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Processing ENDF/B-V Uncertainty Data into Multigroup Covariance Matrices

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PROCESSING ENDF/B-V UNCERTAINTY DATA INTO MULTIGROUP COVARIANCE MATRICES*

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ABSTRACT

The purpose of this work is to develop and demonstrate the capability of processing Evaluated Nuclear Data File, system B, version five (ENDF/B-V) uncertainty data into multigroup covariance matrices. These covariances may then be folded with sensitivity coefficients to obtain uncertainties in selected integral parameters such as K-effective and breeding ratio.

The project consisted of separating the previous uncertainty processor (PUFF) from the basic nuclear data cross section processor (MINX), updating the uncertainty processor to the ENDF/B-V format, programming the processor for new uncertainty data, and demonstrating the processor capabilities by producing a multigroup covariance library. These capabilities were verified in various ways including hand calculations and comparisons with other known results.

A computer code named PUFF-II was written to perform the task described above. The code is capable of processing all uncertainty data currently entered in ENDF/B-V. The only limitation of the code is the treatment of uncertainties in resonance data.

CHAPTER I

INTRODUCTION

The basic nuclear data in the Evaluated Nuclear Data Files System B (ENDF/B) has been broadened and improved upon for many years, by new discoveries, better understanding, and improved technical capabilities. However, improvements in ENDF/B data are still needed.[1] Specifically, it s now evident that some means must be developed to indicate just how good the basic nuclear data are. This measure of the goodness of data has been to include estimated uncertainties in the evaluated microscopic data in ENDF/B files in a standard manner. These uncertainty files, after processing, may be used in conjunction with sensitivity analysis to allow for propagation of uncertainties in basic nuclear data (i.e., ENDF/B) to uncertainties in reactor performance parameters such as K-effective and breeding ratio, thus allowing for systematic adjustment processes. This uncertainty analysis will also allow for valuable feedback to the nuclear data community as to which measurements and/or evaluations most need further refinement.

The objective of this thesis project is to develop the capability of processing uncertainty data in ENDF/B version 5 (ENDF/B-V). Just as the microscopic nuclear data of ENDF/B is processed according to specified algorithms into multigroup form, so is the uncertainty data processed by specific algorithms into multigroup covariance matrices. A covariance shall be defined statistically as the expected value of the product of the deviations of two random variables (may be the same random variable) from their respective means. Each variable is allowed to have its own energy intervals which forms the two dimensions of a covariance matrix.

Previous work in this field consisted of processing limited ENDF/B-IV data (ENDF/B-IV contained uncertainties for nitrogen, oxygen, and carbon only) using an uncertainty processor, PUFF[2], developed by extending the MINX[3] cross section processor. Many additional unofficial cross section uncertainty evaluations were prepared at ORNL in an ENDF/B-IV format.[4] From this data and the PUFF code, three multigroup covariance libraries were produced, which are available through the Radiation Shielding Information Center (RSIC) at ORNL. These three libraries are the fission spectrum covariance matrix library (with GODIVA[5,6] weighting), the LMFBR core physics covariance matrix library (with ZPR-6/7[7] weighting), and the LMFBR shielding covariance library (with 1/E weighting). These libraries are in a standard format, COVERX,[8] for use in the FORSS[9] system. The FORSS system is a collection of codes used in sensitivity and uncertainty analysis.

In the present work, the capability of processing newly formatted ENDF/B-V data has been developed. Specifically, processing capabilities have been added for new uncertainty relationships, explicit cross reaction and cross material relationships (cross is used to indicate that the two random variables are not the same), and derived uncertainties. Derived is used here in the context that a reaction type (and therefore its uncertainties) may be determined by summing other reaction types (e.g., the total cross section is the sum of its partial cross sections). Derived is also used in the context that some reaction types are determined by ratio measurements to a reference reaction type (e.g., ^{239}Pu fission cross section is measured as a ratio to the ^{235}U fission cross section). Capabilities have also been added to produce the off-diagonal submatrices resulting from derived (in the context of summing) uncertainties. Processing uncertainties in the average number of neutrons per fission ($\bar{\nu}$) and in the resolved resonance parameters (for infinitely dilute systems only) have also been included. Finally, an important accomplishment of this work has been to separate the uncertainty processing from the cross section processing, originally suggested by Las Alamos Scientific Laboratory (LASL), to provide not only for a modular code system, but to reduce computing costs.

This new processing capability has been implemented in a new version of the PUFF code named PUFF-II and requires that the user supply only the multigroup cross sections (e.g., VITAMIN-C or -E libraries[10,11]) with corresponding flux spectrum and, of course, the uncertainty file data of ENDF/B-V.

The text of this thesis is organized into six chapters. Chapter II includes definitions for some of the terminology used in the remainder of this thesis. Chapter III explains the basic formats for the uncertainty data expressed in ENDF/B-V. Chapter IV explains the specific processing techniques that are used to produce multigroup covariance matrices. Varification of PUFF-II is described in Chapter V. Chapter VI shows some typical results produced by PUFF-II. The conclusions of this work and recommendations for future work are given in the final chapter.

CHAPTER II

DEFINITIONS

Because ENDF/B is, in effect, breaking new ground in the computation and recording of uncertainty data, several new terms will appear which need to be clearly defined.

Given two variables, X_i and Y_j, which, for this case, represent the multigroup cross section of reaction type X, energy group i, and reaction type Y, energy group j, the covariance matrix (or absolute covarience matrix), COV of such may be described as

$$\mathrm{Cov}(X_i,Y_j) \equiv \langle (X_i-\hat{X}_i)\ (Y_j-\hat{Y}_j)\rangle, \qquad (1)$$

where the diamond shaped bracket and the tilde indicate the expectation (mean) value. From this, several other qualities may be defined, namely the relative covariance matrix, Rel.Cov,

$$\mathrm{Rel.\ Cov}(X_i,Y_j) = \frac{\mathrm{COV}(X_i,Y_j)}{X_i\ Y_j} \quad , \qquad (2)$$

the standard deviation, Std.Dev,

$$\mathrm{Std.Dev.}(X_i) = \sqrt{\mathrm{Cov}(X_i,X_i)}, \qquad (3)$$

and the relative standard deviation, Rel.Std.Dev.,

$$\mathrm{Rel.Std.Dev}(X_i) = \frac{\mathrm{Std.Dev}(X_i)}{X_i} \quad . \qquad (4)$$

Also, a correlation matrix, Corr, may be defined as:

$$\mathrm{Corr}(X_i,Y_j) = \frac{\mathrm{Cov}(X_i,Y_j)}{(\mathrm{Std.Dev}(X_i))(\mathrm{Std.Dev}(Y_j))}, \qquad (5.1)$$

or

$$\text{Corr}(X_i, Y_j) = \frac{\text{Rel.Cov}(X_i, Y_j)}{(\text{Rel.Std.Dev.}(X_i))(\text{Rel.Std.Dev.}(Y_j))}. \tag{5.2}$$

The correlation matrix shows quantitatively the degree of correlation between X_i and Y_j. The correlation matrix is bounded by unity, i.e.,

$$| \text{Corr}(X_i, Y_j) | \leq 1. \tag{6}$$

When $\text{Corr}(X_i, Y_j) = 0$, the variables X_i and Y_j are said to be totally uncorrelated. When $\text{Corr}(X_i, Y_j) = +1$ or -1, the variables are said to be fully correlated or fully anti-correlated, respectively.

It should also be noted that the term covariance and uncertainty are used interchangeably.

CHAPTER III

ENDF/B-V UNCERTAINTY DATA FORMATS

In the ENDF/B system the microscopic data are grouped into files according to the type of data. For example, file 1 contains the microscopic data for $\bar{\nu}$, file 2 contains the resolved resonance parameters, and file 3 is for the "smooth" microscopic cross sections. The uncertainty file number is determined by adding 30 to the respective microscopic data file number. Thus, file 31 contains uncertainty data for $\bar{\nu}$, file 32 contains uncertainties in the resolved resonance parameters, and file 33 contains uncertainties for the smooth microscopic cross sections. As a side note, these three uncertainty files are the current extent of the uncertainty data in ENDF/B-V, although future plans are to include uncertainties in the fission spectrum χ, and in secondary energy and angular distributions.

Files 31 and 33 have identical formats in the ENDF/B-V system and may thus be described together.

Files 31 and 33 are broken down into sections, subsections and sub-subsections. A section completely describes a specific reaction type which is classified by an MT number (e.g., MT=1 is the total cross section, MT=2 is the elastic scattering cross section, etc.). Thus, for example, a section related to the total cross section, MT=1, completely describes the uncertainty related to MT=1.

A subsection completely describes a single covariance matrix. A sub-subsection describes the various components of the covariance matrix and are independent of each other.

Two different types of sub-subsections are used in ENDF/B-V and are referred to as "NI-type" and "NC-type" sub-subsections. The "NI-type" is used to explicitly describe the various components of the covariance matrix of the subsection. The "NC-type" is used to indicate that some or all of the contributing components to the covariance matrix, described in the subsection, are to be found in a different subsection already in the ENDF/B-V data. The idea behind this is, of course, to eliminate the large portion of the uncertainty data that would otherwise have to be repeated as "NI-type" sub-subsections. In each "NI-type" sub-subsection there is a flag which indicates the type of correlations as a function of energy described in the sub-subsection. The flag is called a LB number of which six are permitted in ENDF/B-V:[12]

LB=0 Absolute components only correlated within each E_k interval

$$\mathrm{Cov}(X_i,Y_j) = \sum_k P^{i;k}_{j;k}\, F_{xy,k} \quad , \tag{7}$$

LB=1 Relative components only correlated within each E_k interval

$$\mathrm{Cov}(X_i,Y_j) = \sum_k P^{i;k}_{j;k}\, F_{xy,k}\, X_i\, Y_j \quad , \tag{8}$$

LB=2 Relative components correlated over all E_k intervals

$$\mathrm{Cov}(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'}\, F_{xy,k}\, F_{xy,k'}\, X_i\, Y_j, \tag{9}$$

LB=3 Relative components correlated over E_k and E_ℓ intervals

$$\mathrm{Cov}(X_i,Y_j) = \sum_{k,\ell} P^{i;k}_{j;\ell}\, F_{x,k}\, F_{y,\ell}\, X_i\, Y_j, \tag{10}$$

LB=4 Relative components correlated over all E_ℓ intervals within each E_k interval

$$\mathrm{Cov}(X_i,Y_j) = \sum_{k,\ell,\ell'} P^{i;k,\ell}_{j;k,\ell'}\, F_k\, F_{xy,\ell} F_{xy,\ell'} X_i\, Y_j, \tag{11}$$

and

LB=5 Relative covariance matrix components

$$\mathrm{Cov}(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'} F_{xy;k,k'} X_i Y_j . \quad (12)$$

Here the X_i and Y_j are as previously defined, the F's are the uncertainty components which come directly from the uncertainty file data, and the dimensionless operator P is defined in terms of the operator S as

$$P^{i;k,\ell,\ldots}_{j;m,n,\ldots} \equiv S_i^{\,k} S_i^{\,\ell} \ldots S_j^{\,m} S_j^{\,n} \ldots , \quad (13)$$

where,

$S_i^{\,k}=1$ when the energy E_i is in the interval E_k to E_{k+1} of an E_k energy "table."

or

$S_i^{\,k}=0$ when the energy E_i is outside the range of E_k to E_{k+1} of an E_k energy "table."

Again, the "NC-type" sub-section is used to describe the covariance matrices in the energy ranges where the reaction type desired may be derived in terms of other evaluated reaction types in the same energy ranges. The evaluated cross section refered to here is one in which the covariance matrix is given explicitly ("NI-type") over the energy range of interest.

The "NC-type" sub-subsections are further broken down into two categories, as aluded to earlier. The first is the "derived redundant reaction types", indicated in ENDF/B-V by the flag LTY=0. Here the reaction type, MT, of a certain material, MAT (materials are designated by MAT numbers in ENDF/B), is obtained as a linear combination of other evaluated reaction types having the same MAT number but different MT values in the energy ranges given by E1 and E2 in the uncertainty file. That is

$$X_{MT}^{MAT}(E) = \sum_{i=1}^{NCI} C_i \, X_{MTi}^{MAT}(E), \quad (14)$$

where the C_i's are constant over the whole energy range of E1 to E2, and NCI designates the number of "NC-type" sub-subsections of interest.

The second type of "NC-type" sub-subsection is referred to as "covariances of cross sections derived via ratio measurements", flagged in ENDF/B-V as either LTY=1,2,or 3. Cross section evaluation by means of ratio measurements is a standard method in ENDF/B and one of the main sources of cross material correlations. This relationship can be shown for the cross section X_{MT}^{MAT} derived, in the energy range E1 to E2, through the evaluation of ratio measurements of the "standard" cross section X_{MTR}^{MATR} as

$$X_{MT}^{MAT}(E) = R(E) \, X_{MTR}^{MATR}(E) \quad (15)$$

where R(E) is the measured ratio at energy E. LTY=1 is then used in one subsection of X_{MT}^{MAT} to indicate a ratio measurement to X_{MTR}^{MATR}. LTY=2 is used to indicate a correlation between X_{MT}^{MAT} and X_{MTR}^{MATR}. LTY=3 is used in the reference materials subsection to indicate a correlation between X_{MTR}^{MATR} and X_{MT}^{MAT}.

The final type of uncertainty file to be described is file 32, the uncertainties in the resolved resonance parameters. In file 32, the data necessary for both multi- and single-level Breit-Wigner representations and the correlated uncertainties in these data are given. Covariances are given for the resonance energy, E_r, the total angular momentum of the resonance, J, the neutron width, Γn, the radiation width, $\Gamma \gamma$, and the fission width, Γf. This data is then propagated through to an uncertainty in a resonance cross section. These uncertainties are then added to the uncertainties formulated from file 33, the smooth cross section covariances, to form a complete covariance matrix.

CHAPTER IV

PROCESSING ENDF/B-V UNCERTAINTY DATA INTO MULTIGROUP FORMALISM

Processing ENDF/B-V uncertainty data is a straightforward but strict operation. The matrix operations necessary must follow certain mathematical relationships or errors are prone to occur. With this in mind, and before describing the computational procedures, a brief explanation of the various energy grids used is necessary.

The first energy grid is the cross section energy grid. This grid is, of course, associated with the energy structure on which the multigroup cross sections have been processed. The multigroup cross sections may be in any group structure desired and are not necessarily dependent upon any other grid to be described.

The second energy grid is the user energy grid. This is the energy structure on which the code user wants to have the final multigroup covariances.

A third energy structure is associated with the various energy levels on which the evaluator has expressed the uncertainties. This energy structure will be referred to as the uncertainty file energy structure or grid.

A fourth energy structure, necessary for a unified energy grid on which the cross sections (and flux) are expressed, is called the "supergrid." This grid is the union of the user grid and the uncertainty file energy grid. The supergrid is also necessary, as will be explained later, to process covariances due to ratio measurements.

The fifth and final energy grid is named the super-user grid. This grid is the union of the user energy grid and the energy boundaries of the "derived redundant reaction type" covariances; the E1's and E2's. The super-user grid is necessary, as will be explained later, to process covariances which are linear summing operations.

Another area that should be discussed before describing the covariance computational procedures is that of interpolation of the multigroup cross sections and corresponding flux. In order to use the multigroup processing algorithms, the multigroup cross sections and flux must be expressed on the supergrid. One of the most convenient methods of interpolating the multigroup cross sections on to the supergrid, and the method chosen in PUFF-II, is to energy weight the cross section and collapse (or expand) as described below

$$\bar{\sigma}_{sb} = \frac{\sum_i \sigma_{Mi}\phi_{Mi}\left(\frac{E_{sb} - E_{M,i}}{E_{M,i+1} - E_{M,i}}\right)}{\sum_i \phi_{Mi}\left(\frac{E_{sb} - E_{M,i}}{E_{M,i+1} - E_{M,i}}\right)} \qquad i = 1, 2, \ldots, \text{Multi} \tag{16}$$

where $\bar{\sigma}_{sb}$ is the supergrid cross section for energy group b, $\sigma_{M,i}$ is the multigroup cross section for energy group i and ϕ_{Mi} is the corresponding flux, E_{sb} is a lower energy boundary for the supergrid, $E_{M,i}$ is the energy boundaries for the ith energy group in the multigroup cross section energy grid, and Multi is the number of groups in the multigroup energy grid.

The computation of multigroup covariances from files 31 and 33 using covariances from the "NI-type" sub-subsections is performed according to the different LB flags and are given in multigroup formalism as shown below

LB = 0
$$\mathrm{Cov}(X_i,Y_j) = \frac{\sum_{k\epsilon i,j} F_{xy,k}\phi_{i,k}\phi_{j,k}}{\phi_i\ \phi_j} \tag{17}$$

LB = 1
$$\mathrm{Cov}(X_i,Y_j) = \frac{\sum_{k\epsilon i,j} F_{xy,k}\phi_{i,k}X_{i,k}\phi_{j,k}Y_{j,k}}{\phi_i\ \phi_j} \tag{18}$$

LB = 2
$$\mathrm{Cov}(X_i,Y_j) = \frac{\left(\sum_{k\epsilon i} F_{xy,k}\phi_{i,k}X_{i,k}\right)\left(\sum_{k'\epsilon j} F_{xy,k'}\phi_{j,k'}Y_{j,k'}\right)}{\phi_i\ \phi_j} \tag{19}$$

LB = 3
$$\mathrm{Cov}(X_i,Y_j) = \frac{\left(\sum_{k\epsilon i} F_{x,k}\phi_{i,k}X_{i,k}\right)\left(\sum_{\ell\epsilon j} F_{y,\ell}\phi_{j,\ell}Y_{j,\ell}\right)}{\phi_i\ \phi_j} \tag{20}$$

LB = 4
$$\mathrm{Cov}(X_i,Y_j) = \frac{\sum_{k\epsilon i,j} F_k\left(\sum_{\ell\epsilon i} F_{xy,\ell}\phi_{i,\ell}X_{i,\ell}\right)\left(\sum_{\ell'\epsilon j} F_{xy,\ell'}\phi_{j,\ell'}Y_{j,\ell'}\right)}{\phi_i\ \phi_j} \tag{21}$$

and

LB = 5
$$\mathrm{Cov}(X_i,Y_j) = \frac{\sum_{k\epsilon i}\sum_{k'\epsilon j} F_{xy;k,k'}\phi_{i,k}X_{i,k}\phi_{j,k'}Y_{j,k'}}{\phi_i\ \phi_j}\ . \tag{22}$$

The derivation of Eqs. (17-21) is fully described in Ref. 13. Equation (22) is obvious from the definition of covariance given earlier and from equation (12). The notation used here is:

$Cov(X_i,Y_j)$ = multigroup covariance between reaction X group i and reaction Y, group j.

ϕ_i = multigroup flux per super-user group (or supergrid) i.

$X_{i,k}$ = multigroup cross section for reaction X for a supergrid (i,k) constructed from the union of energy boundaries of the uncertainty file and those from the the user grid. $\phi_{i,k}$ is the flux for this group.

F's = components of covariance taken directly from the uncertainty file.

The "NI-type" sub-subsections are the basis for construction of the "NC-type" sub-subsections and are therefore by necessity processed first. The use of the "NI-type" sub-subsections for the production of the "NC-type" derived redundant cross section covariances is demonstrated as follows: let X be the cross section of interest expressed as a linear combination of n evaluated cross sections, Y, in the energy range from E1 to E2

$$X_i = \sum_{M=1}^{n} Y_{M,i}K_M \tag{23}$$

where i is the energy group index and K_M's are constant values, usually +1 or -1. Then, to express the uncertainty in X we have

$$dX_i = \sum_{M=1}^{n} dY_{M,i}K_M, \tag{24}$$

where dX_i represents $(X_i-\hat{X}_i)$, the uncertainty in X_i; similarly for $Y_{M,i}$. To find the covariance of X_i, Eq. (24) is squared, changing the second index of i to j (where i and j represent the same group structure) and then expectation values are taken

$$\langle dX_i dX_j \rangle = \sum_{M=1}^{n} \sum_{M'=1}^{n} K_M K_{M'} \langle dY_{M,i} dY_{M,j} \rangle \ . \qquad (25)$$

The diamond bracketed items in Eq. (25) are the covariances and may be more conveniently expressed as

$$\mathrm{Cov}(X_i, X_j) = \sum_{M=1}^{n} \sum_{M'=1}^{n} K_M K_{M'} \mathrm{Cov}(Y_{M,i}, Y_{M',j}) \ . \qquad (26)$$

Similarly, taking the expected value of the product of X_i and the $Y_{M,i}$'s gives

$$\langle dX_i, dY_{M,j} \rangle = \sum_{M'=1}^{n} K_{M'} \langle dY_{M',i} dY_{Mj} \rangle \qquad M = 1,2\ldots,n \qquad (27)$$

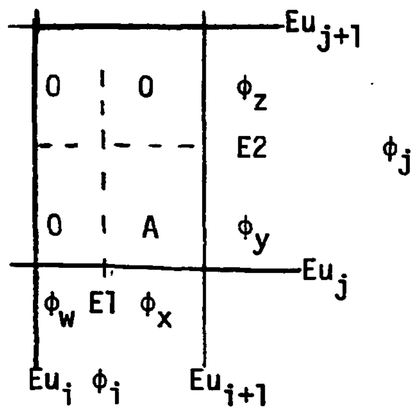
or

$$\mathrm{Cov}(X_i, Y_{M,j}) = \sum_{M'=1}^{n} K_{M'} \mathrm{Cov}(Y_{M',i}, Y_{M,j}) \quad M = 1,2,\ldots n \ . \qquad (28)$$

Equation (26) is the mathematical expression of the processing procedure to produce the multigroup covariances for the derived redundant cross section covariances. Equation (28) is the mathematical expression of the process to produce the multigroup covariances between the reaction of interest, X_i, and each of the reaction types, $Y_{M,i}$'s, from which X_i is evaluated.

Each of the derived redundant cross section covariances are derived for an explicit energy range, E1 to E2. Outside of this energy range the derived covariance matrix is zero. In effect, this requires that the multigroup covariances be produced on an energy grid that not only contains the desired energy boundaries of the user, but must also contain the E1's and E2's. This grid was defined as the super-user grid.

If the derived energy range points are not present numerical errors occur. This may best be explained pictorially as is shown in this partial covariance matrix



where Eu represents the user-energy boundaries for group i and j, E1 and E2 are as explained before, ϕ_w is the super-user grid flux, ϕ_i is the sum of ϕ_w and ϕ_x, likewise for ϕ_j, and A is the covariance element produced from Eq. (26) or (28) (all other elements are zero). If the derived redundant cross section energy boundaries were not present (in the energy grid scheme), the covariance element for user covariance group i,j would simply be A, which is incorrect. The correct covariance value for user group i,j is given in general as

$$\mathrm{Cov}(X_i,Y_j) = \frac{\phi_x\ A\ \phi_y}{(\phi_w+\phi_x)(\phi_y+\phi_z)} , \tag{29}$$

where the covariance element A is flux weighted and collapsed to the user covariance group i,j.

In the second type of "NC-type" sub-subsection, covariances may be wholly or partially derived from measurements made on the relationship one cross section of a certain material has to a reference cross section of another material. This is known as a ratio measurement. To illustrate this, let X_i be the cross section of interest and Z_i be the cross section from which X_i is evaluated, and then

$$X_i = R_i Z_i , \tag{30}$$

where R_i is the measured ratio of X_i to Z_i at energy group i. Then the uncertainty in X_i may be determined with use of the chain rule as

$$dX_i = dR_i Z_i + R_i dZ_i \quad . \tag{31}$$

With this, the covariance of X may be determined as

$$\begin{aligned} \langle dX_i dX_j \rangle &= \langle dR_i dR_j \rangle Z_i Z_j + 2R_i Z_j \langle dR_i dZ_j \rangle \\ &\quad + \langle dZ_i dZ_j \rangle R_i R_j \quad . \end{aligned} \tag{32}$$

Rearrangement of Eq. (32) gives

$$\begin{aligned} \frac{\langle dX_i dX_j \rangle}{R_i R_j Z_i Z_j} = \frac{\langle dR_i dR_j \rangle}{R_i R_j} &+ \frac{2\langle dR_i dZ_j \rangle}{R_j Z_i} \\ &+ \frac{\langle dZ_i dZ_j \rangle}{Z_i Z_j} \quad . \end{aligned} \tag{33}$$

R and Z (or R and any other cross section) are assumed to be uncorrelated (i.e., $\langle dR_i dZ_j \rangle = 0$) and the three remaining terms follow from the definition of a relative covariance matrix; thus

$$\text{Rel. Cov}(X_i, X_j) = \text{Rel. Cov}(R_i, R_j) + \text{Rel. Cov}(Z_i, Z_j) \quad . \tag{34}$$

Also, from Eq. (31) a covariance may be derived between X and Z, namely,

$$\text{Rel. Cov}(X_i, Z_j) = \text{Rel. Cov}(Z_i, Z_j) \quad . \tag{35}$$

Other relationships[12] exist due to ratio measurements, but Eqs. (34) and (35) represent the basic mathematical expressions for processing covariances due to ratio measurements. Equation (34) states that the relative covariance of X is determined by adding the relative covariance of the ratio, R, to the relative covariance of the reference cross section, Z. The uncertainties in R are given in "NI-type" sub-subsections in the subsection given for X. The uncertainties for the reference cross section are in the "NI-type" sub-subsections of Z.

Normal processing procedures of summing two collapsed multigroup covariance matrices cannot be followed in processing ratio measurements. This is because forming a collapsed multigroup covariance for the ratio, R, requires having the covariance matrix for X, which is the desired result. Instead, the covariance matrices of R and Z must be summed while in the supergrid structure. The covariance matrix of X is then collapsed to the user group structure.

This concludes a description of the processing procedures necessary to form multigroup covariances from files 31 or 33. The multigroup covariances due to the uncertainties in the resolved resonance parameters, file 32, must now be formed and added to the smooth cross section covariances of file 33.

The processing of the resolved resonance parameter uncertainties requires an uncertainty analysis approach. The basic equation is the single-level Breit-Wigner formula given as

$$\sigma_i = \frac{\pi}{k^2} g \frac{\Gamma_n \Gamma_i}{(E-E_r)^2+(1/4)\Gamma_T^2}, \tag{36}$$

where Γ_n is the neutron width, Γ_i is the radiation or fission width (i.e., $i = \gamma$ or f), E_r is the resonance energy, and Γ_T is the resonance total width given by

$$\Gamma_T = \Gamma_n + \Gamma_f + \Gamma_\gamma . \tag{37}$$

σ_i is the capture or fission cross section, g is the statistical spin factor given as

$$g = \frac{2J+1}{2(2I+1)} , \tag{38}$$

where J is the spin of compound nucleus, or the total angular momentum and I is the spin of the target nucleus. K is given in ENDF/B as

$$K = (2.196771 \times 10^{-3}) \left(\frac{AWRI}{AWRI+1.0}\right) \sqrt{E_r} \tag{39}$$

where AWRI is the ratio of the mass of a particular isotope to that of a neutron. Only the single-level Breit-Wigner formulae is used because no data have been cast in multi-level form to date.

Equation (36) is then integrated from -∞ + to + ∞ to obtain a representation for the resonance area given as

$$A_i = \frac{2\pi^2}{K^2} g \frac{\Gamma_n \Gamma_i}{\Gamma_T} \tag{40}$$

where A_i is the resonance area in barns^2-eV for capture or fission reactions (i.e., $i = \gamma$ or f). Sensitivities are then taken with respect to each parameter for which uncertainties are expressed (see Chapter III).

For example, the sensitivity of A_i to Γ_n may be shown as

$$\frac{\partial A_i}{\partial \Gamma_n} = \frac{2\pi^2}{K^2} g \, \Gamma_i \, (1 - \Gamma_n/\Gamma_T) \ . \qquad (41)$$

Similar expressions are derived for each of the other parameters which have uncertainties in file 32 and a matrix is formed which looks like

$$H \equiv \begin{bmatrix} \frac{\partial A_\gamma}{\partial \Gamma_\gamma} & \frac{\partial A_\gamma}{\partial \Gamma_n} & \frac{\partial A_\gamma}{\partial \Gamma_f} & \frac{\partial A_\gamma}{\partial J} & \frac{\partial A_\gamma}{\partial E_r} \\ \frac{\partial A_f}{\partial \Gamma_\gamma} & \frac{\partial A_f}{\partial \Gamma_n} & \frac{\partial A_f}{\partial \Gamma_f} & \frac{\partial A_f}{\partial J} & \frac{\partial A_f}{\partial E_r} \end{bmatrix} . \qquad (42)$$

The covariance matrix of the resolved resonance parameters is defined as

$$D = \begin{bmatrix} DG^2 & & & & \\ DNDG & DN^2 & & & \\ DGDF & DNDF & DF^2 & & \\ DJDG & DJDN & DJDF & DJ^2 & \\ 0 & 0 & 0 & 0 & DE^2 \end{bmatrix} , \qquad (43)$$

where

DG^2 is the variance of Γ_γ, [ev^2],

DN^2 is the variance of Γ_n, [ev^2],

DF^2 is the variance of Γ_f, [ev^2],

DJ^2 is the variance of J,

DE^2 is the variance of E_r [ev^2],

DNDG is the covariance of Γ_n and Γ_γ [ev^2],

DGDF is the covariance of Γ_γ and Γ_f [ev^2],

DNDF is the covariance of Γ_n and Γ_f [ev^2],

DJDG is the covariance of J and Γ_γ [ev], DJDN is the covariance of J and Γ_n [ev],

and DJDF is the covariance of J and Γ_f [ev] .

The covariance of E_r and the other parameters is very small, in practice, and therefore set to zero.[12] Also, the D matrix is symmetric (i.e., DNDG = DGDN, etc.).

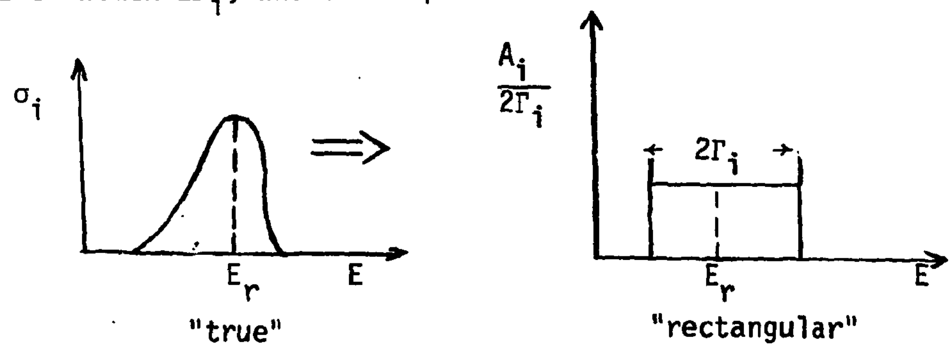
A covariance matrix for the resonance area is produced by folding the sensitivity matrix, H, with the covariance matrix, D, and is given as

$$<dAdA^T> = \begin{bmatrix} <dA_\gamma dA_\gamma> & <dA_\gamma dA_f> \\ <dA_f dA_\gamma> & <dA_f dA_f> \end{bmatrix} . \quad (44)$$

As shown in Eq. (44), not only is a covariance matrix formed for the capture and fission area, but a cross reaction covariance is given between capture and fission. The matrix shown in equation (44) is also symmetric (i.e., $<dA_f dA_\gamma> = <dA_\gamma dA_f>$).

The matrix described in Eq. (44) is summed for each resonance, ℓ-state (neutron angular momentum quantum number), and isotope within each super-user grid (or supergrid) K (if more than one isotope exists, the abundance is used to weight the contribution). This expression is then divided by the square of the width of energy group K (i.e., $(E_{k+1} - E_k)^2$) to form the cross section covariances due to the resolved resonance parameters. These covariances are then summed to the proper absolute covariances of the smooth cross sections formed from file 33.

The approach described above assumes a constant or flat weighting for each resonance within energy group k. A second approach, suggested by Y. Yeivin and J. J. Wagschal[14] is to give each resonance an 1/E weighting. In this approach, the model for averaging a resonance cross section, σ_i, consists of replacing the "true" cross section by a "rectangular" one of width $2\Gamma_i$, where $i = \gamma$ or f.



Letting E_{k+1} and E_k be the upper and lower kth group boundaries, the average cross section would be given by

$$\bar{\sigma}_i = \int_{E_k}^{E_{k+1}} \sigma_i(E)\, \frac{dE}{E} \Bigg/ \int_{E_k}^{E_{k+1}} \frac{dE}{E} \tag{45}$$

$$\cong \frac{A_i}{2\Gamma_i} \ln\left(\frac{E_r+\Gamma_i}{E_r-\Gamma_i}\right) \Bigg/ \ln\left(\frac{E_{k+1}}{E_k}\right) \qquad i = \gamma \text{ or } f\ . \tag{46}$$

Sensitivities are formed from Eq. (46) in the same fashion as described in the first approach and folded with the covariance matrix, D, Eq. (43). This time the covariance matrix of the resonance cross section is formed directly. The rest of the processing is the same as for the constant weighting approach. Both processing modes are allowed in PUFF-II.

Several assumptions have been made in processing the resolved resonance data. One of the more important assumptions is that no uncertainties are due to self-shielding. Normally, self-shielding is accounted for by Bonderinko f-factors[15], which are functions that relate cross section behavior to temperature and material compositions. Inclusion for these f-factors would require not only some very complicated analysis scheme, but would force the covariance calculations to become problem-dependent, which is not the intent for the processor.

Other assumptions are (1) only Breit-Weigner resonance representation (and of course the assumptions of a Breit-Weigner representation such as widely spaced resonances) are applicable, and (2) the resonance area is assumed to lie fully within the energy group k.

Using the procedures described above, the ENDF/B-V uncertainty data may be processed into multigroup covariances. However, due to situations which arise in the "NC-type" sub-subsections, the covariances are produced on an energy grid associated with either the super-user grid or supergrid. The matrices must then be collapsed to the user grid as described by Eq. (29). Finally, the collapsed matrices are prepared for output which usually consists of a COVERX file and correlation matrices.

CHAPTER V

VERIFICATION OF THE PUFF-II CODE

The objective in developing the PUFF-II code -- namely, to process ENDF/B-V uncertainty data into multigroup covariance matrices -- precludes "easy" evaluation and verification of the code because of the following two reasons. First, standard computational benchmark problems with known solutions, which could be solved by PUFF-II to check if the code is working properly, simply do not exist. Secondly, other codes which perform the same tasks as PUFF-II and, therefore, could be used to produce results for comparison with PUFF-II results, simply do not exist. In other words, standard techniques for verification of a newly developed code are not possible in this work.

However, it is possible to compare some PUFF-II results with results of hand calculations. This was done for the covariance of the Aluminum total elastic scattering cross section to the total inelastic scattering cross section. The hand calculated result and the PUFF-II result were identical.

It is also possible to evaluate LB=3 and LB=5 processing from the standpoint of internal consistency. Specifically, uncertainty files in LB=3 format, where E_k and E_ℓ energy intervals (see Chapter III, Eq. 10) are the same, were converted to LB=5 and then processed using PUFF-II. The results from both formats were compared and shown to be identical.

Finally ENDF/B-V results obtained with PUFF-II were compared with ENDF/B-IV results obtained with the old PUFF code. Differences between the two results should, of course, exist because the basic input data is different for the two cases. However, the two results should be at least similar in appearance. This similarity is demonstrated in Figs. 1 and 2 which show a six group representation of the correlation matrix for the ^{239}Pu fission cross section based on ENDF/B-V and ENDF/B-IV, respectively. Note that the version V result is less correlated in the low energy range than the version IV result. In particular, version V exhibits little or no off-diagonal correlation in the low energy range while version IV's off-diagonal low energy correlation ranges from 27% to 50%. Also, the standard deviation of the version V ^{239}Pu fission cross section is ~4% higher in energy group 1 while it is ~2% lower in energy group 6 than the version IV results. The differences in the intermediate energy ranges are less significant than those of the extremes.

Some of the discrepancy in the standard deviations presented in Fig. 1 and 2 is due to the use of different weighting spectrums. Also, the discrepancy in the degree of correlation in the low energy range is due to the fact that the version IV result assumed a long range correlation (i.e., a correlation over a large energy range) at low energy whereas in the ENDF/B-V ^{239}Pu (n,f) uncertainty file, no such assumption was made.

In summary, the verification checks described in this chapter and the results presented in the next chapter, which appear quite reasonable from a physical point of view, lead us to conclude that the new code, PUFF-II, works properly.

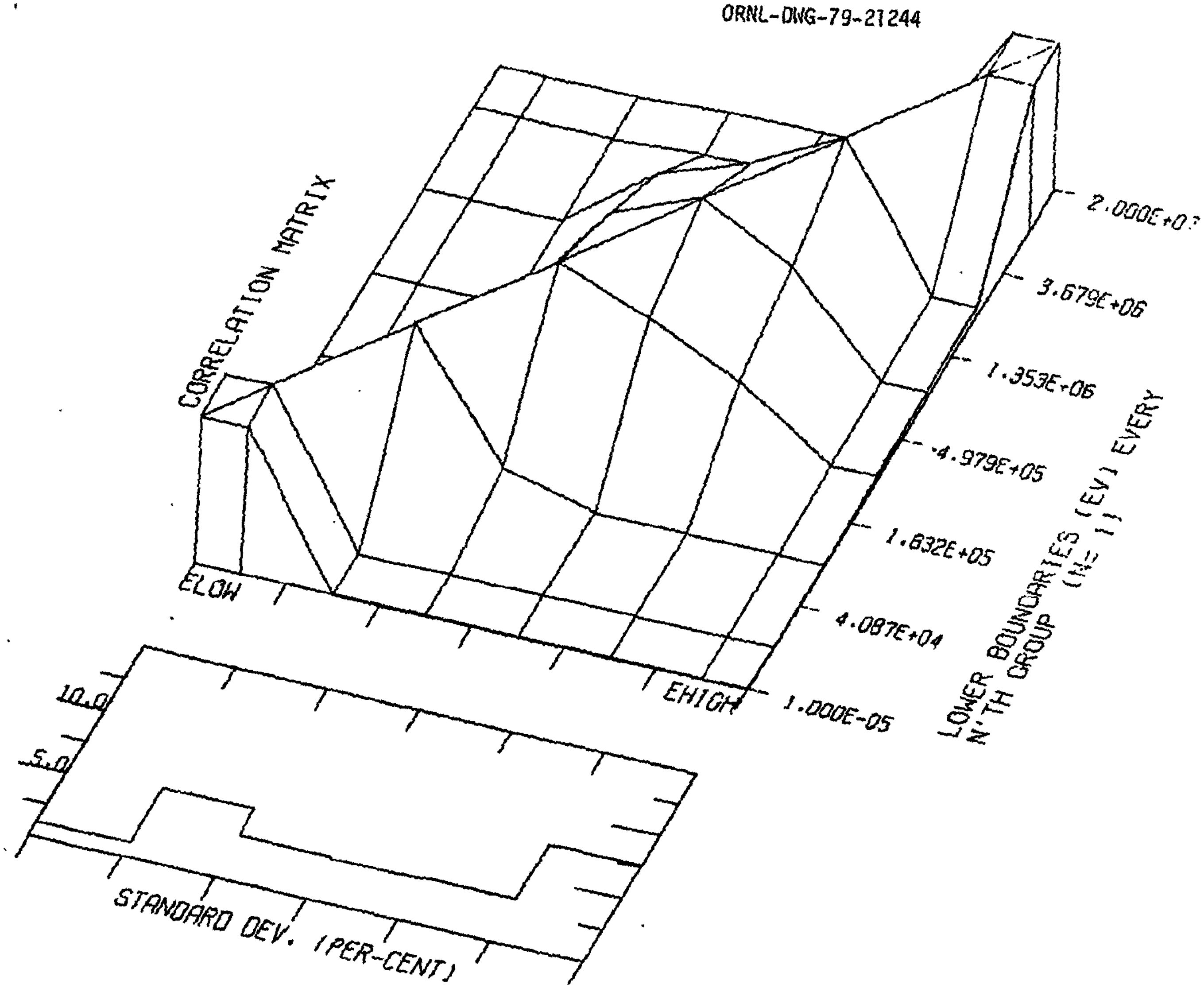


Fig. 1. Standard Deviation and Correlation Matrix of the $^{239}Pu(n,f)$ Cross Sections -- ENDF/B-V

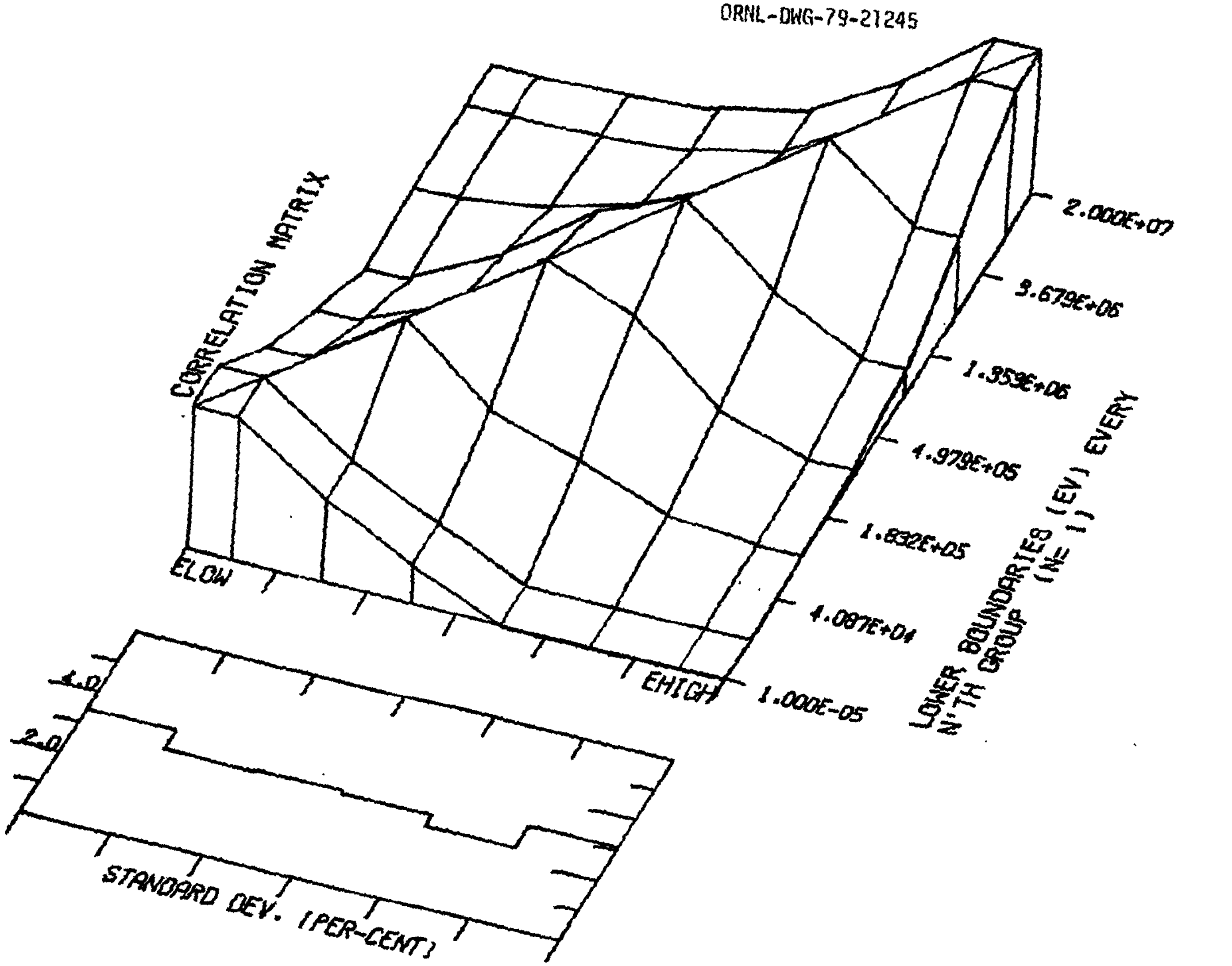


Fig. 2. Standard Deviation and Correlation Matrix of the $^{239}Pu(n,f)$ Cross Sections -- ENDF/B-IV

CHAPTER VI

RESULTS

One of the most illustrative ways of demonstrating the results of PUFF-II is by plotting the correlation matrices. These plots are produced by inputting the COVERX file into a program called PLTCOR, which was developed by Francis Perey and Jim Drischler. In these plots, the energy boundaries of the reaction (or reactions) of interest form the "X and Y" dimensions and the correlation coefficiencies are plotted in the "Z" direction. Also produced on the plots are the relative standard deviations for a correlation matrix of a specific material and reaction relative to itself (i.e., not for a cross material or cross reaction).

An illustration of this plotting and of the 52 group covariance matrix library[16] produced by PUFF-II is shown in Fig. 3. Fig. 3 is a correlation matrix plot for B-10 (MAT number 1305) (n,α) reaction (MT number 107). Note that it is fully correlated from 1.000×10^{-5} ev to about 6.738×10^{4} ev. From 6.738×10^{4} to about 1.353×10^{6} ev the off-diagonal elements are between 0 and 1. From $\sim 1.353 \times 10^{6}$ ev to higher energies, the uncertainty in the B-10 (n,α) reaction is zero in ENDF/B-V uncertainty file 33. Since, in ENDF/B-V, the B-10 (n,α) cross section is given over the full energy range (1.0×10^{-5} ev to 2.0×10^{7}ev) and is non-zero,[18] it is highly unlikely that there is no uncertainty in the cross section above 1.353×10^{6}ev. In other words, the covariance of B-10 (n,α) is incomplete, either because the uncertainty in this high ev region is difficult to determine or the evaluator was unsure of how to express the uncertainty.

Also note that the relative standard deviation indicates that the

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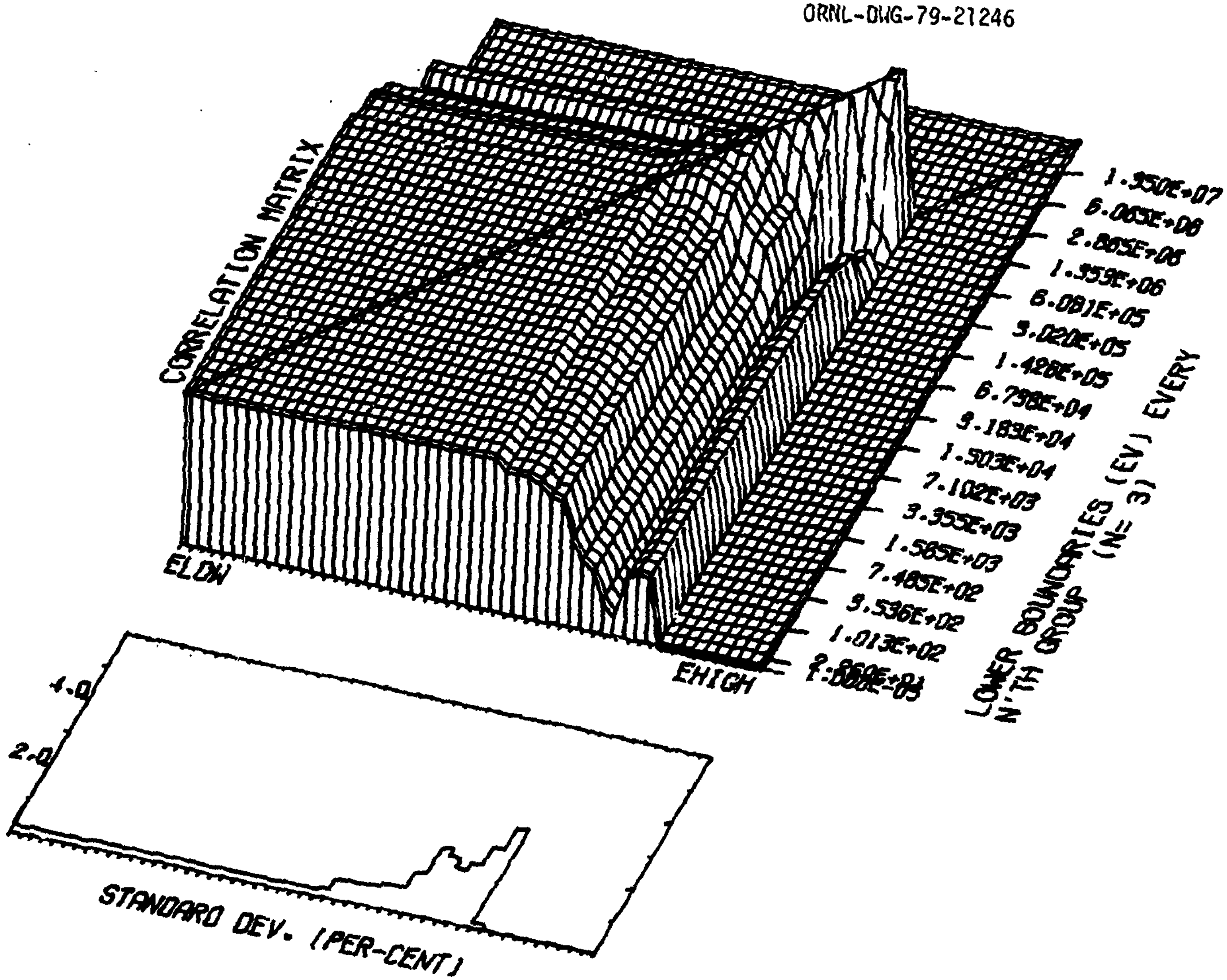

Fig. 3. Standard Deviation and Correlation Matrix of the $^{10}B(n,\alpha)$ Cross Section

cross section is fairly well known (less than 1% uncertainty) from 1.0×10^{-5}ev to about 6.738×10^{4}ev and is known to within 4% (relative standard deviation) for energies greater than 6.738×10^{4}ev but less than 1.353×10^{6}ev.

Figs. 4 and 5 represent the correlation matrix for Fe-56 (MAT number 1326) capture cross section (MT number 102) with and without the resolved resonance uncertainty data, respectively. As can be seen, the addition of the resolved resonance uncertainty increases the relative standard deviation in the resolved resonance uncertainty increases the relative standard deviation in the resolved resonance region. This also causes the off-diagonal elements not to be fully correlated (see equation 5.2). Also note that the relative standard deviation is off the chart in the Mev region. This merely indicates a relative standard deviation greater than 30%.

Fig. 6 is an illustration of a reaction which has been partially derived from ratio measurements; in particular, the capture covariance of U-238 (MAT number 1398). The U-238 capture cross section is derived via ratio measurements from B-10 (n,α) in the energy range of 4.0×10^{3}ev to 2.0×10^{4}ev. Also note the blank area of the U-238 capture covariance. In this case the uncertainty has been set to zero in the ENDF/B-V uncertainty file and referenced as to where this missing data may be found.[19]

Fig. 7 illustrates the correlation between U-238 capture (rows) and B-10 (n,α) (columns). Note here that while the U-238 capture uncertainty is for a fixed energy interval (4.0×10^{3}ev to 2.0×10^{4}ev), the uncertainty in B-10 (n,α) is for the entire energy range (1.0×10^{-5}ev to 1.964×10^{7}ev).

Figs. 8 and 9 ill··rate two $\bar{\nu}$ relationships. Fig. 8 is the correlation matrix for U-238 prompt $\bar{\nu}$ (MT number 456). Fig. 9 is the correlation matrix between U-238 prompt $\bar{\nu}$ and Pu-240 (MAT number 1380) $\bar{\nu}$ (MT number 452). This is an explicit cross material relationship given in ENDF/B-V.

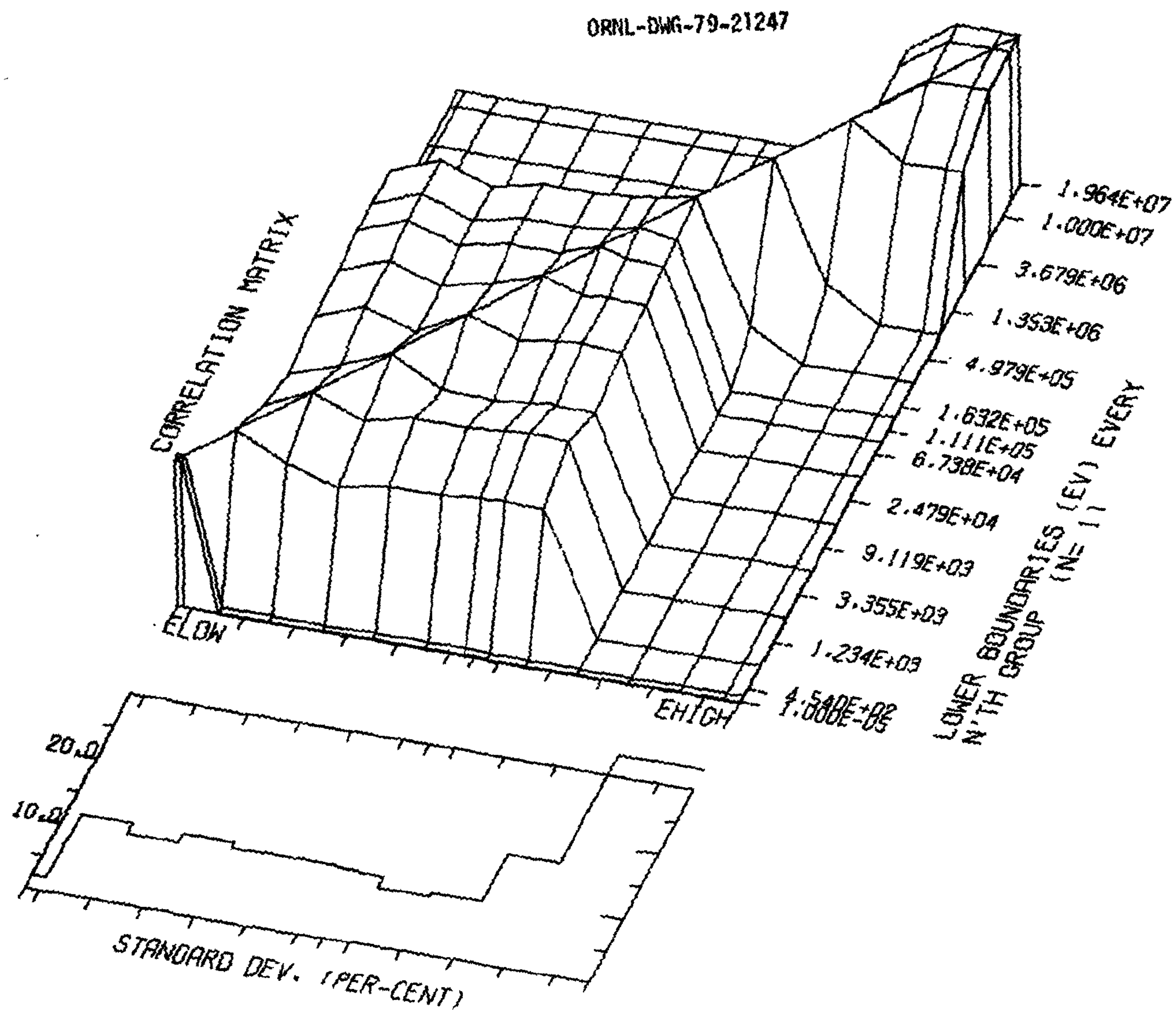

Fig. 4. Standard Deviation and Correlation Matrix of the $^{56}Fe(n,\gamma)$ Cross Section with Resonance Data

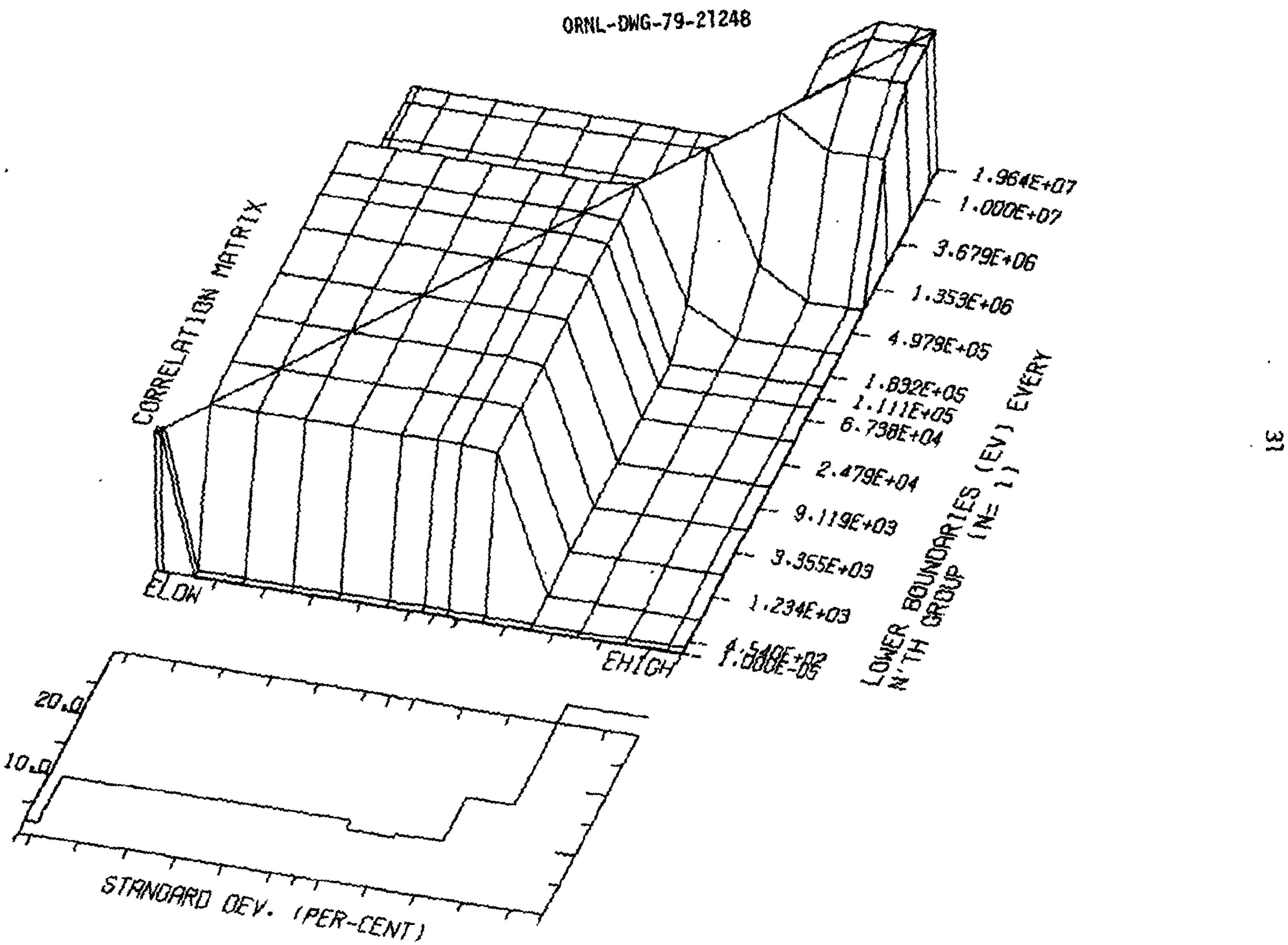

Fig. 5. Standard Deviation and Correlation Matrix of the $^{56}Fe(n,\gamma)$ Cross Section without Resonance Data

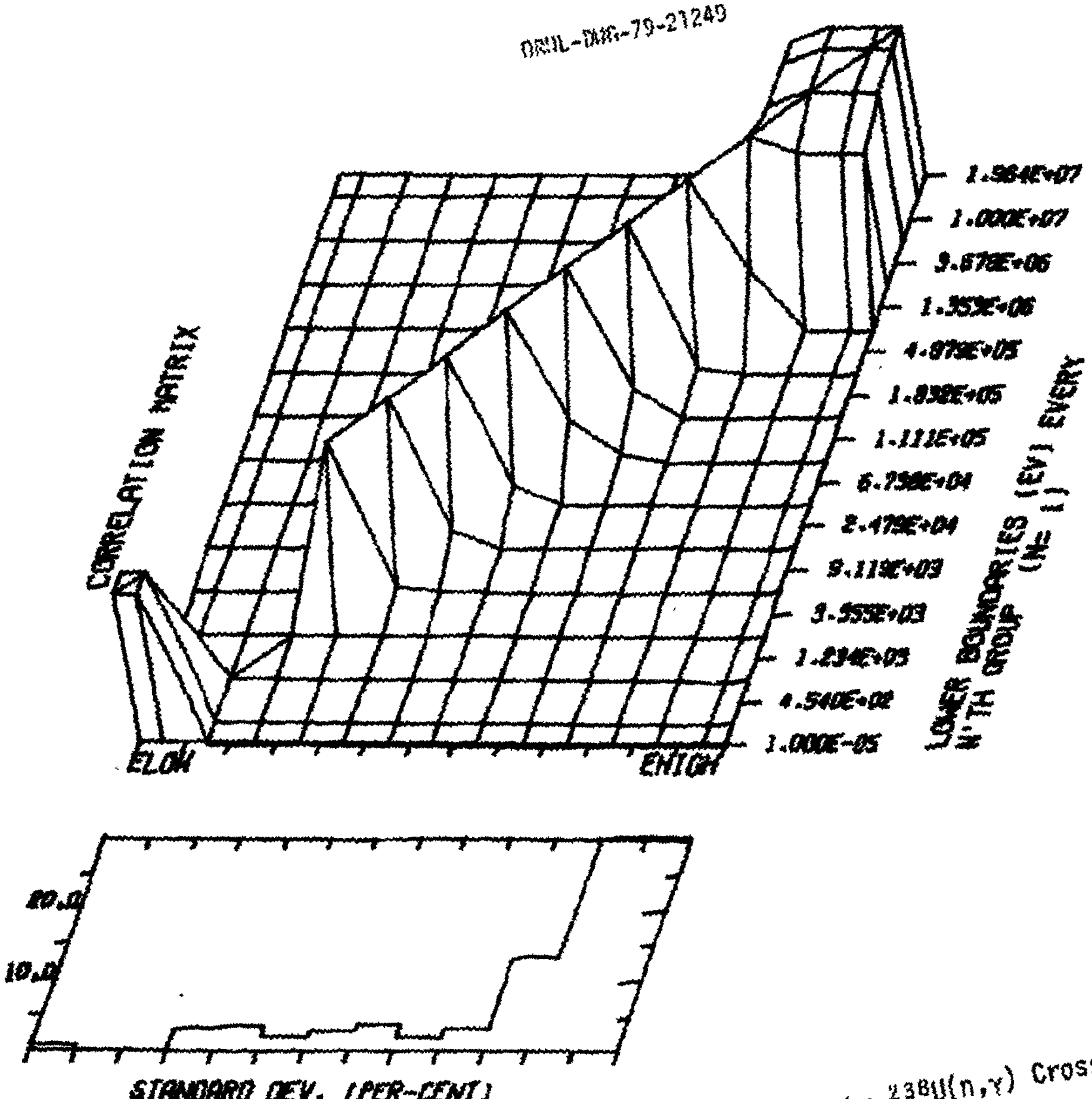

Fig. 6. Standard Deviation and Correlation Matrix of the $^{238}U(n,\gamma)$ Cross Section

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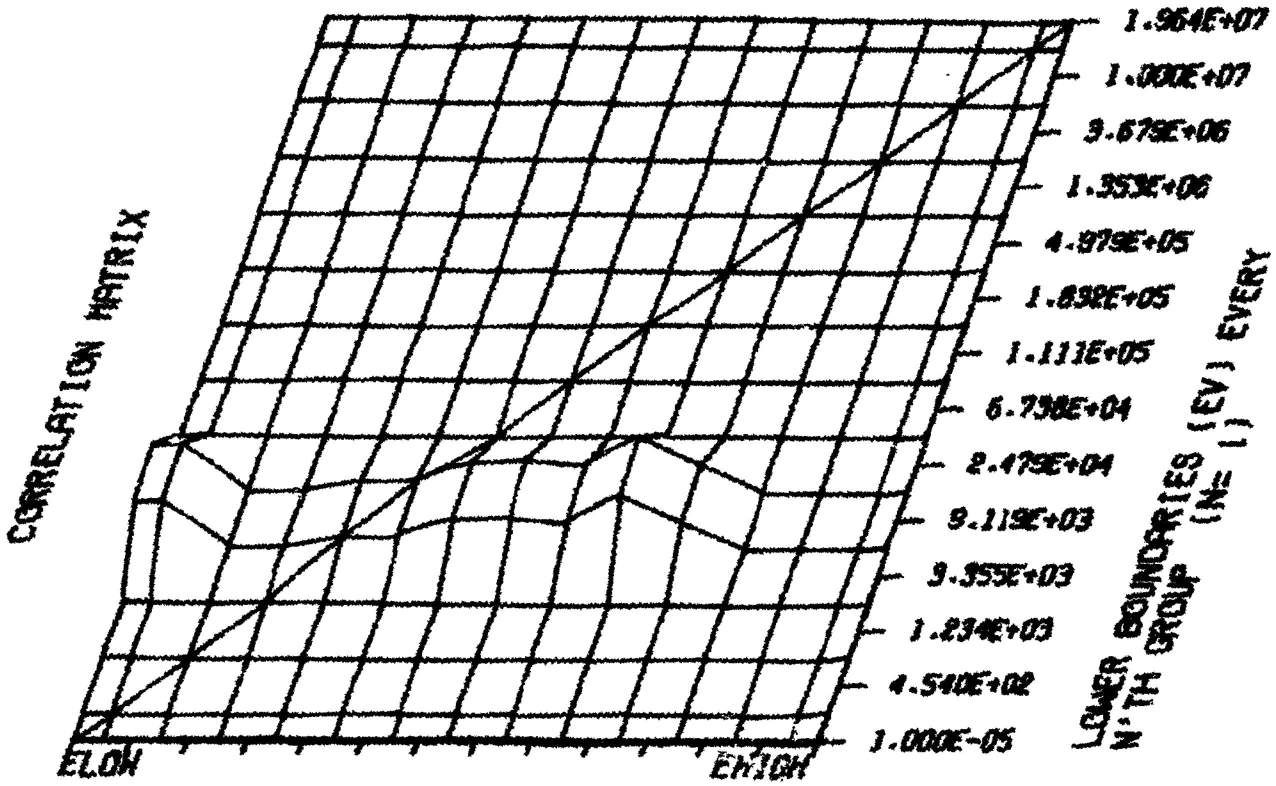

Fig. 7. Correlation Matrix Between $^{238}U(n,\gamma)$ and $^{10}B(n,\alpha)$ Cross Sections (row = $^{238}U(n,\gamma)$)

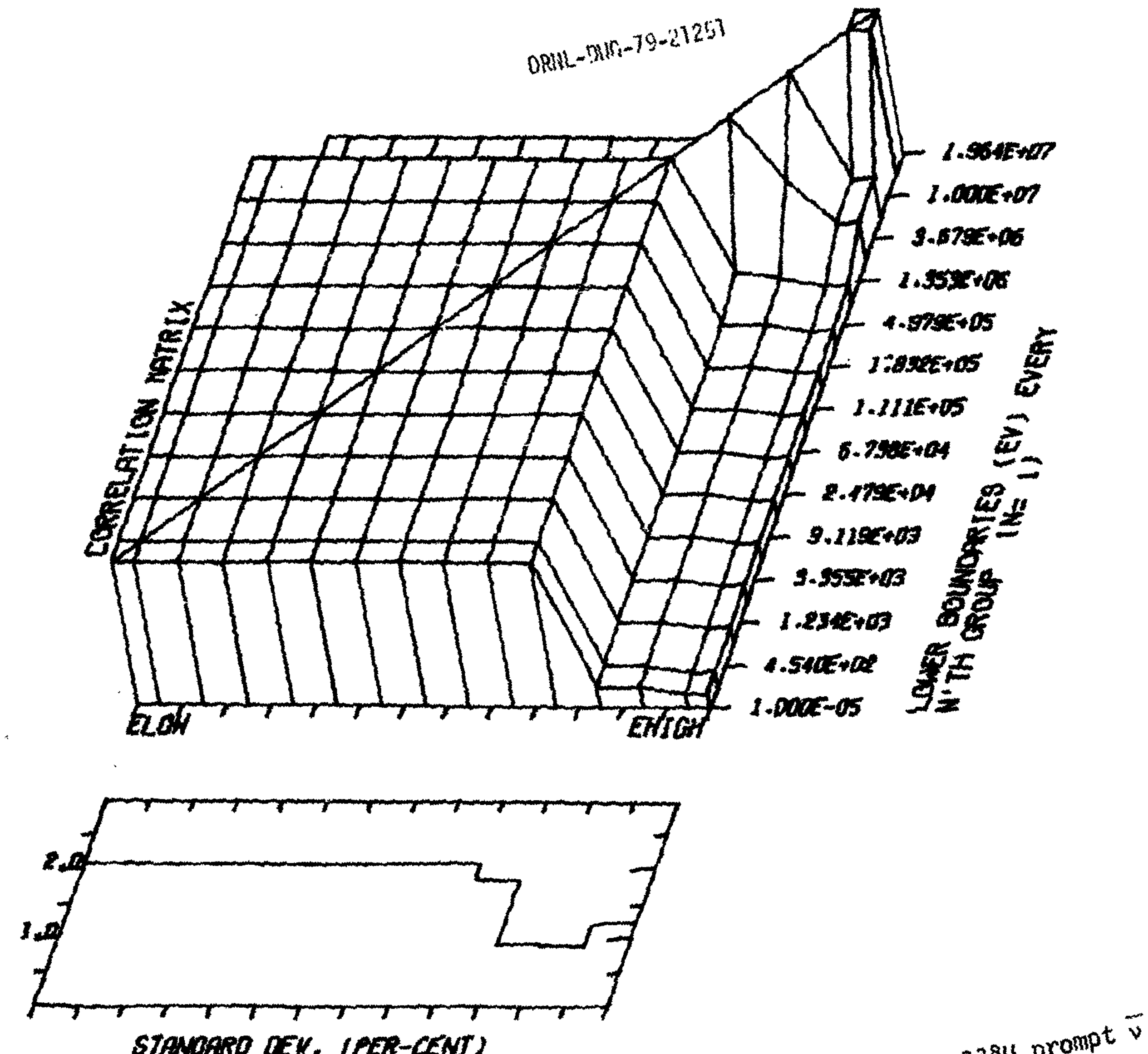

Fig. 8. Standard Deviation and Correlation Matrix of the ^{238}U prompt $\bar{\nu}$

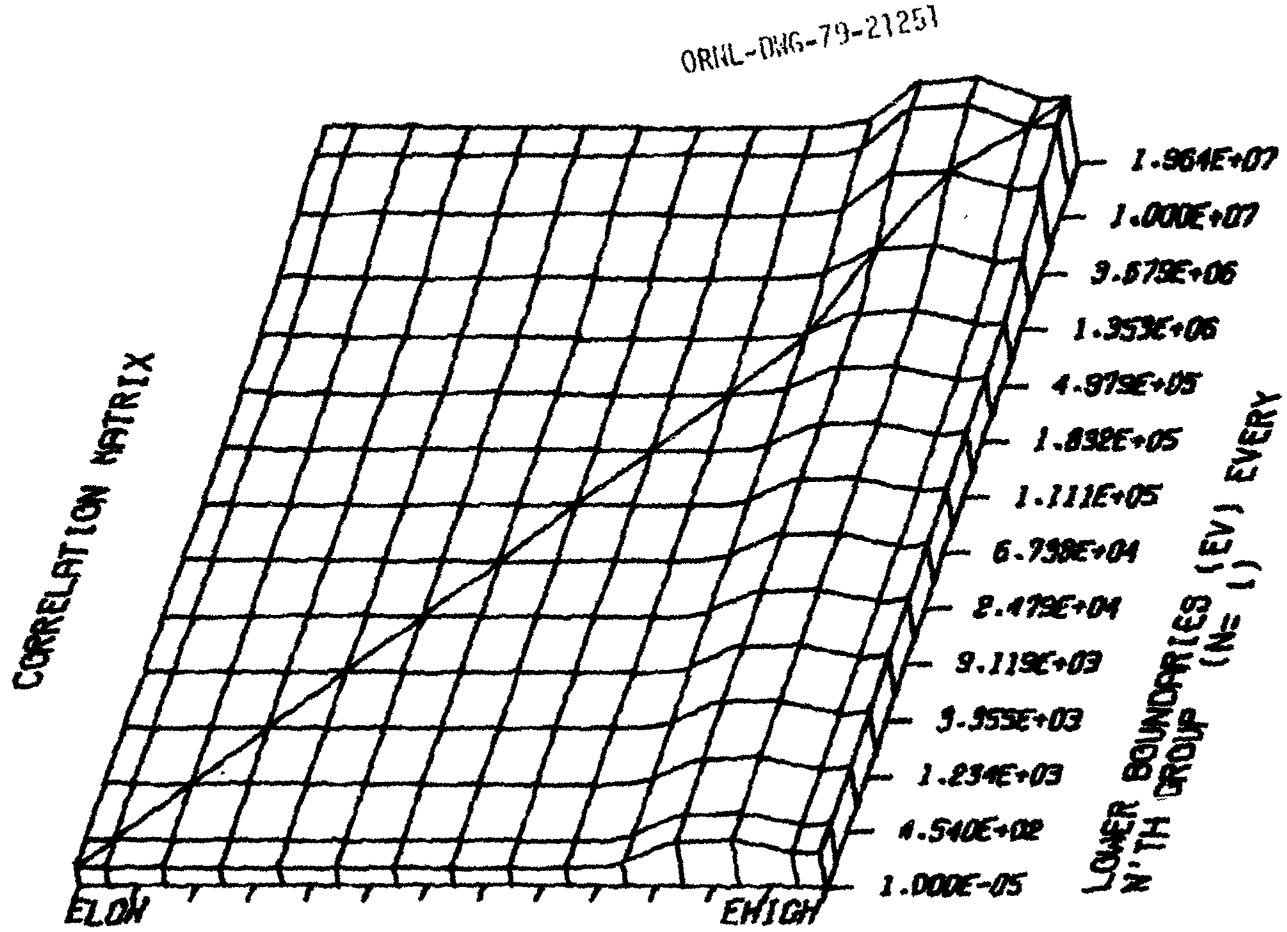

Fig. 9. Correlation Matrix Between ^{238}U prompt $\bar{\nu}$ and ^{240}Pu $\bar{\nu}$ (row = ^{238}U($\bar{\nu}$))

As a demonstration of the use of these covariance matrices, the 52 group covariance library was collapsed to 26 groups[16,20] and folded with sensitivity data[9] produced from ENDF/B-V cross sections to produce an uncertainty in K_{eff} for an experimental reactor (ZPR 6/7)[7]. The calculated K_{eff} is .985 with a standard deviation of 1.574%. The experimental value for K_{eff} is 1.0 with a standard deviation of .1%. Thus it is seen that the standard deviation of the calculated value due to uncertainties in cross sections can account for the entire discrepancy between the calculated and experimental value.

The results presented above from the PUFF-II code were obtained on a PDP-10 timesharing system requiring approximately 50K of core. Typical time requirements in cpu ranged from ∿1 minute for a single 52 group covariance matrix to ∿3 hours for a multiple 52 group covariance matrices. The coding language is FORTRAN IV.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

PUFF-II is a stand alone module capable of processing all types of uncertainty data currently present in ENDF/B-V (i.e., files 31 through 33). Specifically, processing capabilities have been added for new uncertainty relationships, explicit cross reaction and cross material relationships, and derived uncertainties. Capabilities for processing uncertainties in $\bar{\nu}$ and in the resolved resonance parameters (for infinitely dilute system only) have also been included. A final important accomplishment of this work has been to separate the uncertainty processing from the cross section processing to provide for a modular code system and reduce computing costs. The actual processing time and core requirement has been kept to a minimum by minimizing the size of the energy grid on which the covariance matrices must first be processed.

The only current limitation of the code involves the treatment of uncertainties in resolved resonance data. Specifically, the code will process only infinitely dilute resonance data.

The code has been evaluated by hand calculations and by comparison to ENDF/B-IV results for reasonableness. Results of the evaluation indicate that the code works correctly.

It should be pointed out that a problem may result from the use of the multigroup covariance matrices produced by PUFF-II. In particular, a cross section may be present for each of the user energy groups while the standard deviation determined from the uncertainty data may be zero. This problem occurs in one of three instances: 1.) The uncertainty data is incomplete;

2.) The multigroup cross section is produced in an energy structure in which one group includes the threshold energy boundary of the reaction and a user group is specified such that its upper boundary is smaller than the threshold energy and is contained within the boundaries of the larger group; or 3.) There is not a resonance energy present for one or more of the user energy groups and no uncertainty is given for the smooth cross sections in file 33 for this energy range or ranges.

Thus, the following recommendations are made regarding future work: 1.) A more detailed analysis should be given to the resolved resonance data uncertainties; specifically, a multi-level Breit-Wigner formalism should be programmed assuming future data uses this form and a treatment should be given for the uncertainties in the Bordorenko f-factors in conjunction with the resonance cross section; and 2.) The problem described above regarding the use of the multigroup covariances should be solved by writing a subroutine in the COVERX service module[21] to eliminate discrepancies between cross sections and uncertainties.

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APPENDIX A

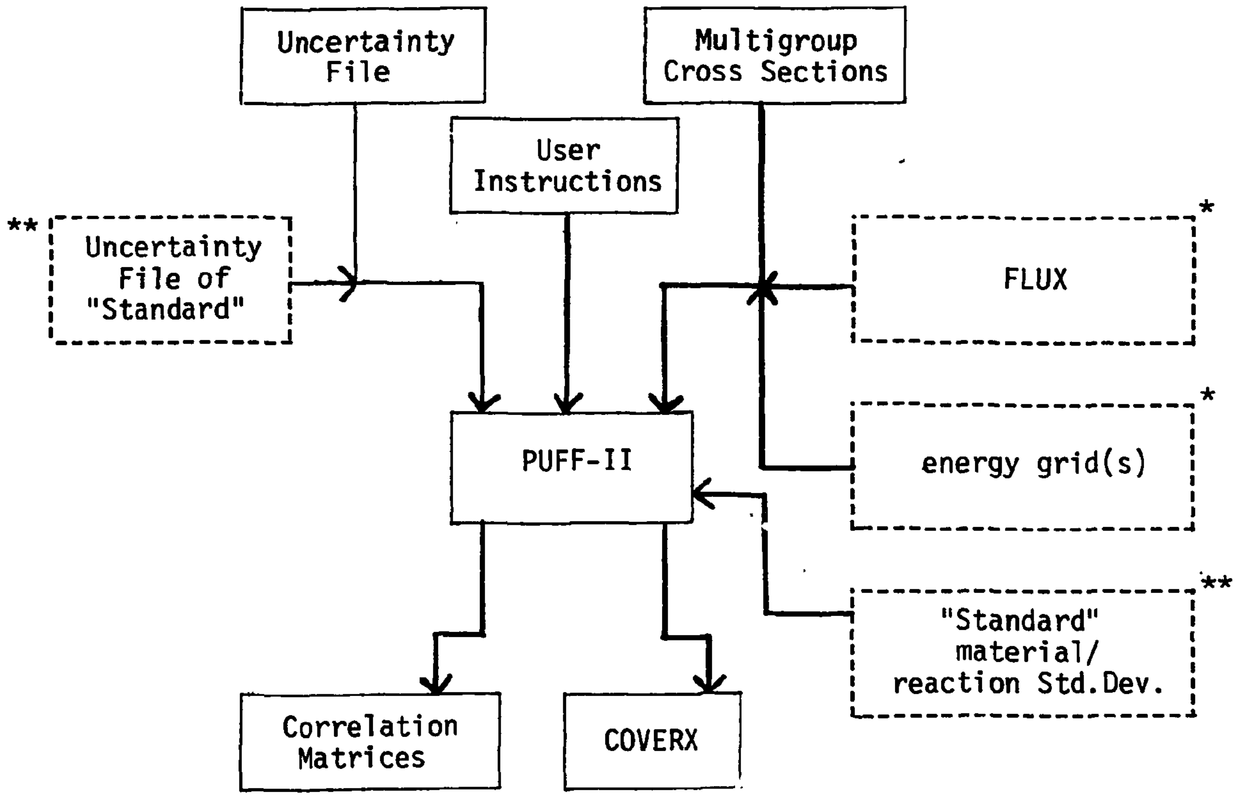
USER'S MANUAL FOR PUFF-II ON THE PDP-10

PUFF-II was written to process ENDF/B-V uncertainty files into multigroup covariance matrices. The multigroup covariance matrices are formed according to the procedures outlined in the body of this report.

Three basic types of input are required by PUFF-II; the ENDF/B-V uncertainty data, the multigroup cross sections, and the user instructions. The ENDF/B-V data may be obtained from the Radiation Shielding Information Center (RSIC) at ORNL and from many other locations. This data may be reduced to just the desired input results by RIGEL.[22] Multigroup cross sections are read in from a file containing cross sections punched by PAL[22] with the fixed format option. An option allowing for the reading of cross sections libraries in AMPX[22] master interface formats is also incorporated into PUFF-II; however, this is not considered practical while on the PDP-10 and will not be described. The user input instructions, as described below, are dependent upon the material to be processed.

Two basic types of output are also supplied by PUFF-II. The first, which may be used to check the results is a printout consisting of the user group structure, cross sections, standard deviations, and correlation matrices for each reaction(s) for which cross sections <u>and</u> uncertainties have been supplied. The second type of output is the COVERX formatted files. This data contains relative covariance matrices and is useful for sensitivity investigations in the FORSS system. The basic inputs and outputs are illustrated in Fig. A-1.

This description of how to use PUFF-II will be based on a batch



*Dashed lines indicate that the input is optional

**This input is needed only for cross material processing

Fig. A-1. Input and Output of PUFF-II

processing mode for the PDP-10. Batch processing is performed by creating a file consisting of the responses one would normally type in directly and then submitting this file to the queue. Also, for this time-sharing system certain liberties have been taken which are not currently possible on a non-interacting system.

The ENDF/B-V uncertainty file data is read in subroutine DELTA (see Fig. A-2) and is converted to binary with appropriate flags for subsequent processing. The input file is defined explicitly by an open statement in DELTA for unit IØ32 (IØ32=60). If the material to be processed has a reaction which is derived via ratio measurements to a referenced material's reaction, the reference material's reaction must be in a separate file in the user's area. This file is also defined explicitly by an open statement in DELTA for unit 19.

The energy grids are handled by subroutine RUSEGY. RUSEGY first forms the user grid. The user grid is formed in one of two ways. The user grid may be selected as one of nine grids stored in RUSEGY or may be read in from a separate file. If read in, the file is explicitly defined by an open statement in RUSEGY for unit 20. The energy grid may be either low to high or high to low energy in a 6E12.5 format. RUSEGY then continues to form the super-user grid and/or supergrid as flagged by the binary uncertainty file. Next, the cross section grid is formed. The cross section grid may again be chosen as one of nine optional grids or may be read in from a separate file as described above. If both the user grid and cross section grid are to be read in, then the user grid should be "stacked" on top of the cross section grid.

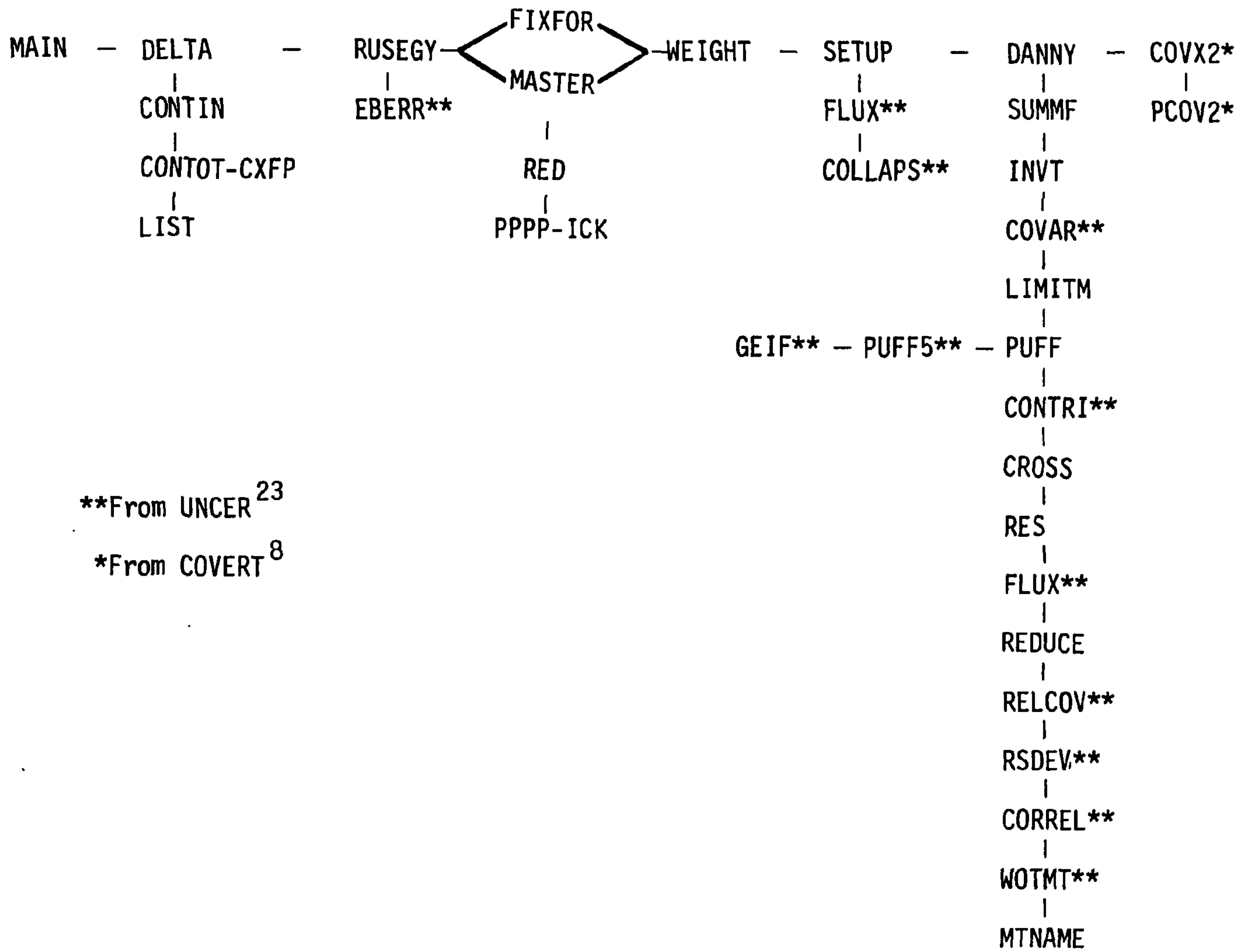


Fig. A-2. Flow Chart for PUFF-II

The multigroup cross sections are read in by subroutine FIXFOR. Here again the cross section file is defined explicitly by an open statement in FIXFOR for unit 10.

The flux may be read in and/or produced in subroutine WEIGHT. If read in, the file is defined explicitly by an open statement in WEIGHT for unit 50 and is given in a 6E12.5 format. Other options are explained below.

Two other input files may be required. The first is involved with cross material processing. If correlations exist between reactions of different materials, then the standard or reference material must be processed first and its standard deviation saved on unit 16. This file is then defined explicitly in subroutine DANNY by an open statement for unit 17. Note that the user grid must be the same for both the reference material processing and the material desired.

The second file is associated with resonance data uncertainty processing. If resonance data uncertainty processing is to take place, the file containing the data must be defined explicitly in subroutine RES for unit IØ32. Note that this is the same unit and usually the same file as that which was defined explicitly in subroutine DELTA.

The first of the output units containing the correlation matrices is unit IØ6 (IØ6=6). This unit is the line printer unit and creates a file named Q??.LPT for each run, where ? represents a letter or interger variable.

The second type of output is for the COVERX file. Both a card image and a binary file are created in COVERX format on units 26 and 27 respectively.

The user instructions depend upon the desired results and the type material to be processed. The first response is to give the number of groups in the user group structure and the weighting option desired where the numerical response and the options are shown below as

1 : $1/E$,

2 : $1/(E\ \sigma_T)$,

3 : input weighting/E,

or

4 : input weighting,

where E is the energy points associated with the cross sections and σ_T is the total corss section. The second response is the option to read an AMPX master library or not where 0=No and 1=Yes. The third response is to give the number of energy groups associated with the cross sections. The fourth response is the option to read either file 31 or 33, where 0=file 33 and 1= file 31. The fifth response is the option to process file 32, where 0=No and 1=Yes. The sixth response is to give the MAT number of the material to be processed. The seventh response is to give the optional user energy grid desired where the numerical response and the associated energy grid is given as

1 : input grid,

2 : 240 group structure,

3 : GAM2 (99 groups),

4 : SAND2 (620 groups),

5 : LASL (30 groups),

6 : GAM1 (68 groups),

7 : Vitamin-C (171 groups),

8 : 26 groups (ORNL-TM 5517),

9 : 100 groups (GE Library),

and

10 : 6 groups (ENDF/B-IV cross section covariances)

where the actual group structures may be found in subroutine RUSEGY. The eighth response is to give the cross section energy grid where the options are the same as described above for the user grid. The ninth response is to tell the number of reactions to be read in from the cross section file. The tenth response is to give a title to the COVERX file (limited to 72 characters) and the final response is to give the weighting option used so that, when the COVERX file is formed, there is some reference to the weighting used in its production.

As an illustration of the user instructions and of a sample problem the following batch file is shown:

```
EX PUFF2.FOR
*6 4
*Ø
*1ØØ
*Ø
*Ø
*1399
*1Ø
*9
*3
*PU-239 WITH CROSS MATERIAL
*4
```

where it is seen that a six group user structure is desired using 100 group cross sections and a flux which is read in and that the material to be processed is Pu-239 (MAT#1399). Pu-239 is known from the uncertainty file to have a cross material relationship to U-235 so a set up run for U-235 was produced first.

For each run executed in the batch system a log is kept of the transactions between the batch file and the computer system. This log is created under the same file name as the batch file with an extension of .LOG. The log file for this sample problem is shown on the following page.

```
TY BATCH.LOG

13:39:48 BAJOB  BATCON VERSION 13(1071)-2 RUNNING BATCH SEQUENCE 3585 IN
 STREAM 2
13:39:48 BAFIL  INPUT FROM ORELØ:BATCH.[104,1134]
13:39:48 BAFIL  OUTPUT TO  ORELØ:BATCH.LOG[104,1134]
13:39:48 BASUM  JOB PARAMETERS
                TIME:01:00:00   UNIQUE:YES      RESTART:NO

13:39:48 MONTR
13:39:48 MONTR  .LOGIN 104,1134 /CHARGE:18075 /SPOOL:ALL/TIME:3600/NAME:
"JDS   6010"
13:39:49 USER   JOB 16 ORELA/602.3 TTY63
13:39:49 USER   [LGNJSP OTHER JOBS SAME PPN:13]
13:39:49 USER   CHARGE = 18075
13:39:49 USER   1339    30-OCT-79       TUE
13:39:51 MONTR
13:39:51 MONTR  .EX PUFF2.FOR
13:39:53 USER   LINK:   LOADING
13:40:24 USER   [LNKXCT PUFF2 EXECUTION]
13:40:24 USER    GIVE # OF GROUPS IN USER GROUP STRUCTURE AND AND TYPE O
F WEIGHTING SPECTRUM DESIRED, WHERE 1=1/E, 2=1/(E*SIGMA TOTAL), 3=1/E*IN
PUT,AND 4=INPUT.>*6 4
13:40:26 USER    SPECIFY OPTION TO READ MASTER LIBRARY (Ø=NO,1= YES).>*Ø
13:40:27 USER    GIVE # OF X-SEC GROUPS>*100
13:40:27 USER   READ FILE 31(NUBAR) OR FILE 33?(Ø=33;1=31)>*Ø
13:40:28 USER   PROCESS FILE 32 ?(Ø=NO;1=YES)>*Ø
13:40:28 USER    MAT # OF MATERIAL PROCESSING>*1399
13:40:46 USER   SPECIFY TYPE OF USER GRID STRUCTURE(I FORMAT), 1-ARBITRA
RY,2-240 GROUP,3-GAM2(99 GRPS),4-SAND2(620 GRPS), 5-LASL(30 GRPS),6-GAM1
(68 GRPS),7-171 GROUPS,8-26 GROUPS, 9-100 GROUPS,10- 6 GROUPS.>*10
13:40:53 USER   SPECIFY THE TYPE GROUP STRUCTURE THE CROSS SECTIONS ARE
ON( SAME OPTIONS AS FOR USER GRID).>*9
13:40:55 USER    GIVE # OF MT >*3
13:43:59 USER   TYPE IN FILE DESCRIPTION, 1 CARD FORMAT(12A6)
13:43:59 USER   >*PU-239 WITH CROSS MATERIAL
13:44:00 USER   TYPE IN NUMBER CORRESPONDING TO WEIGHTING FUNCTION (I5)
>*4
13:44:04 USER   STOP
13:44:05 USER
13:44:05 USER   END OF EXECUTION
13:44:05 USER   CPU TIME: 2:4.58        ELAPSED TIME: 3:40.33
13:44:06 MONTR  EXIT
13:44:06 MONTR
13:44:06 MONTR  .KJOB ORELØ:BATCH.LOG=/W/B/Z:4/VR:10/VS:3585/VL:200/VP:1
Ø/VD:D
13:44:07 KJOB   OTHER JOBS SAME PPN
13:44:07 LGOUT  JOB 16, USER [104,1134]  LOGGED OFF TTY63    1344  30-OC
T-79
13:44:07 LGOUT  ANOTHER JOB STILL LOGGED IN UNDER [104,1134]
13:44:07 LGOUT  CPU  TIME =  2.22 MINUTES
13:44:07 LGOUT  CON  TIME =  0.07 HOURS
13:44:07 LGOUT  KILO CORE =  2.12 HOURS
13:44:07 LGOUT  JOB  COST =  5.30 DOLLARS
13:44:07 LGOUT  PRIME RATES
```

Tables A-1 through A-5 illustrates the output from PUFF-II which contains the standard deviations and correlation matrices. Table A-6 illustrates the COVERX formatted output file from PUFF-II.

The computer code PUFF-II has been checked by hand calculations and by comparison of results to previous ENDF/B-IV results for reasonableness. Running time varies and is dependent upon the order of the matrices and on the amount of correlations between reactions. For the sample problem which has been used for illustration thus far, a cpu time of two minutes and ~four seconds was recorded on the PDP-10. The coding language is Fortran IV. The only limitation of PUFF-II, at the present, is the limited treatment given to the resonance data uncertainty.

Table A-1. Correlation Matrix and Standard Deviations for ^{239}Pu(n,f) to ^{235}U(n,f)

MATERIAL 1= 1399, REACTION 1= 18 , MATERIAL 2= 1395, REACTION 2= 18

GRØUP	E HIGH	E LØW	X-IØN(1)	X-IØN(2)	REL.S.D.(1)	REL.S.D.(2)
1	2.0000E+07	3.6790E+06	2.5270E+00	2.0500E+00	7.1807E-02	5.2079E-02
2	3.6790E+06	1.3530E+06	1.9055E+00	1.2550E+00	3.1328E-02	2.3702E-02
3	1.3530E+06	4.9790E+05	1.6996E+00	1.1749E+00	3.4220E-02	2.7380E-02
4	4.9790E+05	1.8320E+05	1.5423E+00	1.2700E+00	3.3301E-02	2.7812E-02
5	1.8320E+05	4.0870E+04	1.5770E+00	1.6328E+00	5.2803E-02	2.6331E-02
6	4.0870E+04	1.0000E-05	6.8942E+02	4.9976E+02	1.1159E-02	3.3689E-03

*** CØRRELATIØN MATRIX ***

CØLUMN=MATERIAL 1 RØW=MATERIAL 2

RØW \ CØLUMN	1	2	3	4	5	6
1	141	135	9	0	0	0
2	35	756	389	186	0	0
3	3	367	797	581	0	0
4	0	173	576	784	0	0
5	0	32	150	356	0	0
6	0	0	0	0	0	0

Table A-2. Correlation Matrix and Standard Deviation for $^{239}Pu(n,f)$

MATERIAL 1= 1399, REACTIØN 1= 18 , MATERIAL 2= 1399, REACTIØN 2= 18

GRØUP	E HIGH	E LØW	X-IØN(1)	X-IØN(2)	REL.S.D.(1)	REL.S.D.(2)
1	2.0000E+07	3.6790E+06	2.5270E+00	2.5270E+00	7.1807E-02	7.1807E-02
2	3.6790E+06	1.3530E+06	1.9055E+00	1.9055E+00	3.1328E-02	3.1328E-02
3	1.3530E+06	4.9790E+05	1.6996E+00	1.6996E+00	3.4220E-02	3.4220E-02
4	4.9790E+05	1.8320E+05	1.5423E+00	1.5423E+00	3.3301E-02	3.3301E-02
5	1.8320E+05	4.0870E+04	1.5770E+00	1.5770E+00	5.2803E-02	5.2803E-02
6	4.0870E+04	1.0000E-05	6.8942E+02	6.8942E+02	1.1159E-02	1.1159E-02

*** CØRRELATIØN MATRIX ***

CØLUMN=MATERIAL 1 RØW=MATERIAL 2

RØW \ CØLUMN	1	2	3	4	5	6
1	1000	79	50	45	0	0
2	79	1000	674	491	0	0
3	50	674	1000	810	0	0
4	45	491	810	1000	123	0
5	0	0	0	123	1000	0
6	0	0	0	0	0	1000

Table A-3. Correlation Matrix and Standard Deviations for $^{239}Pu(n,\gamma)$ to $^{235}U(n,f)$

MATERIAL 1= 1399, REACTIØN 1= 102 , MATERIAL 2= 1395, REACTIØN 2= 18

GRØUP	E HIGH	E LØW	X-IØN(1)	X-IØN(2)	REL.S.D.(1)	REL.S.D.(2)
1	2.0000E+07	3.6790E+06	2.4085E-03	2.0500E+00	3.0843E-01	5.2079E-02
2	3.6790E+06	1.3530E+06	7.3689E-03	1.2550E+00	3.0156E-01	2.3702E-02
3	1.3530E+06	4.9790E+05	5.0417E-02	1.1749E+00	1.8340E-01	2.7380E-02
4	4.9790E+05	1.8320E+05	1.6607E-01	1.2700E+00	2.0272E-01	2.7812E-02
5	1.8320E+05	4.0870E+04	3.1099E-01	1.6328E+00	2.0735E-01	2.6331E-02
6	4.0870E+04	1.0000E-05	2.7055E+02	4.9976E+02	3.2777E-02	3.3689E-03

*** CØRRELATIØN MATRIX ***

CØLUMN=MATERIAL 1 RØW=MATERIAL 2

RØW \ CØLUMN	1	2	3	4	5	6
1	33	10	1	0	0	0
2	8	72	65	28	0	0
3	1	41	170	88	0	0
4	0	17	131	127	0	0
5	0	3	35	59	0	0
6	0	0	0	0	0	0

Table A-4. Correlation Matrix and Standard Deviation for $^{239}Pu(n,\gamma)$

MATERIAL 1= 1399, REACTIØN 1= 102 , MATERIAL 2= 1399, REACTIØN 2= 102

GRØUP	E HIGH	E LØW	X-IØN(1)	X-IØN(2)	REL.S.D.(1)	REL.S.D.(2)
1	2.0000E+07	3.6790E+06	2.4085E-03	2.4085E-03	3.0843E-01	3.0843E-01
2	3.6790E+06	1.3530E+06	7.3689E-03	7.3689E-03	3.0156E-01	3.0156E-01
3	1.3530E+06	4.9790E+05	5.0417E-02	5.0417E-02	1.8340E-01	1.8340E-01
4	4.9790E+05	1.8320E+05	1.6607E-01	1.6607E-01	2.0272E-01	2.0272E-01
5	1.8320E+05	4.0870E+04	3.1099E-01	3.1099E-01	2.0735E-01	2.0735E-01
6	4.0870E+04	1.0000E-05	2.7055E+02	2.7055E+02	3.2777E-02	3.2777E-02

*** CØRRELATIØN MATRIX ***

CØLUMN=MATERIAL 1   RØW=MATERIAL 2

RØW \ CØLUMN	1	2	3	4	5	6
1	1000	969	196	2	0	0
2	969	1000	211	8	0	0
3	196	211	1000	972	924	0
4	2	8	972	1000	956	0
5	0	0	924	956	1000	0
6	0	0	0	0	0	1000

Table A-5. Correlation Matrix and Standard Deviations for $^{239}Pu(n,f)$ to $^{239}Pu(n,\gamma)$

MATERIAL 1= 1399, REACTIØN 1= 18 , MATERIAL 2= 1399, REACTIØN 2= 102

GRØUP	E HIGH	E LØW	X-IØN(1)	X-IØN(2)	REL.S.D.(1)	REL.S.D.(2)
1	2.0000E+07	3.6790E+06	2.5270E+00	2.4085E-03	7.1807E-02	3.0843E-01
2	3.6790E+06	1.3530E+06	1.9055E+00	7.3689E-03	3.1328E-02	3.0156E-01
3	1.3530E+06	4.9790E+05	1.6996E+00	5.0417E-02	3.4220E-02	1.8340E-01
4	4.9790E+05	1.8320E+05	1.5423E+00	1.6607E-01	3.3301E-02	2.0272E-01
5	1.8320E+05	4.0870E+04	1.5770E+00	3.1099E-01	5.2803E-02	2.0735E-01
6	4.0870E+04	1.0000E-05	6.8942E+02	2.7055E+02	1.1159E-02	3.2777E-02

*** CØRRELATIØN MATRIX ***

CØLUMN=MATERIAL 1 RØW=MATERIAL 2

CØLUMN

RØW	1	2	3	4	5	6
1	232	19	12	11	0	0
2	7	99	73	51	0	0
3	9	119	204	171	0	0
4	7	78	126	163	25	0
5	0	0	0	23	258	0
6	0	0	0	0	0	-375

PUFF PRØCESSING CØMPLETED

Table A-6. Sample COVERX file

```
0V CØVERX CØVERX*ØRNL - FØRSS*         1
1D       6       6       0       2       2       5       5
2D *PU-239 WITH CRØSS MATERIAL           *
3D   0.2000E+08  0.3679E+07  0.1353E+07  0.4979E+06  0.1832E+06
  4.0870E+04  1.0000E-05
5D   1399     18      4   1399    102      4
6D   0.2527E+01  0.1905E+01  0.1700E+01  0.1542E+01  0.1577E+01
  6.8943E+02  7.1807E-02  3.1328E-02  3.4220E-02  3.3301E-02  5.2803E-02
  1.1159E-02
6D   0.2409E-02  0.7369E-02  0.5042E-01  0.1661E+00  0.3110E+00
  2.7055E+02  3.0844E-01  3.0156E-01  1.8340E-01  2.0272E-01  2.0735E-01
  3.2777E-02
7D   1399     18   1395     18      1
8D       6       1       6       2       6       3       6       4       6       5       6
     6       6
9D   0.5256E-03  0.5994E-04  0.5904E-05  0.3307E-06  0.3658E-07
  0.0000E-01  2.2059E-04  5.6112E-04  3.1519E-04  1.5050E-04  2.6206E-05
  0.0000E-01  1.5923E-05  3.1589E-04  7.4648E-04  5.4840E-04  1.3548E-04
  0.0000E-01  2.7077E-07  1.4659E-04  5.2944E-04  7.2653E-04  3.1184E-04
  5.0867E-11  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01
  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01
  0.0000E-01
7D   1399     18   1399     18      1
8D       6       1       6       2       6       3       6       4       6       5       6
     6       6
9D   0.5156E-02  0.1779E-03  0.1240E-03  0.1084E-03  0.0000E+00
  0.0000E-01  1.7792E-04  9.8144E-04  7.2275E-04  5.1274E-04  0.0000E-01
  0.0000E-01  1.2402E-04  7.2275E-04  1.1710E-03  9.2279E-04  0.0000E-01
  0.0000E-01  1.0839E-04  5.1274E-04  9.2279E-04  1.1090E-03  2.1610E-04
  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  2.1610E-04  2.7881E-03
  6.1044E-11  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  6.1044E-11
  1.2452E-04
7D   1399    102   1395     18      1
8D       6       1       6       2       6       3       6       4       6       5       6
     6       6
9D   0.5305E-03  0.6019E-04  0.5826E-05  0.3551E-06  0.4393E-07
  0.0000E-01  1.5549E-04  5.1331E-04  3.3768E-04  1.4556E-04  2.6384E-05
  0.0000E-01  6.4966E-06  2.8125E-04  8.5504E-04  6.6841E-04  1.6726E-04
  0.0000E-01  2.3163E-07  1.3554E-04  4.9092E-04  7.1516E-04  3.1742E-04
  5.4195E-11  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01
  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01
  0.0000E-01
7D   1399    102   1399    102      1
8D       6       1       6       2       6       3       6       4       6       5       6
     6       6
9D   0.9513E-01  0.9016E-01  0.1108E-01  0.1068E-03  0.0000E+00
  0.0000E-01  9.0162E-02  9.0936E-02  1.1649E-02  4.8904E-04  0.0000E-01
  0.0000E-01  1.1077E-02  1.1649E-02  3.3637E-02  3.6122E-02  3.5131E-02
  1.4304E-09  1.0677E-04  4.8904E-04  3.6122E-02  4.1097E-02  4.0196E-02
  1.6287E-09  0.0000E-01  0.0000E-01  3.5131E-02  4.0196E-02  4.2993E-02
  1.6808E-09  0.0000E-01  0.0000E-01  1.4304E-09  1.6287E-09  1.6808E-09
  1.0743E-03
7D   1399     18   1399    102      1
8D       6       1       6       2       6       3       6       4       6       5       6
     6       6
9D   0.5144E-02  0.1616E-03  0.1208E-03  0.1060E-03  0.0000E+00
  0.0000E-01  1.7896E-04  9.3385E-04  6.8386E-04  4.9390E-04  0.0000E-01
  0.0000E-01  1.2473E-04  7.4912E-04  1.2815E-03  8.7607E-04  0.0000E-01
  0.0000E-01  1.0913E-04  5.0818E-04  1.0461E-03  1.1000E-03  1.5933E-04
  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  2.6594E-04  2.8283E-03
  4.4394E-11  0.0000E-01  0.0000E-01  0.0000E-01  0.0000E-01  7.1726E-11
 -1.3718E-04
```