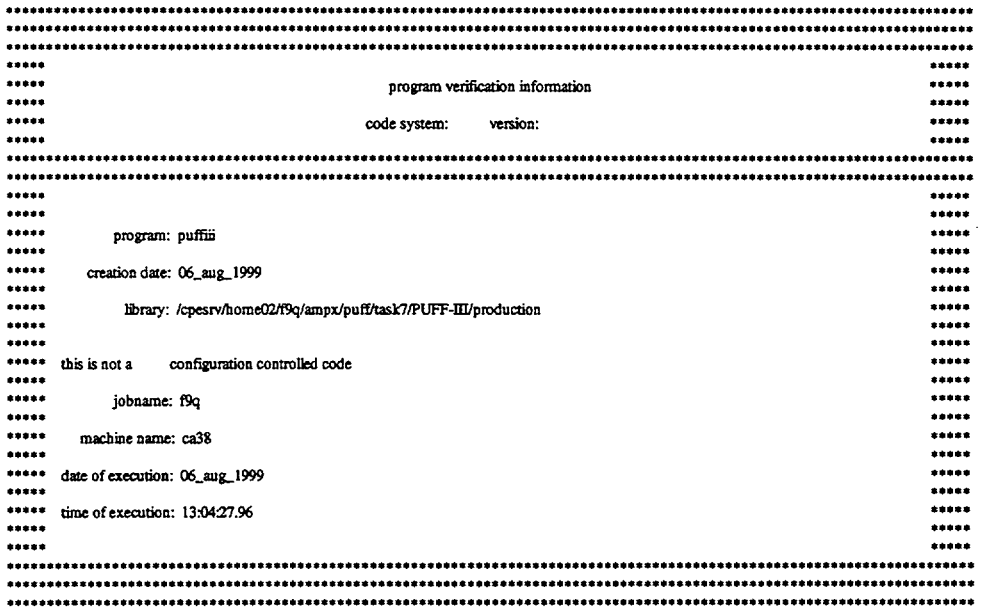

Figure 5.2 Example program verification information output

5.3 Problem Verification Information

Execution of PUFF-III requires the development of a user input file, as described in Sect. 4. Because of the possibility of typing errors, incorrect unit specification, etc., the code provides a problem or input verification table in the output. This section should be evaluated to ensure the desired input information is provided. Following the program verification information is the problem verification information. An example of the problem verification information is provided in Figure 5.3. As shown in Figure 5.3, the amount of storage that is allocated for PUFF-III is printed. Furthermore, the output indicates the type of run requested by the user (e.g., directory only or process the covariance data). In addition, the requested unit numbers are displayed for the COVERX output file, as well as the units associated with the standard uncertainty information. Also, the unit numbers for the AMPX master library and ENDF uncertainty file are printed in the problem verification information. Following the unit number specifications is the requested processing information. In particular, the requested material ID and the source of the user and cross-section group structure is printed. If the source designation is "internal," the user has requested a library group structure that is available with PUFF-III (e.g., ENDF/B-V 44 group structure). Additional processing information includes the flux-weighting spectrum, source of cross-section data, requested ENDF

uncertainty data files and the number of reaction pairs to process. In Figure 5.3, the user has requested that "all" covariance reactions be processed.

```
PUFF-III has been allocated    500000 words of core

The following input parameters are specified:
Directory only run:                          no
Unit for COVERX output:                      1
Unit for group std. dev. (standard):         0
Unit for standard uncertainty file:          0
Unit for AMPX master library:                4
Unit for ENDF uncertainty file:              8
Material to process:                         1125
Source of user group structure:              internal
Source of cross-section group structure:     AMPX
Weighting:                                   1/E
Source of cross sections:                    AMPX
Process:                                     File 33
Process:                                     File 32
Number of reaction pairs to process:         All
```

Figure 5.3 Example problem verification information output

5.4 Directory of Uncertainty File

One of the new features in the latest version of PUFF is the capability to print a detailed directory of the ENDF uncertainty data. An example of an abbreviated PUFF-III directory output is provided in Figure 5.4. If an LTY = 0 sub-subsection is specified in the covariance data, PUFF-III identifies the reaction and provides a list of the reactions that are used to derive the covariance matrix. Although not shown in this example, PUFF-III also identifies any LTY = 1, 2 or 3 sub-subsections and identifies the standard material as appropriate. As shown in Figure 5.4, a directory of the explicitly and implicitly defined covariance matrices is also provided in the output. The last portion of the directory information pertains to the resonance parameter uncertainty data. If resonance parameter uncertainty data are available, PUFF-III indicates that File 32 data are available for processing. In most cases, the directory print option will be used prior to processing the ENDF covariance data. By invoking the directory option, the code identifies the possible covariance matrices as well as the standard material data that are needed to process covariance matrices derived from ratio measurements. Once the directory information is obtained, the user can construct an input file for a specific application of interest.

The following reactions are needed to process LTY = 0 for 1125 – 2:
1. 16. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 91. 102. 103. 107.

The following reactions are needed to process LTY = 0 for 1125 – 3:
16. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 91. 102. 103. 107.

The following reactions are needed to process LTY = 0 for 1125 – 4:
51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 91.

Directory of ENDF File 31/33 Data for MAT: 1125
27 Explicitly Defined Covariances:

MAT1	MF1	MT1	MAT2	MF2	MT2
1125	33	1	1125	33	1
1125	33	2	1125	33	2
1125	33	3	1125	33	3
1125	33	4	1125	33	4
1125	33	16	1125	33	16
1125	33	51	1125	33	51
1125	33	52	1125	33	52
1125	33	53	1125	33	53
1125	33	54	1125	33	54
1125	33	55	1125	33	55
1125	33	56	1125	33	56
1125	33	57	1125	33	57
1125	33	58	1125	33	58
1125	33	59	1125	33	59
1125	33	60	1125	33	60
1125	33	61	1125	33	61
1125	33	62	1125	33	62
1125	33	63	1125	33	63
1125	33	64	1125	33	64
1125	33	65	1125	33	65
1125	33	66	1125	33	66
1125	33	67	1125	33	67
1125	33	68	1125	33	68
1125	33	91	1125	33	91
1125	33	102	1125	33	102
1125	33	103	1125	33	103
1125	33	107	1125	33	107

69 Implicitly Defined Covariances from LTY = 0 sub-subsections:

MAT1	MF1	MT1	MAT2	MF2	MT2
1125	33	2	1125	33	1
1125	33	2	1125	33	16
		•			
		•			
		•			
		•			
1125	33	4	1125	33	67
1125	33	4	1125	33	68
1125	33	4	1125	33	91
1125	33	2	1125	33	3
1125	33	2	1125	33	4
1125	33	3	1125	33	4

File 32 resonance parameter uncertainty data are available

Figure 5.4 Example directory information output

5.5 Energy Grid Information

A listing of the energy grids is provided in the output following the directory information. A complete description of the energy grid definitions is provided in Sect. 2.2.2.3. PUFF-III prints the energy information in descending order (i.e., high to low). An example of the printout of the energy-grid information is provided in Figure 5.5. Initially, the user grid structure is provided followed by the supergrid and cross-section grid structures.

```
user group structure contains-- 44 groups
 2.00000E+07 8.18730E+06 6.43400E+06 4.80000E+06 3.00000E+06 2.47900E+06
 2.35400E+06 1.85000E+06 1.40000E+06 9.00000E+05 4.00000E+05 1.00000E+05
 2.50000E+04 1.70000E+04 3.00000E+03 5.50000E+02 1.00000E+02 3.00000E+01
 1.00000E+01 8.10000E+00 6.00000E+00 4.75000E+00 3.00000E+00 1.77000E+00
 1.00000E+00 6.25000E-01 4.00000E-01  3.75000E-01  3.50000E-01  3.25000E-01
 2.75000E-01  2.5000E-01  2.25000E-01  2.00000E-01  1.50000E-01  1.00000E-01
 7.00000E-02  5.00000E-02 4.00000E-02  3.00000E-02  2.53000E-02  1.00000E-02
 7.50000E-03  3.00000E-03 1.00000E-05

0

supergroup structure contains-- 123 groups
 2.00000E+07 1.80000E+07 1.60000E+07 1.50000E+07 1.45000E+07 1.40000E+07
 1.35000E+07 1.29500E+07 1.25000E+07 1.20000E+07 1.15000E+07 1.10000E+07
 1.05000E+07 1.04000E+07 1.00000E+07 9.60000E+06 9.00000E+06 8.50000E+06
 8.18730E+06 8.13180E+06 8.00000E+06 7.50000E+06 7.42200E+06 7.00000E+06
 6.54510E+06 6.50000E+06 6.43400E+06 6.34520E+06 6.30000E+06 6.21630E+06
 6.10000E+06 6.01270E+06 6.00000E+06 5.80000E+06 5.77260E+06 5.61600E+06
 5.00000E+06 4.97930E+06 4.80000E+06 4.62440E+06 4.50000E+06 4.20000E+06
 4.05020E+06 4.03560E+06 4.00000E+06 3.84150E+06 3.80000E+06 3.75480E+06
 3.50000E+06 3.40000E+06 3.30000E+06 3.11390E+06 3.00000E+06 2.82370E+06
 2.75580E+06 2.60000E+06 2.49800E+06 2.47900E+06 2.40000E+06 2.35400E+06
 2.16920E+06 1.85000E+06 1.65000E+06 1.50000E+06 1.40000E+06 1.20000E+06
 1.00000E+06 9.00000E+05 8.50000E+05 7.50000E+05 6.60000E+05 5.00000E+05
 4.59310E+05 4.10000E+05 4.00000E+05 3.80000E+05 3.10000E+05 2.98000E+05
 2.95000E+05 2.90000E+05 1.00000E+05 5.60000E+04 5.00000E+04 3.30000E+04
 2.50000E+04 1.70000E+04 5.00000E+03 3.10000E+03 3.00000E+03 2.50000E+03
 6.00000E+02 5.50000E+02 1.00000E+02 5.00000E+01 3.00000E+01 1.00000E+01
 8.10000E+00 6.00000E+00 5.00000E+00 4.75000E+00 3.00000E+00 1.77000E+00
 1.00000E+00 6.25000E-01  4.00000E-01  3.75000E-01  3.50000E-01  3.25000E-01
 2.75000E-01  2.50000E-01  2.25000E-01  2.00000E-01  1.50000E-01  1.00000E-01
 7.00000E-02  5.00000E-02  4.00000E-02  3.00000E-02  2.53000E-02  2.00000E-02
 1.00000E-02  7.50000E-03  3.00000E-03  1.00000E-05

0

cross section structure contains-- 44 groups
 2.00000E+07 8.18730E+06 6.43400E+06 4.80000E+06 3.00000E+06 2.47900E+06
 2.35400E+06 1.85000E+06 1.40000E+06 9.00000E+05 4.00000E+05 1.00000E+05
 2.50000E+04 1.70000E+04 3.00000E+03 5.50000E+02 1.00000E+02 3.00000E+01
 1.00000E+01 8.10000E+00 6.0000E+00  4.75000E+00 3.00000E+00 1.77000E+00
 1.00000E+00 6.25000E-01  4.00000E-01  3.75000E-01  3.50000E-01  3.25000E-01
 2.75000E-01  2.50000E-01  2.25000E-01  2.00000E-01  1.50000E-01  1.00000E-01
 7.00000E-02  5.00000E-02  4.00000E-02  3.00000E-02  2.53000E-02  1.00000E-02
 7.50000E-03  3.00000E-03  1.00000E-05
```

Figure 5.5 Example energy-grid structure output

5.6 Calculated Correlation Matrices

The majority of the PUFF-III output is comprised of the calculated correlation matrices for the material of interest. The output for each correlation matrix is separated into two sections. In the first section, the first and second reactions of the matrix are identified, followed by the multigroup cross-section values and corresponding relative standard deviations. An example of the first section is provided in Figure 5.6. As shown in Figure 5.6, the subsequent matrix represents the correlation between the total cross section of material 1125 with itself. Prior to the correlation matrix, the multigroup cross sections are provided with the relative standard deviations. In addition, the energy boundaries of each energy group are provided in the output. In the second portion of the output, the correlation matrix is provided for reaction 1 of material 1 crossed with reaction 2 of material 2. An example of the correlation matrix output is provided in Figure 5.6. PUFF-III also evaluates the eigenvalues of the correlation matrix and categorizes the matrix based on the calculated eigenvalues.

1 material 1= 1125, reaction 1= 4 , material 2= 1125, reaction 2= 4

group	e high	e low	x-sec(1)	x-sec(2)	rel.s.d.(1)	rel.s.d.(2)
1	2.0000E+07	8.1873E+06	7.4080E-01	7.4080E-01	9.9574E-02	9.9574E-02
2	8.1873E+06	6.4340E+06	9.4732E-01	9.4732E-01	6.1968E-02	6.1968E-02
3	6.4340E+06	4.8000E+06	8.9214E-01	8.9214E-01	7.4444E-02	7.4444E-02
4	4.8000E+06	3.0000E+06	8.7261E-01	8.7261E-01	7.3450E-02	7.3450E-02
5	3.0000E+06	2.4790E+06	7.1755E-01	7.1755E-01	1.5112E-01	1.5112E-01
6	2.4790E+06	2.3540E+06	6.4984E-01	6.4984E-01	1.2751E-01	1.2751E-01
7	2.3540E+06	1.8500E+06	6.6509E-01	6.6509E-01	1.6055E-01	1.6055E-01
8	1.8500E+06	1.4000E+06	4.6389E-01	4.6389E-01	1.4929E-01	1.4929E-01
9	1.4000E+06	9.0000E+05	4.6921E-01	4.6921E-01	1.7464E-01	1.7464E-01
10	9.0000E+05	4.0000E+05	1.6618E-01	1.6618E-01	1.2734E-01	1.2734E-01
11	4.0000E+05	1.0000E+05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
12	1.0000E+05	2.5000E+04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
13	2.5000E+04	1.7000E+04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
14	1.7000E+04	30000E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
15	3.0000E+03	5.5000E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
16	5.5000E+02	1.0000E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
17	1.0000E+02	3.0000E+01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
18	3.0000E+01	1.0000E+01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
19	1.0000E+01	8.1000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
20	8.1000E+00	6.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
21	6.0000E+00	4.7500E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
22	4.7500E+00	3.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
23	3.0000E+00	1.7700E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
24	1.7700E+00	1.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
25	1.0000E+00	6.2500E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
26	6.2500E-01	4.0000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
27	4.0000E-01	3.7500E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
28	3.7500E-01	3.5000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
29	3.5000E-01	3.2500E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
30	3.2500E-01	2.7500E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
31	2.7500E-01	2.5000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
32	2.5000E-01	2.2500E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
33	2.2500E-01	2.0000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
34	2.0000E-01	1.5000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
35	1.5000E-01	1.0000E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
36	1.0000E-01	7.0000E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
37	7.0000E-02	5.0000E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
38	5.0000E-02	4.0000E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
39	4.0000E-02	3.0000E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
40	3.0000E-02	2.5300E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
41	2.5300E-02	1.0000E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
42	1.0000E-02	7.5000E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
43	7.5000E-03	3.0000E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
44	3.0000E-03	1.0000E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

Figure 5.6 Example multigroup cross-section values and relative standard deviations output

1 *** correlation matrix ***
column=material 1 row=material 2

0 column

row	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1	1000	65	3	3	2	3	2	3	2	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	65	1000	360	129	44	56	45	49	42	51	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	3	360	1000	416	60	77	62	68	58	70	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	3	129	416	1000	291	284	95	103	88	107	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	2	44	60	291	1000	895	81	88	75	91	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	3	56	77	284	895	1000	509	415	257	310	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	2	45	62	95	81	509	1000	772	436	527	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	3	49	68	103	88	415	772	1000	671	580	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	2	42	58	88	75	257	436	671	1000	603	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	3	51	70	107	91	310	527	580	603	1000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

0 column

row	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

WARNING
Correlation Matrix <1125, 4;1125, 4> is positive semidefinite
smallest eigenvalue: 0.0000E+00

Figure 5.7 Example correlation matrix output

5.7 Termination of Output File

The remaining portion of the output file identifies the completion of the calculation. Once the last correlation matrix is printed, a "processing completed" message is printed. The CPU time for calculating the covariance matrices is provided in seconds followed by the total CPU time for the problem. If the problem has executed successfully, the final message, "PUFF-III has terminated normally," is printed in the last line of the output file. An example of the termination information is provided in Figure 5.8.

```
1              ******************************
               *                            *
               *  puff processing completed *
               *                            *
               ******************************
1

CPU time for calculating  covariance matrices:   89.00 seconds
Total CPU time required for  PUFF-III:   90.00 seconds

PUFF-III has terminated normally
```

Figure 5.8 Example termination output

6 MESSAGES

PUFF-III provides warning and error messages that indicate problems with program execution. The warning messages may indicate a possible error; however, the code can continue the calculation despite the message. The user should evaluate the warning message to determine if a problem exists. When an error is encountered, the code prints the appropriate message and stops execution if the error is too severe. The warning and error messages that are presented in this section may provide an underscore to indicate the appropriate data.

6.1 Warning Messages

SCOPE:

Warning: no COVERX output unit specified. COVERX output will be in binary form on unit 1.

This message indicates that a COVERX output file was not specified in the input file. If a unit number was specified, this message may indicate a problem in another location in the input file.

LUMPER:

Warning: cross section not found for mat = _____ mt = _____ .

Lumped reaction covariance data are specified in File 33; however, LUMPER could not locate the noted partial cross sections for the lumped reaction. The program will continue, but the code alerts the user to the data deficiency.

Cross sections for mat = _____ lumped reaction cross section _____ are all zero. These cross sections will not be included in covariance matrix.

This message is intended to alert the user to the data deficiency for the lumped reaction cross section. To correct this problem, the appropriate cross sections must be provided.

REDUN:

No File 33 reactions on ENDF tape

The input requested File 33 processing, but no File 33 reactions are present on the ENDF uncertainty file.

SUMMER:

Cannot construct redundant cross section for MT: _____ . The constituents are not on the cross-section tape.

PUFF-III has attempted to construct the noted cross section by summing the partial reactions; however, all of the partial reactions could not be located on the tape. This message is intended to alert the user of the data deficiency.

DANNY:

Cross section not found for mat = _____ mt = _____ .

The message indicates that the code cannot locate the noted cross sections on the master library or as input.

Rel. std. dev. not found for mat = _____ mt = _____ .

The relative standard deviations cannot be located for the noted material and reaction. The calculation will continue, but the results may not be correct.

****error*** standard x-sec r.s.d. not found mat2 = _____ mt2 = _____ .*

The relative standard deviations for the standard material cannot be located for the noted material and reaction. The calculation will continue, but the results may not be correct.

REDUCE:

error: sum of the group flux = 0 in reduce.

REDUCE collapses the covariance matrices from the supergrid to the super-user grid. This message indicates that there is a problem in the collapsing procedure.

HQR:

Too many iterations in hqr

HQR is used to calculate the eigenvalues of the correlation matrix. This message indicates that the eigenvalue calculation has not converged. Consequently, the eigenvalues may not be correct for the corresponding correlation matrix.

6.2 Error Messages

PUFFIII:

unable to get _____ words for PUFF-III.

Subroutine ALOCAT is unable to get the requested storage for execution. On unix machines, the stacksize may need to be increased for the problem.

SCOPE:

****Error***: IXS flag indicates read AMPX master library but no master library is specified.*

This message indicates that an inconsistency exists in the input file. If IXS = -11, an AMPX master library must be provided.

Storage exceeded --- used = _____ assigned = _____ .

This message indicates that additional storage space is needed. Increase the core allocation in the 0$ block and resubmit the problem.

Common /data/ array dat storage exceeded --- used = _____ assigned = _____ .

This message indicates that a problem exists in the data common block.

DELTA:

File not found for mat = _____ .

This message is provided by subroutine DELTA and indicates that the ENDF uncertainty data could not be located for the material specified.

File _____ not found for standard mat = _____ mt = _____ .

PUFF-III could not locate the standard uncertainty data for the material specified on the file.

Error: this version of PUFF-III cannot process LTY = _____ with WEI = _____.

The ENDF/B-VI formats permit the overlap of energy ranges for different LTY ≥ 1 sub-subsections. At the time of development, no evaluations had overlapping energy ranges for LTY values ≥ 1. Consequently, PUFF-III does not process these NC sub-subsections.

COCO:

Need at least _____ more words of storage

The storage limit has been exceeded. Increase the core allocation in the 0$ block and resubmit the problem.

RUSEGY:

Stop 123

RUSEGY sets an internal limit of 300 points in the supergrid structure. This stop code indicates that the internal limit has been exceeded.

EBERR:

Error: user grid lower boundary is _____ , but uncertainty data have energies below this value.

EBERR combines two data vectors into a single vector. This message indicates that the lower energy bound of the uncertainty data is outside the range of the user grid. The user grid should be modified accordingly.

Error: user grid has upper energy of _____ , but uncertainty data have energies above this value.

EBERR combines two data vectors into a single vector. This message indicates that the upper energy bound of the uncertainty data is outside the range of the user grid. The user grid should be modified accordingly.

MASTER:

Storage exceeded --- used = _____ assigned = _____ .

This message indicates that additional storage space is needed. Increase the core allocation in the 0$ block and resubmit the problem.

LUMPER:

Storage exceeded in lumper --- used = _____ assigned = _____ .

This message indicates that additional storage space is needed for LUMPER. Increase the core allocation in the 0$ block and resubmit the problem.

WEIGHT:

Error on weighting --- total x. sec. not found.

This message occurs if IWT = 2, and the total cross section is not provided.

DANNY:

Storage exceeded --- used = _____ assigned = _____ .

This message indicates that additional storage space is needed. Increase the core allocation in the 0$ block and resubmit the problem.

Error LB = 8 NI sub-subsection is specified for the covariance between MAT: _____ MT: _____ and MAT1: _____ MT1: _____.

This message indicates that LB = 8 is specified for a cross-covariance calculation. This violates the current ENDF/B-VI rules.[3]

Stop 9333

DANNY limits the number of LTY = 3 sub-subsections for processing (ibub). If ibub exceeds 20 the code stops execution.

ni15 equals _____ but the number of covariances equals _____ .

This message indicates that the internal counter of the number of covariance matrices on I15 has been exceeded.

CROSSMT:

The number of pairs of points is equal to _____ so you need to increase the dimension of know in sub. crossmt to at least this value.

CROSSMT limits the number of reactions for an LTY = 0 sub-subsection to 50. This message indicates that the array size has been exceeded.

ni57 equals _____ but the number of cross covariances equals _____ .

This message indicates that the internal counter of the number of cross-covariance matrices on I57 has been exceeded.

RES:

File 32 not found for mat = _____ .

PUFF-III could not locate the File 32 data for the noted material.

Resonance energy is _____ which is below the 0.414 eV cut-off energy and therefore this resonance will not be processed.

This is a historical message that is present in earlier versions of PUFF. Resonance energies below 0.414 eV are not included in the contribution to the covariance matrix.

7 REFERENCES

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2. J. D. Smith III, *Processing ENDF/B-V Uncertainty into Multigroup Covariance Matrices*, ORNL/TM-7221, Union Carbide Corp., Oak Ridge National Lab., June 1980.

3. *ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6*, BNL-NCS-44945, Rev. 10/91 (ENDF/B-VI), Brookhaven National Laboratory, October 1991.

4. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation,* NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols. I, II, and III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

5. Letter Correspondence, B. L. Broadhead, ORNL, to D. W. Muir, LANL, November 17, 1983.

6. W. H. Press, W. T. Vetterling, S. A. Teukolsky and B. P. Flannery, *Numerical Recipes in FORTRAN The Art of Scientific Computing*, Second Edition, Cambridge University Press, 1992.

APPENDIX A

ALPHABETICAL INDEX OF SUBROUTINES

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ALPHABETICAL INDEX OF SUBROUTINES

This section provides an alphabetical index of the subroutines used by PUFF-III. For each entry, a list of subroutines that call the given subroutine is provided, as well as a list of subroutines called by the given subroutine.

Table A.1 Index of subroutines

Subroutine	Calling subroutine	Called subroutine
ADDVAR	DANNY	
ALOCAT	PUFFIII	SCOPE
CHECKER	DANNY	ELMHES HQR
CLOSDA	PUFFIII	
COCO	SCOPE	
COLAPS	SETUP	
CONTIN	DELTA	
CONTRI	DANNY	
CORREL	DANNY	
COVAR	DANNY	
COVX2	SCOPE	PCOV2
CROSSMT	DANNY SUBCALC	DART FINDER

Table A.1 (continued)

Subroutine	Calling subroutine	Called subroutine
DANNY	SCOPE	ADDVAR CHECKER CONTRI CORREL COVAR CROSSMT DART FLUXER INVT INVTDIAG LIMITDIAG LIMITM OPENDA PUFF REDUCE RELCOV REPOZ RES RSDEV SUBMAT SUMMF WRITCO WRITCORR WOTMT
DART	CROSSMT DANNY REDUCE RES SUBMAT WRITCO	REED RITE
DELTA	SCOPE	CONTIN LIST
EBERR	RUSEGY	
ELMHES	CHECKER	
FFPACK	FFREAD	
FFREAD	FIDAS	FFPACK Y0TRNS

Table A.1 (continued)

Subroutine	Calling subroutine	Called subroutine
FIDAS	FIXFOR MASTER PUFFIII RUSEGY WEIGHT	FFREAD
FINDER	CROSSMT SUBMAT	
FIXFOR	SCOPE	FIDAS
FLUXER	DANNY SETUP	
HQR	CHECKER	
INVT	DANNY REDUCE	
INVTDIAG	DANNY	
JSTIME	PUFFIII SCOPE	
LIMITDIAG	DANNY	
LIMITM	DANNY	
LIST	DELTA	
LUMPER	SCOPE	
MASTER	SCOPE	FIDAS RED PPPP
MESAGE	PUFFIII	
MTZ	SUMMER	
OPENDA	DANNY	
OPNFIL	PUFFIII SCOPE	
PCOV2	COVX2	
PPPP	MASTER	
PUFF	DANNY	PUFF5

Table A.1 (continued)

Subroutine	Calling subroutine	Called subroutine
PUFF5	PUFF	
PUFFIII		ALOCAT CLOSDA FIDAS JSTIME MESAGE OPNFIL
RED	MASTER	
REDUCE	DANNY	DART INVT
REDUN	SCOPE	SUMMER
REED	DART	
RELCOV	DANNY	
REPOZ	DANNY SUBCALC SUBMAT	
RES	DANNY	DART
RITE	DART	
RSDEV	DANNY	
RUSEGY	SCOPE	EBERR FIDAS
RXSEC	SUMMER	
SCOPE	ALOCAT	CLOSDA COCO COVX2 DANNY DELTA FIXFOR JSTIME LUMPER MASTER OPNFIL REDUN RUSEGY SETUP WEIGHT

Table A.1 (continued)

Subroutine	Calling subroutine	Called subroutine
SETUP	SCOPE	COLAPS FLUXER
SUBCALC	SUBMAT	CROSSMT REPOZ
SUBMAT	DANNY	DART FINDER REPOZ SUBCALC
SUMMER	REDUN	MTZ RXSEC
SUMMF	DANNY	
WEIGHT	SCOPE	FIDAS
WOTMT	DANNY	
WRITCO	DANNY	DART
WRITCORR	DANNY	
Y0TRNS	FFREAD	

APPENDIX B

SAMPLE PROBLEMS

APPENDIX B

SAMPLE PROBLEMS

This appendix contains sample problems that demonstrate the procedures to execute PUFF-III. Four sample problems are presented that demonstrate the features of PUFF-III. In particular, sample input files are presented for ^{23}Na, ^{241}Pu and ^{235}U. Because the sample problems were developed in a unix environment, the input for each sample problem is provided using lower case letters. In addition, the FIDO input method, which is described in Appendix C, is used to specify the input options for each sample problem. Because PUFF-III is typically used to process one or two isotopes at a time, using an abbreviated AMPX master library that only has the desired isotopes may be more efficient. In order to create a condensed master library, the AMPX module AJAX can be used to read the desired cross-section data from a larger AMPX library and write the selected data to a different unit. The problem-specific cross-section library can be used in the subsequent covariance calculations.

Sample Problem 1:

The first sample case considers the ENDF/B-VI evaluation for ^{23}Na (MAT = 1125), and the objective of the sample problem is to process the available uncertainty information for ^{23}Na using the following sequence of operations:

Step 1:

Prior to processing the covariance information, the directory feature of PUFF-III is used to identify the covariance information on the ENDF tape. A directory of the available covariance information for ^{23}Na can be obtained with the following input:

```
0$$ 8
1$$ a6 1125 e t
```

In the above input, the ENDF uncertainty file is located on unit 8 and identified in the 0$ block. Because only a directory of the uncertainty information will be produced, the MAT number is the only entry required in the 1$ block.

Step 2:

Based on the results from Step 1 (refer to Figure 5.4 of Sect. 5), ^{23}Na has resonance parameter uncertainty information as well as cross-section data uncertainty (i.e., Files 32 and 33, respectively). In File 33, there are 27 explicitly defined covariance matrices with an additional 69 covariance matrices that are implicitly defined from the LTY = 0 sub-subsections. All of the possible covariance matrices can be calculated with the following input:

```
1$$ 1 0 0 4 8 1125 -12 -11 1 1 0 1 3r0 -1 e t
coverx file for na23
```

In the above input, the AMPX master library and ENDF uncertainty files are located on units 4 and 8, respectively. The -12 entry in the 1$ block selects the 44-group structure for the final output, and the -11 entry specifies that the input cross-section group structure is obtained from the AMPX master library. The ninth entry in the 1$ block specifies that $1/E$ weighting is used to collapse the matrices to the user-group

structure, and the tenth entry specifies that AMPX cross sections are used in the calculation. By setting JOPT1 equal to zero and JOPT2 equal to 1 in the 1$ block, the File 33 and File 32 data on unit 8 will be processed. Because NMT is set to -1 in the sixteenth entry of the 1$ array, all available covariance matrices in File 33 will be generated.

Sample Problem 2:

The second sample case considers the ENDF/B-VI evaluation for ^{241}Pu (MAT = 9443).

Step 1:

Following the procedure of the previous example, a directory of the ^{241}Pu uncertainty information can be obtained with the following input file:

```
0$$ 8
1$$ a6 9443 e t
```

The directory for ^{241}Pu has the following information:

Note: LTY = 1; the covariance data for 9443 -- 18 are derived from material 9228 -- 18

Note: LTY = 2; data provided for the covariance of 9443 -- 18 with the standard: 9228 -- 18

Directory of ENDF File 31/33 Data for MAT: 9443
10 Explicitly Defined Covariances:

MAT1	MF1	MT1	MAT2	MF2	MT2
9443	31	452	9443	31	452
9443	31	452	1380	31	452
9443	31	452	1390	31	452
9443	31	452	1395	31	452
9443	31	452	1398	31	456
9443	31	452	1399	31	452
9443	33	18	9443	33	18
9443	33	18	9443	33	102
9443	33	18	9228	33	18
9443	33	102	9443	33	102

No Implicitly Defined Covariances

No File 32 resonance parameter uncertainty data.

Based on the directory output, the ^{241}Pu fission cross section is derived by ratio measurements to the fission cross section for ^{235}U (MAT = 9228). As a result, there is a LTY = 1 sub-subsection and a LTY = 2 sub-subsection in File 33 for ^{241}Pu, and there should be a corresponding LTY = 3 sub-subsection defined in File 33 for ^{235}U. Before PUFF can process MAT = 9443, the standard deviations in the ^{235}U fission cross-section data must be obtained.

Step 2:

A directory of the ^{235}U uncertainty information can be obtained with the following input file:

```
0$$ 9
1$$ a6 9228 e t
```

The directory for ^{235}U has the following information:

Note: LTY = 3; the following covariance data are derived from this material 9437 -- 18

Note: LTY = 3; the following covariance data are derived from this material 9440 -- 18

Note: LTY = 3; the following covariance data are derived from this material 9443 -- 18

Note: LTY = 3; the following covariance data are derived from this material 9446 -- 18

Note: LTY = 3; the following covariance data are derived from this material 9543 -- 18

Directory of ENDF File 31/33 Data for MAT: 9228
13 Explicitly Defined Covariances:

MAT1	MF1	MT1	MAT2	MF2	MT2
9228	31	452	9228	31	452
9228	31	452	1380	31	452
9228	31	452	1381	31	452
9228	31	452	1390	31	452
9228	31	452	1398	31	456
9228	31	452	1399	31	452
9228	33	18	9228	33	18
9228	33	18	9437	33	18
9228	33	18	9440	33	18
9228	33	18	9443	33	18
9228	33	18	9446	33	18
9228	33	18	9543	33	18
9228	33	102	9228	33	102

10 Implicitly Defined Covariances from LTY = 3 sub-subsections:

MAT1	MF1	MT1	MAT2	MF2	MT2
9437	33	18	9440	33	18
9437	33	18	9443	33	18
9437	33	18	9446	33	18
9437	33	18	9543	33	18
9440	33	18	9443	33	18
9440	33	18	9446	33	18
9440	33	18	9543	33	18
9443	33	18	9446	33	18
9443	33	18	9543	33	18
9446	33	18	9543	33	18

No File 32 resonance parameter uncertainty data.

Based on the directory information for ^{235}U, there is an LTY = 3 sub-subsection that describes the covariance between the ^{235}U fission cross section and the ^{241}Pu fission cross section.

Step 3:

In order to process the ^{241}Pu covariance data, the fission covariance matrix for ^{235}U must be generated. The following input is used to calculate <9228,18; 9228, 18>:

```
1$$ -1 0 0 4 9 9228 -12 -11 1 1 0 4r0 1 0 0 t
4** 9228 18 t
coverx file for u235
```

In the above input, a single reaction pair (i.e., MAT = 9228 and MT =18) is specified in the 4* array. For this sample problem, the AMPX master library that has the ^{235}U and ^{241}Pu cross-section data is located on unit 4. After calculating the ^{235}U fission covariance matrix, the fission cross-section standard deviations are stored on unit 16.

Step 4:

The standard deviations from the previous step are used as input for the ^{241}Pu covariance data calculation. In particular, the ^{235}U fission cross section standard deviations, which are stored on unit 16 in the previous step, are moved to a different unit that will be designated as the input standard deviations in the ^{241}Pu input file. The following input is used to calculate all of the File 33 covariance matrices for ^{241}Pu:

```
1$$ -1 30 9 4 8 9443 -12 -11 1 1 0 4r0 -1 0 0 t
coverx file for pu241
```

In the above input, the ^{235}U fission cross-section standard deviations are located on unit 30, and the ENDF uncertainty files for ^{235}U and ^{241}Pu are located on units 9 and 8, respectively. Since NMT is set to -1 in the sixteenth entry of the 1$ array, all of the File 33 covariance matrices are calculated.

Sample Problem 3:

Based on the ^{235}U covariance data directory from Step 2 of Sample Problem 2, a cross-material-covariance matrix exists between the ^{235}U fission cross section and the ^{241}Pu fission cross section (i.e., <9228, 18; 9443, 18>). This covariance matrix is defined by an LTY = 3 sub-subsection in File 33 for ^{235}U. Two approaches can be used to obtain the cross-material-covariance matrix. In the first approach, the results from the previous sample problem can be used to obtain the desired covariance matrix. By processing the covariance data for ^{241}Pu in Sample Problem 2, PUFF-III calculates the cross-material-covariance matrix between the ^{241}Pu fission cross section and the ^{235}U fission cross section (i.e., <9443, 18; 9228, 18>). Based on the results from Sample Problem 2, the matrix <9228, 18; 9443, 18> can be obtained by writing a short program to read and transpose the matrix <9443, 18; 9228, 18>. To avoid transposing the covariance matrix from Sample Problem 2, an alternative approach is available to process the matrix defined by the LTY = 3 sub-subsection of a standard material. The following sequence of steps can be used to calculate the covariance matrix <9228, 18; 9443, 18>.

Step 1:

Before the cross-material-covariance matrix between the ^{235}U fission cross section and the ^{241}Pu fission cross section can be calculated, the standard deviations of the ^{241}Pu fission cross-section data must be calculated. However, the covariance data for the ^{241}Pu fission cross section are defined in terms of the ^{235}U covariance data by an LTY = 1 sub-subsection in File 33 of the ^{241}Pu data. Consequently, the covariance matrix for the ^{235}U fission cross section must be calculated to obtain the standard deviations in the ^{235}U fission cross-section data. The input file from Step 3 of Sample Problem 2 can be used to calculate the matrix <9228,18; 9228, 18>.

Step 2:

As noted in the previous step, the standard deviations in the ^{241}Pu fission cross-section data are needed in the subsequent calculation. Therefore, the standard deviations from Step 1 are used as input for the ^{241}Pu covariance data calculation. Unit 16 from the previous step is moved to a different unit that will be designated as the input ^{235}U standard deviations in the ^{241}Pu input file. The following input is used to calculate the fission covariance matrix for ^{241}Pu:

```
1$$ -1 30 9 4 8 9443 -12 -11 1 1 0 4r0 1 0 0 t
4** 9443 18 t
coverx file for pu241
```

In the above input, the ^{235}U fission cross-section standard deviations are located on unit 30, and the ENDF uncertainty files for ^{235}U and ^{241}Pu are located on units 9 and 8, respectively.

Step 3:

In the final step of the calculation sequence, the ^{235}U data are processed again to obtain the cross-material-covariance matrix <9228, 18; 9443, 18>. The following input is used to calculate the covariance matrix between the ^{235}U fission cross section and the ^{241}Pu fission cross section:

```
1$$ -1 31 0 4 9 9228 -12 -11 1 1 0 4r0 2 0 0 t
4** 9228 9443 2r18 t
coverx file for u235
```

The ^{241}Pu standard deviations from Step 2 are located on unit 31 in the above input file, and the ^{235}U ENDF uncertainty file is located on unit 9. In the preceding input file, two MAT-MT reaction pairs are specified in the 4* array (i.e., 9228 18 and 9443 18).

Sample Problem 4:

Based on the directory information for ^{235}U in Step 2 of Sample Problem 2, covariance information is available for the neutron multiplicity data. In particular, File 31 defines the covariance matrix for ν_t. The following input file can be used to calculate the covariance matrix for MT = 452:

```
1$$ -1 0 0 4 9 9228 -12 -11 1 1 1 4r0 1 0 0 t
4** 9228 452 t
coverx file for u235
```

In the preceding input, the AMPX master library and the ENDF uncertainty data are located on units 4 and 9, respectively. Since File 31 is to be processed, JOPT1 is set equal to 1 in the eleventh entry of the 1$ array. To obtain the covariance matrix for ν_t, the appropriate MAT-MT reaction pair is specified in the 4* array.

APPENDIX C

FIDO INPUT

APPENDIX C

FIDO INPUT

C.1 INTRODUCTION

The FIDO input method is specially devised to allow entering or modifying large data arrays with minimum effort. Advantage is taken of patterns of repetition or symmetry wherever possible. The FIDO system was patterned after the input method used with the FLOCO coding system at Los Alamos and was first applied to the DTF-II code. Since that time, numerous features requested by users have been added, a free-field option has been developed, and the application of FIDO has spread to innumerable codes.

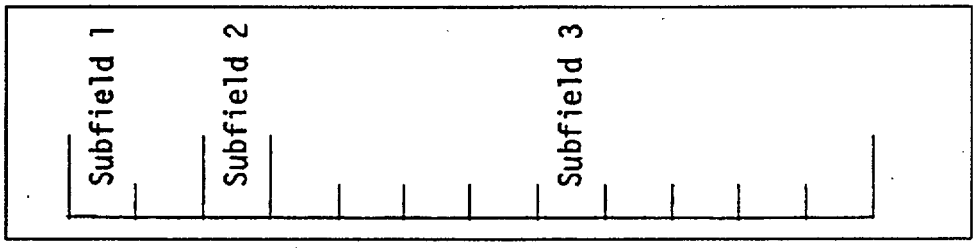
The data are entered in units called "arrays." An array comprises a group of contiguous storage locations that are to be filled with data at the same time. These arrays usually correspond on a one-to-one basis with FORTRAN arrays used in the program. A group of one or more arrays read with a single call to the FIDO package forms a "block," and a special delimiter is required to signify the end of each block. Arrays within a block may be read in any order with respect to each other, but an array belonging to one block must not be shifted to another. The same array can be entered repeatedly within the same block. For example, an array could be filled with "0" using a special option, and then a few scattered locations could be changed by reading in a new set of data for that array. If no entries to the arrays in a block are required, the delimiter alone satisfies the input requirement.

Three major types of input are available: fixed-field input, free-field input, and user-field input.

C.2 FIXED-FIELD INPUT

The fixed-field input option is documented here for completeness. **The use of fixed-field input is NOT recommended. Use the free-field input option documented in Sect. C.3.**

Each card is divided into six 12-column data fields, each of which is divided into three subfields. The following sketch illustrates a typical data field. The three subfields always comprise 2, 1, and 9 columns, respectively.



To begin the first array of a block, an array originator field is placed in any field on a card:

Subfield 1: An integer array identifier <100 specifying the data array to be read in.

Subfield 2: An array-type indicator:
"$" if the array is integer data
"*" if the array is real data
"#" if the array is double-precision data

Subfield 3: Blank

Data are then placed in successive fields until the required number of entries has been accounted for. A sample data sheet shown in Table C.1 illustrates this point.

In entering data, it is convenient to think of an "index" or "pointer" as a designator that is under the control of the user and which specifies the position in the array into which the next data entry is to go. The pointer is always positioned at array location #1 by entering the array originator field. The pointer subsequently moves according to the data operator chosen. Blank fields are a special case in that they do not cause any data modification and do not move the pointer.

A data field has the following form:

Subfield 1: The data numerator, an integer <100. We refer to this entry as N_1 in the following discussion.

Subfield 2: One of the special data operators listed below.

Subfield 3: A nine-character data entry, to be read in F9.0 format. It will be converted to an integer if the array is a "$" array or if a special array operator such as Q is being used. Note that an exponent is permissible but not required. Likewise, a decimal is permissible but not required. If no decimal is supplied, it is assumed to be immediately to the left of the exponent, if any; and otherwise to the right of the last column. This entry is referred to as N_3 in the following discussion.

A list of data operators and their effect on the array being input follows:

"Blank" indicates a single entry of data. The data entry in the third subfield is entered in the location indicated by the pointer, and the pointer is advanced by one. However, an entirely blank field is ignored.

"+" or "–" indicates exponentiation. The data entry in the third field is entered and multiplied by $10^{\pm N_1}$, where N_1 is the data numerator in the first subfield, given the sign indicated by the data operator itself. The pointer advances by one. In cases where an exponent is needed, this option allows the entering of more significant figures than the blank option.

"&" has the same effect as "+".

"R" indicates that the data entry is to be repeated N_1 times. The pointer advances by N_1.

"I" indicates linear interpolation. The data numerator, N_1, indicates the number of interpolated points to be supplied. The data entry in the third subfield is entered, followed by Nj interpolated entries equally spaced between that value and the data entry found in the third subfield of the next nonblank field. The pointer is advanced by $N_1 + 1$. The field following an "I" field is than processed normally, according to its own data

Table C. 1 General example of FIDO input

Name General Example of FIDO Input Charge _____ Date _____ Page _____

	IDENTIFICATION	REMARKS (DO NOT PUNCH)
1 1 $		Begin the 1$ array, fixed-field, integral
13 1		Enter 1
25 F 2		Fill array with 2
37 2 *		Begin the 2* array fixed-field, real
49 1 . 2 3 4	73 80	Enter 1.234
61 1 2 . 3 4 - 1	1 0	" "
1 5 - 1 2 3 4 + 0 2		" "
13 3 - 1 2 3 4		" "
25 7		" 7.0
37		A blank field is always ignored
49 T	73 80	Terminate this block
61	2 0	No entries may follow T on a card
1 3 *		Begin 3* array, fixed-field real
13 9 I 0		Enter 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 10, 10
25 3 R 1 0		as real numbers
37 3 * * 1 0 S 1 0		Repeat 3* in free-field, skip
49 1 1 1 2	73 80	to 11th entry, correct sequence to
61	3 0	--- 9, 10, 11, 12
1 4 * * 2 I 1 4 . 0		Begin 4* array, free-field, real
13 2 Q 4		Enter 1, 2, 3, 4, 1, 2, 3, 4, 1, 2, 3, 4
25 E		End reading this array; remainder of array unchanged.
37 T		Terminate this block
49	73 80	
61	4 0	

R - REPEAT I - INTERPOLATE S - SKIP T - TERMINATE

operator. The "I" entry is especially valuable for specifying a spatial mesh. In "$" arrays, interpolated values will be rounded to the nearest integer.

"L" indicates logarithmic interpolation. The effect is the same as that of "I" except that the resulting data are evenly separated in log-space. This feature is especially convenient for specifying an energy mesh.

"Q" is used to repeat sequences of numbers. The length of the sequence is given by the third subfield, N_3. The sequence of N_3 entries is to be repeated N_1 times. The pointer advances by N_1*N_3. If either N_1 or N_3 is 0, then a sequence of $N_1 + N_3$ is repeated one time only, and the pointer advances by $N_1 + N_3$. This feature is especially valuable for geometry specification.

The "N" option has the same effect as "Q," except that the order of the sequence is reversed each time it is entered. This feature is valuable for the type of symmetry possessed by S_n quadrature coefficients.

"M" has the same effect as "N," except that the sign of each entry in the sequence is reversed each time the sequence is entered. For example, the entries

1 2 3 2M2

would be equivalent to

1 2 3 -3 -2 2 3.

This option is also useful in entering quadrature coefficients.

"Z" causes $N_1 + N_3$ locations to be set at 0. The pointer is advanced by $N_1 + N_3$.

"C" causes the position of the last array entered to be printed. This is the position of the pointer, less 1. The pointer is not moved.

"O" causes the print trigger to be changed. The trigger is originally off. Successive "O" fields turn it on and off alternately. When the trigger is on, each card image is listed as it is read.

"S" indicates that the pointer is to skip N_1 positions leaving those array positions unchanged. If the third subfield is blank, the pointer is advanced by N_1. If the third subfield is nonblank, that data entry is entered following the skip, and the pointer is advanced by $N_1 + 1$.

"A" moves the pointer to the position, N_3 specified in the third subfield.

"F" fills the remainder of the array with the datum entered in the third subfield.

"E" skips over the remainder of the array. The array length criterion is always satisfied by an E, no matter how many entries have been specified. No more entries to an array may be given following an "E," except that data entry may be restarted with an "A."

The reading of data to an array is terminated when a new array origin field is supplied, or when the block is terminated. If an incorrect number of positions has been filled, an error edit is given; and a flag is set which will

later abort execution of the problem. FIDO then continues with the next array if an array origin was read. Otherwise, control is returned to the calling program.

A block termination consists of a field having "T" in the second subfield. Entries following "T" on a card are ignored, and control is returned from FIDO to the calling program.

Comment cards can be entered within a block by placing an apostrophe (') in column 1. Then columns 2–80 will be listed, with column 2 being used for printer carriage control. Such cards have no effect on the data array or pointer.

C.3 FREE-FIELD INPUT

With free-field input, data are written without fixed restrictions as to field and subfield size and positioning on the card. The options used with fixed-field input are available, although some are sightly restricted in form. In general, fewer data cards are required for a problem, the interpreting print is easier to read, a card listing is more intelligible, the cards are easier to keypunch, and certain common keypunch errors are tolerated without affecting the problem. Data arrays using fixed- and free-field input can be intermingled at will within a given block,

The concept of three subfields per field is still applicable to free-field input; but if no entry for a field is required, no space for it need be left. Only columns 1-72 may be used, as with fixed-field input. A field may not be split across cards.

The array originator field can begin in any position. The array identifiers and type indicators are used as in fixed-field input. The type indicator is entered twice to designate free-field input (i.e., "$$," "**," or "##"). The blank third subfield required in fixed-field input is not required. For example,

```
31**
```

indicates that array 31, a real-data array, will follow in free-field format.

Data fields may follow the array origin field immediately. The data field entries are identical to the fixed-field entries with the following restrictions:

1. Any number of blanks may separate fields, but at least one blank must follow a third subfield entry if one is used.

2. If both first- and second-subfield entries are used, no blanks may separate them (i.e., 24S, but not 24 S).

3. Numbers written with exponents must not have imbedded blanks (i.e., 1.0E+4, 1.0-E4, 1.0+4, or even 1+4, but *not* 1.0 E4). A zero should never be entered with an exponent. For example, 0.00-5 or 0.00E-5 will be interpreted as -5×10^{-2}.

4. In third-subfield data entries only 9 digits, including the decimal but not including the exponent field, can be used (i.e., 123456.89E07, but *not* 123456.789E07).

5. The Z entry must be of the form: 738Z, *not* Z738 or 738 Z.

6. The + or - data operators are not needed and are not available.

7. The Q, N, and M entries are restricted: 3Q4, 1N4, M4, but *not* 4Q, 4N, or 4M.

C.4 USER-FIELD INPUT

If the user follows the array identifier in the array originator field with the character "U" or "V," the input format is to be specified by the user. If "U" is specified, the FORTRAN FORMAT to be used must be supplied in columns 1–72 of the next card. The format must be enclosed by the usual parentheses. Then the data for the entire array must follow on successive cards. The rules of ordinary FORTRAN input as to exponents, blanks, etc., apply. If the array data do not fill the last card, the remainder must be left blank.

"V" has the same effect as "U," except that the format read in the last preceding "U" array is used.

C.5 CHARACTER INPUT

If the user wishes to enter character data into an array, at least three options are available. The user may specify an arbitrary format using a "U" and reading in the format. The user may follow the array identifier by a "/". The next two entries into subfield 3 specify the beginning and ending indices in the array into which data will be read. The character data are then read starting with the next data card in an 18A4 format.

Finally, the user may specify the array as a free-form "*" array and then specify the data entries as "nH" character data where n specifies how many characters follow H.

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10. SUPPLEMENTARY NOTES
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11. ABSTRACT *(200 words or less)*

PUFF-III is an extension of the previous PUFF-II code that was developed in the 1970s and early 1980s. The PUFF codes process the Evaluated Nuclear Data File (ENDF) covariance data and generate multigroup covariance matrices on a user-specified energy grid structure. Unlike its predecessor, PUFF-III can process the new ENDF/B-VI data formats. In particular, PUFF-III has the capability to process the spontaneous fission covariances for fission neutron multiplicity. With regard to the covariance data in File 33 of the ENDF system, PUFF-III has the capability to process short range variance formats as well as the lumped reaction covariance data formats that were introduced in ENDF/B-V. In addition to the new ENDF formats, a new directory feature is now available that allows the user to obtain a detailed directory of the uncertainty information in the data files without visually inspecting the ENDF data. Following the correlation matrix calculation, PUFF-III also evaluates the eigenvalues of each correlation matrix and tests each matrix for positive definiteness. Additional new features are discussed in the manual. With the release of PUFF-III, a new and improved covariance processing code is available to process ENDF covariance formats through Version VI.

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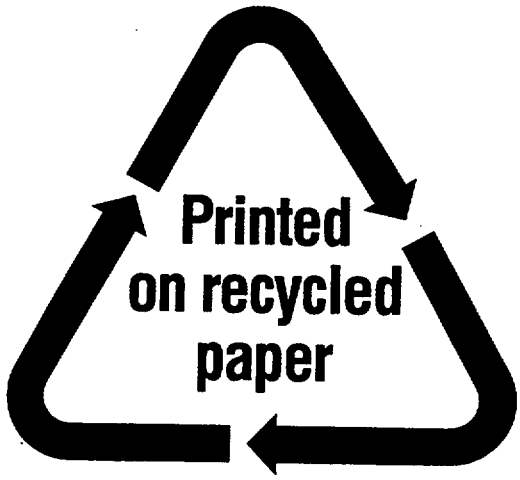

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