



**UNCER: A University of Wisconsin Version of
Uncertainty Files Processor for ENDF/B-V**

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ABSTRACT

A computer code, called UNCER, is written to process data covariance matrices from the ENDF/B-V Files 31 and 33. It has the capability of handling the "NC-type" sub-subsections for the "derived" cross sections and all the flag numbers, the LB flag, allowed in the "NI-type" sub-subsections in these files. A special feature of this code is the employment of the existing RSIC fine group data libraries, e.g., DLC-41B/VITAMIN-C, as a source of the multigroup cross sections used in the computation. By avoiding the time-consuming multigroup cross sections processing procedure, we are able to run this code inexpensively and use a rather small amount of computer core memory which is especially valuable for small computers.

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I. Introduction

The theory and application of sensitivity and uncertainty analysis have been developed extensively over the past decade⁽¹⁾. It has been well-recognized that one of the major problems in applying the theory of sensitivity and uncertainty analysis to nuclear reactor design is the question of availability of the data covariance matrices which are essential for uncertainty analysis. Historically covariance data were first released in version IV of the ENDF files as File 33 for a limited number of materials. Subsequently a computer code, PUFF⁽²⁾, was written to extend the capabilities of the MINX⁽³⁾ multigroup processing code to include processing of the ENDF/B-IV uncertainty files. Due to a great number of requests for the uncertainty files for most of the materials in order to perform uncertainty calculations, more materials will have uncertainty files in version V of the ENDF files which should be released soon.

The format changes of the uncertainty files from ENDF/B-IV to ENDF/B-V⁽⁴⁾ have made the data covariance processing more difficult. This computer code, UNCER, is therefore written to upgrade PUFF to deal with uncertainty files in ENDF/B-V. The following are some major revisions made in an effort to achieve this goal:

- (1) In version IV a dummy sub-subsection of "NC-type" is provided at the beginning of the uncertainty files which gives a set of energy boundaries for the entire uncertainty files. This set of energy boundaries is then

read and combined with the user group structure to form a set of "super-group" energy boundaries for the purpose of generating the supergroup cross sections. In version V one has to read through the entire uncertainty files to pick up all the possible energy boundaries contained in each sub-subsection, both "NC-type" and "NI-type", in order to construct the uncertainty file energy boundaries.

- (2) The implementation of the "NC-type" sub-subsections in ENDF/B-V, used to describe the covariance matrices of cross sections which can be "derived" in terms of other "evaluated" cross sections, has made it difficult to process the uncertainty files. Since the covariance matrices of the "derived" cross sections depend upon that of the "evaluated" cross sections from which the cross sections of interest are "derived", one has to program the code such that it will process the uncertainty files step by step: first of all, the "NI-type" of the same reactions, followed by the "NI-type" of the different reactions, and finally the "NC-type" sub-subsections.
- (3) In the "NI-type" sub-subsections, used to describe explicitly the various components of the covariance matrix, there is an LB flag whose numerical value indicates the nature of the covariance components and their correlations. Since the ENDF/B-V format permits more possible LB flags than ENDF/B-IV, one has to program the computer code to accommodate those additional flag values.

There is a special feature of UNCER which is entirely different from PUFF regarding the philosophy of obtaining the multigroup cross sections in the computation. In UNCER, the multigroup cross sections are extracted from the existing fine group data libraries of the DLC series distributed by the Radiation Shielding Information Center (RSIC), e.g., DLC-41B/VITAMIN-C. By

avoiding the actual processing procedure of generating the multigroup cross sections it is to be expected that this code can be run very inexpensively. In case there are incompatibilities or strong discrepancies between the ENDF/B-V data and that of the RSIC DLC data library chosen, one still has the alternative of using the multigroup cross sections processor to generate cross sections from the ENDF/B-V files and then combine the result with this code to generate covariance matrices.

This version of UNCER is only intended for processing Files 31 and 33 of ENDF/B-V. As far as File 32 is concerned, which is used for describing the "short-range" covariance components in the resolved resonance regions, this capability will be included in a later version.

II. Definitions

Suppose we have two quantities X_i and Y_j which represent the multigroup cross sections of reaction X, group i, and reaction Y, group j; the covariance matrix COV of X and Y can be defined statistically by

$$\text{COV}(X_i, Y_j) = E((X_i - E(X_i))(Y_j - E(Y_j))), \quad (1)$$

where E denotes the expectation value. Subsequently we can define the relative covariance matrix, RCOV, the standard deviation, SD, and the relative standard deviation, RSD, as follows:

$$\text{RCOV}(X_i, Y_j) = \frac{\text{COV}(X_i, Y_j)}{X_i Y_j} \quad (2)$$

$$\text{SD}(X_i) = \sqrt{\text{COV}(X_i, X_i)} \quad (3)$$

$$\text{RSD}(X_i) = \frac{\text{SD}(X_i)}{X_i} \quad (4)$$

The correlation matrix, CORR, which measures quantitatively to what extent X_i and Y_j are correlated, can be defined by

$$\text{CORR}(X_i, Y_j) = \frac{\text{COV}(X_i, Y_j)}{\text{SD}(X_i)\text{SD}(Y_j)} \quad (5)$$

For the extreme cases when $\text{CORR}(X_i, Y_j) = 0, 1,$ or $-1,$ X_i and Y_j are said to be totally uncorrelated, fully correlated, or fully anticorrelated, respectively.

III. Data Formats of Files 31 and 33 in ENDF/B-V

There are two different types of covariance representations permitted in ENDF/B-V, the "NC-type" and "NI-type" sub-subsections. The "NI-type" is used to describe explicitly the various components of the covariance matrix. On the other hand, the "NC-type" may be used to describe the covariance matrices in energy ranges where the cross sections can be "derived" in terms of other "evaluated" cross sections in the same energy range. In the context of Files 31 and 33, an "evaluated" cross section, in a given energy range, is defined as one for which the covariance matrix in that energy range is given entirely in terms of "NI-type" representation.

"NI-type" Sub-subsection

In each "NI-type" sub-subsection there is a flag, the LB flag, whose numerical value indicates whether the components are "relative" or "absolute" and the kinds of correlations as a function of energy. Six LB's are permitted in ENDF/B-V:

LB = 0 Absolute components only correlated within each E_k interval

$$\text{COV}(X_i, Y_j) = \sum_k P_{j;k}^{i;k} F_{XY,k} \quad (6)$$

LB = 1 Fractional components only correlated within each E_k interval

$$\text{COV}(X_i, Y_j) = \sum_k P_{j;k}^{i;k} F_{XY,k} X_i Y_j \quad (7)$$

LB = 2 Fractional components correlated over all E_k intervals

$$\text{COV}(X_i, Y_j) = \sum_{k, k'} P_{j; k'}^{i; k} F_{XY, k} F_{XY, k'} X_i Y_j \quad (8)$$

LB = 3 Fractional components correlated over E_k and E_1 intervals

$$\text{COV}(X_i, Y_j) = \sum_{k, 1} P_{j; 1}^{i; k} F_{X, k} F_{Y, 1} X_i Y_j \quad (9)$$

LB = 4 Fractional components correlated over E_1 intervals within each E_k interval

$$\text{COV}(X_i, Y_j) = \sum_{k, 1, 1'} P_{j; k, 1'}^{i; k, 1} F_k F_{XY, 1} F_{XY, 1'} X_i Y_j \quad (10)$$

LB = 5 Relative covariance matrix components

$$\text{COV}(X_i, Y_j) = \sum_{k, k'} P_{j; k'}^{i; k} F_{XY; k, k'} X_i Y_j \quad (11)$$

where X_i and Y_j represent cross sections X and Y evaluated at energies i and j respectively, the F's represent uncertainty components taken directly from the File 31 or 33 describing the covariances of cross sections X and Y for specific energy intervals. The dimensionless operators P in the above definitions are defined as follows:

$$P_{j; m, n, \dots}^{i; k, l, \dots} = S_i^k S_i^l \dots S_j^m S_j^n \dots, \quad (12)$$

where

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

"NC-type" Sub-subsections

(a) LTY=0, "Derived Redundant Cross Sections"

In this sub-subsection, the cross sections of the material number MAT

and the reaction number MT designated by X_{MT}^{MAT} , were strictly obtained as a linear combination of other "evaluated" cross sections having the same MAT number but different MT values in the energy range bounded by E1 and E2. That is,

$$X_{MT}^{MAT}(E) = \sum_{i=1}^{NCI} C_i X_{MT_i}^{MAT}(E). \quad (13)$$

The C_i 's are constant over the whole range of energy E1 to E2, usually ± 1 .

All the values of C_i 's and MT_i 's, in addition to NCI, E1, and E2, will be provided in this sub-subsection.

(b) LTY=1,2 and 3, "Covariances of Cross Sections Derived via Ratio Measurements"

Evaluation of cross sections by means of "ratio" measurements is one of the main sources of information on covariances of cross sections having different MAT values. Suppose the cross sections X_{MT}^{MAT} are strictly "derived", in the energy range from E1 to E2, through the evaluation of ratio measurements to the "standard" cross sections S_{MTS}^{MATS} , then we have the relationship:

$$X_{MT}^{MAT}(E) = R(E) S_{MTS}^{MATS}(E), \quad (14)$$

where $R(E)$ is the ratio measured at energy E. In this sub-subsection, MATS, MTS, E1 and E2 should be given, while the relevant information on the uncertainty of the ratios will be specified in "NI-type" sub-subsection.

IV. Computation of Multigroup Covariance Matrices from Files 31 and 33

For a "NI-type" sub-subsection the calculation is straight-forward.

That is, for different LB flags:

LB = 0

$$\text{COV}(X_i, Y_j) = \frac{\sum_{k \in i, j} F_{XY, k} \phi_{i, k} \phi_{j, k}}{\phi_i \phi_j} \quad (15)$$

LB = 1

$$\text{COV}(X_i, Y_j) = \frac{\sum_{k \in i, j} F_{XY, k} \phi_{i, k} \phi_{j, k} X_{i, k} Y_{j, k}}{\phi_i \phi_j} \quad (16)$$

LB = 2

$$\text{COV}(X_i, Y_j) = \frac{(\sum_{k \in i} F_{XY, k} \phi_{i, k} \phi_{i, k}) (\sum_{k' \in j} F_{XY, k'} \phi_{j, k'} \phi_{j, k'})}{\phi_i \phi_j} \quad (17)$$

LB = 3

$$\text{COV}(X_i, Y_j) = \frac{(\sum_{k \in i} F_{X, k} \phi_{i, k} X_{i, k}) (\sum_{l \in j} F_{Y, l} \phi_{j, l} Y_{j, l})}{\phi_i \phi_j} \quad (18)$$

LB = 4

$$\text{COV}(X_i, Y_j) = \frac{\sum_{k \in i, j} F_k (\sum_{l \in i} F_{XY, l} \phi_{i, l} X_{i, l}) (\sum_{l' \in j} F_{XY, l'} \phi_{j, l'} Y_{j, l'})}{\phi_i \phi_j} \quad (19)$$

LB = 5

$$\text{COV}(X_i, Y_j) = \frac{\sum_{k \in i} \sum_{k' \in j} F_{XY; k, k'} \phi_{i, k} X_{i, k} \phi_{j, k'} Y_{j, k'}}{\phi_i \phi_j} \quad (20)$$

Here we have used the following definitions:

$\text{COV}(X_i, Y_j)$ = Multigroup covariance of reaction X, group i, and reaction Y, group j.

ϕ_i = Multigroup flux for user group i.

$X_{i, k}$ = Multigroup cross section for reaction X for a supergroup (i, k) constructed from the union of energy boundaries of the E_k table from uncertainty file and those from user

input. $\phi_{i,k}$ is the flux for this group.

F's = Components of covariance taken from F_k table in uncertainty files.

The "NC-type" sub-subsections can be processed by using the results from the "NI-type" calculations. For the case of the derived redundant cross sections, i.e., $LTY = 0$, let X be the cross sections of interest which are expressed as a linear combination of the other evaluated cross sections Y_m :

$$X_i = \sum_{m=1}^{NCI} C_m Y_{m,i} \quad (21)$$

where i is the group index and C_m 's are constant values, usually ± 1 .

Then the covariance matrix of X and the covariance matrices of X and Y_m from the contribution of this type can be easily obtained:

$$COV(X_i, X_j) = \sum_{m=1}^{NCI} \sum_{m'=1}^{NCI} C_m C_{m'} COV(Y_{m,i}, Y_{m',j}), \quad (22)$$

and

$$COV(X_i, Y_{m,j}) = \sum_{m'=1}^{NCI} C_{m'} COV(Y_{m',i}, Y_{m,j}), \quad m=1,2,\dots,NCI. \quad (23)$$

It is clear that our knowledge about the covariance matrices of Y_m and $Y_{m'}$, which should be entered and processed in "NI-type", is a necessity in order to process the "NC-type" sub-subsections.

As stated in the previous section, one of the main sources of information on covariances of cross sections between different materials comes from the ratio measurements. Let X and Y be the cross sections of interest and S be the "standard" cross sections involved in the ratio measurements. In principle, there are three possible cases regarding the covariances between reactions X , Y , and S :

Case 1. Only X Derived from S, $X = R^{XS}S$

$$\text{RCOV}(X_i, X_j) = \text{RCOV}(R_i^{XS}, R_j^{XS}) + \text{RCOV}(S_i, S_j) \quad (24)$$

$$\text{RCOV}(X_i, S_j) = \text{RCOV}(S_i, S_j) \quad (25)$$

Case 2. Both X and Y Derived from S, $X = R^{XS}S$ and $Y = R^{YS}S$

$$\text{RCOV}(X_i, X_j) = \text{RCOV}(R_i^{XS}, R_j^{XS}) + \text{RCOV}(S_i, S_j) \quad (26)$$

$$\text{RCOV}(X_i, S_j) = \text{RCOV}(S_i, S_j) \quad (27)$$

$$\text{RCOV}(Y_i, Y_j) = \text{RCOV}(R_i^{YS}, R_j^{YS}) + \text{RCOV}(S_i, S_j) \quad (28)$$

$$\text{RCOV}(Y_i, S_j) = \text{RCOV}(S_i, S_j) \quad (29)$$

$$\text{RCOV}(X_i, Y_j) = \text{RCOV}(S_i, S_j) \quad (30)$$

Case 3. X Derived from S and Y Derived from X, $X = R^{XS}S$ and $Y = R^{YX}X$

$$\text{RCOV}(X_i, X_j) = \text{RCOV}(R_i^{XS}, R_j^{XS}) + \text{RCOV}(S_i, S_j) \quad (31)$$

$$\text{RCOV}(X_i, S_j) = \text{RCOV}(S_i, S_j) \quad (32)$$

$$\text{RCOV}(Y_i, Y_j) = \text{RCOV}(R_i^{XS}, R_j^{XS}) + \text{RCOV}(R_i^{YX}, R_j^{YX}) + \text{RCOV}(S_i, S_j) \quad (33)$$

$$\text{RCOV}(X_i, Y_j) = \text{RCOV}(R_i^{XS}, R_j^{XS}) + \text{RCOV}(S_i, S_j) \quad (34)$$

$$\text{RCOV}(Y_i, S_j) = \text{RCOV}(S_i, S_j) \quad (35)$$

where R^{XS} , R^{YS} , and R^{YX} are the ratios from the measurements with the assumption that these ratios do not correlate each other and there are no correlations between the ratios and the "standard" cross sections. If these correlations do exist, Eqs. (24-35) would appear in a more complex formation.

V. A Programmer's Guide for UNCER

V-1. General Information

The UNCER processor was written to generate the data covariance matrices from the ENDF/B-V uncertainty files. Multigroup covariance matrices are constructed according to Eqs. (15-35) in the preceding

section. The total covariance matrix for a pair of reaction types, which are designated by (MAT1,MT1) and (MAT2,MT2), is the sum of the partial matrices resulting from the processing of each sub-subsection contained in that particular subsection.

This code is unique in that the source of the fine group reaction cross sections is the DLC series of data libraries in the RSIC collections. Among those libraries, the following are most recommended for the purpose of this code: (1) DLC-41B/VITAMIN-C, 171 neutron and 36 photon groups; (2) DLC-42B/CLEAR, 126 neutron and 36 photon groups; (3) DLC-43B/CSRL, 218 neutron groups; (4) DLC-52/EPRMASTER, 100 neutron groups. These libraries are all in AMPX⁽⁵⁾ master interface format and the relevant contents of the reaction cross section files will be extracted by a program, called DLC1D, to create a fine group reaction cross section file N12 as one of the input units for PUFF-DLC. The binary form of the uncertainty files, stored in unit N13, are constructed by a program ERROR from the original ENDF/B-V files in BCD format. The output file of this code, unit N23, can be used for either plotting the group cross sections, standard deviations, and correlation matrices by program PLOTMOV or converting to COVERX⁽⁶⁾ formats for further uncertainty analysis.

Figure 1 shows the relationship of UNCER with the auxiliary programs and the logical units assigned to the code. Having the same format as the output file, file N17 is used for storing information on the "standard" cross sections and is therefore needed only if the uncertainty files contain covariances involving the ratio measurements. Tables 1, 2, and 3 show the formats for data stored in files N12, N13, and N23, respectively. Four scratch units are also required for this code, i.e., N15, N16, N18, and N22.

Flow diagram by subroutines is presented in Fig. 2. Subroutines SUMMF, INVT, and MTNAME are directly taken from the original PUFF without changes. On the other hand, subroutines DANNY and PUFF, originally from PUFF code, were revised significantly in order to fit the format of ENDF/B-V files. The rest of the subroutines are completely new.

V-2. Input Data

Card No. 1 (10I4)

NGUSER	1-4	number of user groups
IWT	5-8	weighting option
		1: $1/E$
		2: $1/(E\sigma_t)$
		3: input weighting/E
		4: input weighting
N13	9-12	uncertainty file in binary format (default = 13)
N12	13-16	fine group cross sections file (default = 12)
N23	17-20	output file containing cross sections, relative standard deviations, and correlation matrices in user group structure (default = 23)
N22	21-24	scratch file storing supergroup cross sections (default = 22)
N15	25-28	scratch file storing standard deviations (default = 15)
N16	29-32	scratch file storing covariance matrices (default = 16)
N17	33-36	file in the format of N23 containing the information on "standard" cross sections (default = 17)
N18	37-40	scratch file (default = 18)

Card No. 2 (6E12.5) energy boundaries (eV) from high to low in user group structure

EBUSER(1)	1-12	high energy edge for the first group
EBUSER(2)	13-24	high energy edge for the second group
⋮		
EBUSER(NGUSER+1)		low energy edge for the last group

Card No. 3 (6E12.5) weighting function for the fine group cross sections,
 required only if IWT = 3 or 4

PHI(1)	1-12	weighting for the first group
PHI(2)	13-24	weighting for the second group
⋮		
PHI(NGFINE)		weighting for the last group

V-3. Output Descriptions

The output from UNCER lists the energy boundaries of the input user group structure and of the supergroup structure which is the union of the input structure and all the energy edges contained in the uncertainty file. The reaction MT numbers in the uncertainty file are also shown to serve the purpose of program checking. Then the series of result from UNCER processing for each pair of reaction types contained in the uncertainty files will be presented. For the pair of the same reaction types, the output lists the group numbers, high and low energy edges of each group, cross sections, and relative standard deviations in percentage. Also shown in the output is the correlation matrix with the values multiplied by 1000. For the covariances of the different reaction types, two sets of group cross sections and standard deviations will be presented. And the correlation matrix, likely to be asymmetric for the different reactions, will be shown with the column and row indices referring to the group numbers of the first reaction and of the second reaction respectively.

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Table 1. Data Format for File N12

Record No. 1 (R1) energy boundaries (eV) from high to low in fine group structure

NGG,EB(1),EB(2),.....,EB(NGFINE+1),

where, NGFINE is the total number of fine groups. NGG=NGFINE+1.

Record No. 2 (R2) fine group cross sections

MAT,MT,CS(1),CS(2),.....,CS(NGFINE).

⋮

Repeat R2 for all reaction cross sections.

⋮

MAT = 10000 signals the end of file N12.

Table 2. Data Format for File N13

There are three types of records used in file N13:

Record No. 1 (R1) MAT1,MT1,NC,NI,MAT,MF,MT

Record No. 2 (R2) LT, LB, NP2, NP, LTY, E1, E2

Record No. 3 (R3) D(I), I=1, 2, ..., NP2

A single sub-subsection contains two records, R2 and R3. For an "NI-type" sub-subsection, LTY is set to -1, E1 and E2 are two meaningless numbers. For an "NI-type" sub-subsection with LB = 5, we have NE = NP, NT = NP2, and LS = LT, where NE, NT, and LS are defined in Ref. 4.

A subsection has the following structure:

R1
 R2 } repeat NC + NI times.
 R3 }

A section may contain several subsections with different MAT1 and MT1. An R1 record filled with 1000 or 10000 signals the end of a section or the end of file N13, respectively.

Table 3. Data Format for Files N23 and N17

Record No. 1 (R1) energy boundaries (eV) from high to low in user group structure

NGG,EB(1),EB(2),.....,EB(NG+1),

where, NGG=NG+1, and NG is the total number of user groups.

Record No. 2 (R2) file identifications

NG,MAT1,MT1,MAT2,MT2

Record No. 3 (R3) group cross sections

CS1(1),CS1(2),...,CS1(NG); CS2(1),CS2(2),...,CS2(NG).

Record No. 4 (R4) group relative standard deviations (%)

RSD1(1),RSD1(2),...RSD1(NG); RSD2(1),RSD2(2),...,RSD2(NG).

Record No. 5 (R5) correlation matrix

CORR(1,1),CORR(2,1),...,CORR(NG,1),CORR(1,2),...,CORR(NG,NG).

Repeat R2, R3, R4, and R5 for different pairs of reactions.

⋮

MATEND,MATEND,MATEND,MATEND,MATEND.

Note: (1) MATEND = 10000 for signaling the end of file.

(2) For MAT1 = MAT2 and MT1 = MT2, the group cross sections and standard deviations of the second reaction will not be stored.

(3) For the correlation matrix element CORR(i,j), j and i refer to the group indices of the first reaction, designated by (MAT1,MT1), and of the second reaction, designated by (MAT2,MT2), respectively.

Fig. 1. Relationship of UNCER with the Auxiliary Programs

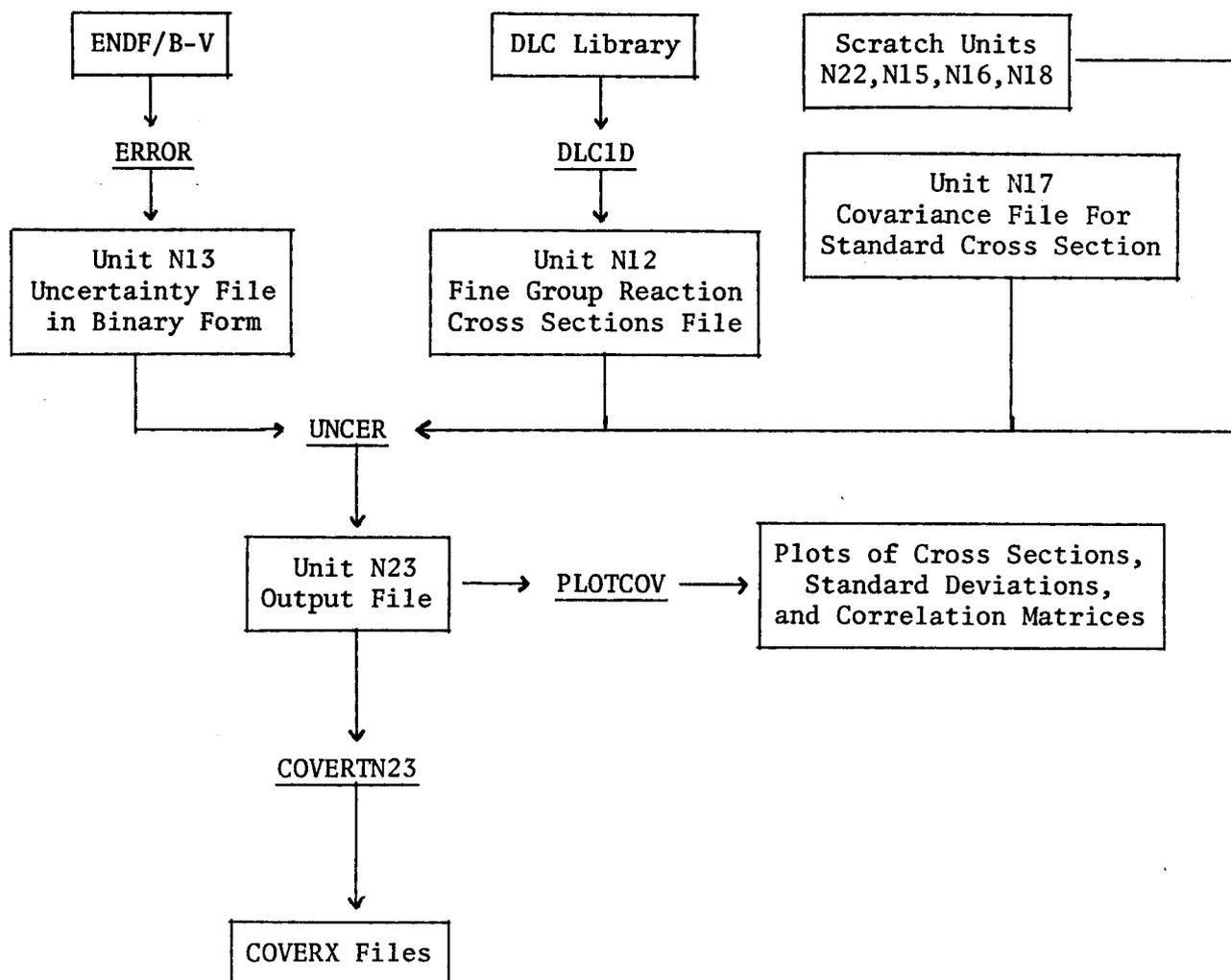
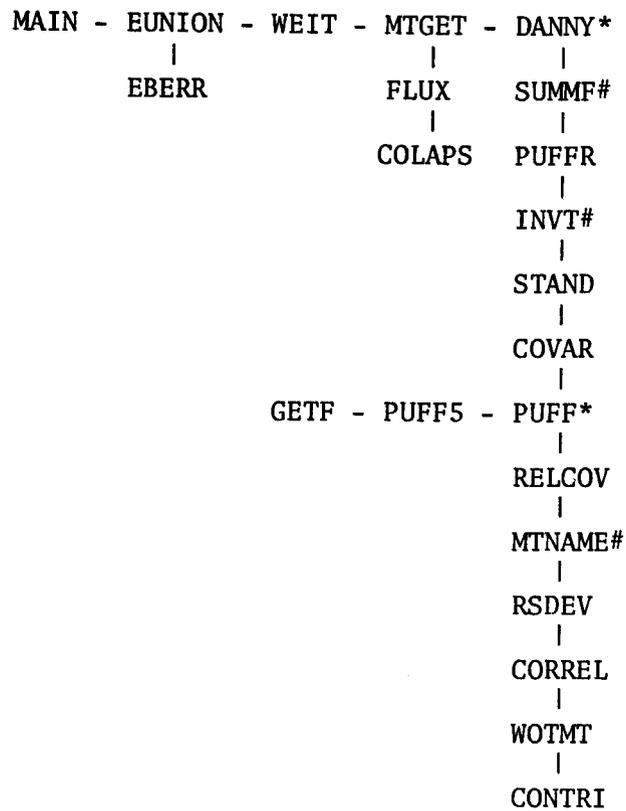


Fig. 2. Hierarchy of Subroutines in the UNCER Code



Directly taken from PUFF.

* Taken from PUFF with modifications

References

1. T. Wu and C.W. Maynard, "The Application of Uncertainty Analysis in Conceptual Fusion Reactor Design," Proc. of RSIC Seminar/Workshop on Theory and Application of Sensitivity and Uncertainty Analysis, August 1978 (to be published), also UWFD-290 (1978).
2. C.R. Weisbin, et al., "Cross Section and Method Uncertainties: The Application of Sensitivity Analysis to Study Their Relationship in Radiation Transport Benchmark Problems," ORNL/TM-4847 (ENDF-218) (1975).
3. C.R. Weisbin, et al., "MINX: A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," LA-6486-MS (ENDF-237) (1976).
4. F.G. Perey, "The Data Covariance Files for ENDF/B-V," ORNL/TM-5938 (ENDF-249) (1977).
5. N.M. Greene, et al., "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron Gamma Libraries from ENDF/B," ORNL/TM-3706 (1976).
6. J.D. Drischler and C.R. Weisbin, "Compilation of Multigroup Cross Section Covariance Matrices for Several Important Reactor Materials," ORNL-5318 (ENDF-235) (1977).

Appendix A.

Computer Code Abstract of UNCER

1. NAME OF CODE

UNCER: A University of Wisconsin Version of Uncertainty Files Processor for ENDF/B-V.

2. CODING LANGUAGE AND COMPUTER

Fortran IV; UNIVAC 1110.

3. NATURE OF PROBLEM SOLVED

Processing of cross section covariance matrices from ENDF/B-V Files 31 and 33⁽¹⁾ by utilizing the RSIC collection of fine group data libraries with AMPX⁽²⁾ interface. The results are then used for uncertainty analysis.

4. METHOD OF SOLUTION

The format of ENDF/B-V Files 31 and 33 allows two different types of sub-subsections, namely, the "NC-type" and "NI-type". The "NI-type" sub-subsections are used to describe explicitly the various components of the covariance matrix with the implementation of flag number, the LB flag, for indicating the nature of various components and their correlations as a function of energy. The processing procedure is therefore straightforward and basically a method of covariance matrix collapsing. On the other hand, the "NC-type" sub-subsections are used to describe the covariance matrices for the cross sections of interest which can be "derived" in terms of other "evaluated" cross sections in a certain energy range. Therefore, the processing procedure is basically a method of combining different covariance matrices within the framework of sta-

tistical theory⁽³⁾. The multigroup cross sections used in the computation are extracted from the RSIC collection of fine group data libraries. It is to be expected that this code should be very inexpensive to run by avoiding the time-consuming multigroup cross section processing procedure.

5. RESTRICTIONS OR LIMITATIONS

The current version of UNCER does not have the capability of processing the covariances of the resonance parameters in ENDF/B-V Files 32.

6. TYPICAL RUNNING TIME

Running time depends on the total number of user groups and the usage of "NC-type" sub-subsections in the uncertainty files. For the sample problem the running time on the UNIVAC 1110 is only several seconds.

7. AUXILARY ROUTINES

ERROR: Converting the uncertainty files from BCD to binary form.

DLC1D: Producing the fine group reaction cross sections from the RSIC data libraries with AMPX interface.

PLOTCOV: Plotting the covariance matrices from the UNCER output unit.

COVERTN23: Converting the output file into the COVERX format for the ORNL FORSS system.⁽⁴⁾

8. MACHINE REQUIREMENTS

UNCER was written in FORTRAN IV for the UNIVAC 1110. It can be run by most computers and is operable in any FORTRAN compiler. The maximum core requirement is less than $3x(NGUSER)^2$ words, where NGUSER is the total number of user groups. Thus for a 100 group problem, it needs less than 30 K words of core memory.

9. REFERENCES

- (1) F.G. Perey, "The Data Covariance Files for ENDF/B-V," ORNL/TM-5938 (ENDF-249) (1977).

- (2) N.M. Greene, et al., "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron Gamma Libraries from ENDF/B," ORNL/TM-3706, Oak Ridge National Laboratory (1976).
- (3) T. Wu and C.W. Maynard, "UNCER: A University of Wisconsin Version of Uncertainty Files Processor for ENDF/B-V," UWFD-291, University of Wisconsin-Madison (1978) (This report).
- (4) C.R. Weisbin, et al., "Application of FORSS Sensitivity and Uncertainty Methodology to Fast Reactor Benchmark Analysis," ORNL/TM-5563 (ENDF-236) (1976).

Appendix B.

Sample Problem

This sample problem is intended to cover all the possible formation in ENDF/B-V Files 31 and 33 and to have the processing result easy to interpret by using a uniform weighting function. A fictitious evaluation of material designated with MAT=9999 is used in this example. Eight reaction types are contained in File 33, i.e., MT=1,2,3,4,16,18,51, and 102. Therefore File 3 of MAT 9999 should at least have evaluations of these reactions. To make the result easy to interpret, the user group structure, fine group structure, and the uncertainty files have the same energy boundaries. Table B-1 shows the energy boundaries and the cross sections for different MT numbers.

Table B-1. Fine Group Cross Sections for MAT 9999

Reaction MT No.	Group No. and Energy Ranges (eV)				
	1	2	3	4	5
	$2 \times 10^7 - 10^7$	$10^7 - 10^6$	$10^6 - 10^5$	$10^5 - 10^4$	$10^4 - 10^{-5}$
1	4	4	4	4	4
2	1	1	1	1	1
3	3	3	3	3	3
4	2	1	0	0	0
16	1	0	0	0	0
18	1	1	1	1	1
51	1	1	0	0	0
102	0	1	2	2	2

Table B-2 summarizes the types of the fictitious covariance evaluations for different reactions. For the case of MT=18, it is assumed that in the energy range from 2×10^7 eV to 10^5 eV the cross sections of interest are derived from the ratio measurement relative to a fictitious "standard" cross section set with MAT=1261 and MT=18. Table B-3 tabulates the relevant information of this "standard" cross section set which is stored in file N17.

Table B-2. Summary of Evaluation of File 33 for MAT 9999

Reaction MT No.	Group No. and Energy Ranges (eV)				
	1	2	3	4	5
	$2 \times 10^7 - 10^7$	$10^7 - 10^6$	$10^6 - 10^5$	$10^5 - 10^4$	$10^4 - 10^{-5}$
1	NI	NI	NI	2+18+102	2+18+102
2	1-3*	1-3	1-3	NI	NI
3	NI	NI	NI	18+102	18+102
4	16+51	16+51	--	--	--
16	NI	--	--	--	--
18	NC(R)#	NC(R)	NC(R)	NI	NI
51	NI	NI	--	--	--
102	--	NI	NI	NI	NI

* Cross section derived as $\sigma(\text{MT}=1) - \sigma(\text{MT}=3)$.

NC-type, ratio measurement.

Table B-4 shows a complete listing of File 33 in BCD format for MAT 9999. It is our intention, in this fictitious evaluation, to have all possible forms allowed in the ENDF/B-V Files 33 except that of the "NC-type" sub-subsection with LTY = 3. This may not be typical of practical ENDF/B-V evaluations of the uncertainty files. The program ERROR is then used to convert File 33 from BCD format to a binary form described in Table 2 as an input file for UNCER.

Table B-3. Cross Sections, Standard Deviations, and
Correlation Matrix of a Fictitious "Standard" Cross
Sections Set

<u>Group No.</u>	<u>Energy Range (eV)</u>	<u>Cross Section</u>	<u>Standard Deviation (%)</u>
1	$2 \times 10^7 - 10^7$	1.0	3.0
2	$10^7 - 10^6$	1.0	3.0
3	$10^6 - 10^5$	1.0	3.0
4	$10^5 - 10^4$	1.0	3.0
5	$10^4 - 10^{-5}$	1.0	3.0

<u>Correlation Matrix</u>					
<u>Group No.</u>	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	<u>5</u>
1	1.0				
2	0.8	1.0			
3	0.09	0.7	1.0		
4	0.008	0.05	0.6	1.0	
5	0	0	0	0.5	1.0

The sample input is listed in Table B-5. Notice that the default values are used for all the logical units and a uniform flux spectrum is employed as the weighting function, i.e., IWT = 4. Table B-6 gives the sample printout from the execution of UNCER for this sample problem and the output file N23 should be saved for the purposes of plotting data covariance matrices or converting into the COVERX files for further uncertainty analysis.

Table B-5. Sample Input

5	4	2.0E07	1.0E07	1.0E06	1.0E05	1.0E04	1.0E-5
		1.	1.	1.	1.	1.	1.

USER ENERGY GROUP STRUCTURE-- 5 GROUPS

2.0000+07 1.0000+07 1.0000+06 1.0000+05 1.0000+04 1.0000-05

SUPER GROUP STRUCTURE (USER + ERROR)-- 5 GROUPS

2.0000+07 1.0000+07 1.0000+06 1.0000+05 1.0000+04 1.0000-05

ERROR FILE CONTAINS THE FOLLOWING REACTIONS

MT= 1 2 3 4 16 18 18 51 102

MATERIAL=9999 REACTION= 16---N,2N

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	1.0000+00	3.0000+01
2	1.0000+07	1.0000+06	0.0000	0.0000
3	1.0000+06	1.0000+05	0.0000	0.0000
4	1.0000+05	1.0000+04	0.0000	0.0000
5	1.0000+04	1.0000-05	0.0000	0.0000

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 16

ROW	COLUMN				
	1	2	3	4	5
1	1000	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0
5	0	0	0	0	0

MATERIAL=9999 REACTION= 18---N,F (TOTAL)

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	1.0000+00	3.7417+00
2	1.0000+07	1.0000+06	1.0000+00	3.7417+00
3	1.0000+06	1.0000+05	1.0000+00	3.3166+00
4	1.0000+05	1.0000+04	1.0000+00	5.0000+00
5	1.0000+04	1.0000-05	1.0000+00	5.0000+00

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 18

ROW	COLUMN				
	1	2	3	4	5
1	1000	871	146	0	0
2	871	1000	588	0	0
3	146	588	1000	0	0
4	0	0	0	1000	1000
5	0	0	0	1000	1000

MATERIAL=9999 REACTION= 51---N,NPRIME1

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	1.0000+00	5.0000+01
2	1.0000+07	1.0000+06	1.0000+00	6.0000+01
3	1.0000+06	1.0000+05	0.0000	0.0000
4	1.0000+05	1.0000+04	0.0000	0.0000
5	1.0000+04	1.0000-05	0.0000	0.0000

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 51

ROW	COLUMN				
	1	2	3	4	5
1	1000	333	0	0	0
2	333	1000	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0
5	0	0	0	0	0

MATERIAL=9999 REACTION= 102---N,GAMMA

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	0.0000	0.0000
2	1.0000+07	1.0000+06	1.0000+00	6.6933+00
3	1.0000+06	1.0000+05	1.0000+00	5.8566+00
4	1.0000+05	1.0000+04	1.0000+00	5.3666+00
5	1.0000+04	1.0000-05	1.0000+00	4.4721+00

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 102

ROW	COLUMN				
	1	2	3	4	5
1	0	0	0	0	0
2	0	1000	1000	0	0
3	0	1000	1000	0	0
4	0	0	0	1000	1000
5	0	0	0	1000	1000

MATERIAL 1=9999 REACTION 1= 18 , MATERIAL 2=1261 REACTION 2= 18

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	1.0000+00	1.0000+00	3.7417+00	3.0000+00
2	1.0000+07	1.0000+06	1.0000+00	1.0000+00	3.7417+00	3.0000+00
3	1.0000+06	1.0000+05	1.0000+00	1.0000+00	3.3166+00	3.0000+00
4	1.0000+05	1.0000+04	1.0000+00	1.0000+00	5.0000+00	3.0000+00
5	1.0000+04	1.0000-05	1.0000+00	1.0000+00	5.0000+00	3.0000+00

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 18 , ROW--MAT2=1261 MT2= 18

	COLUMN				
	1	2	3	4	5
ROW	-----				
1	802	641	81	0	0
2	641	802	633	0	0
3	72	561	905	0	0
4	0	0	0	0	0
5	0	0	0	0	0

MATERIAL=9999 REACTION= 1---TOTAL

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	4.0000+00	1.0000+01
2	1.0000+07	1.0000+06	4.0000+00	5.0000+00
3	1.0000+06	1.0000+05	4.0000+00	5.0000+00
4	1.0000+05	1.0000+04	4.0000+00	3.1004+00
5	1.0000+04	1.0000-05	4.0000+00	2.0917+00

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 1

	COLUMN				
	1	2	3	4	5
ROW	-----				
1	1000	0	0	0	0
2	0	1000	1000	0	0
3	0	1000	1000	0	0
4	0	0	0	1000	954
5	0	0	0	954	1000

MATERIAL=9999 REACTION= 2---ELASTIC

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	1.0000+00	1.3342+02
2	1.0000+07	1.0000+06	1.0000+00	9.9247+01
3	1.0000+06	1.0000+05	1.0000+00	7.0000+01
4	1.0000+05	1.0000+04	1.0000+00	1.0000+01
5	1.0000+04	1.0000-05	1.0000+00	5.0000+00

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 2

	COLUMN				
	1	2	3	4	5
ROW	-----				
1	1000	918	867	0	0
2	918	1000	964	0	0
3	867	964	1000	0	0
4	0	0	0	1000	1000
5	0	0	0	1000	1000

Table B-6. (Continued)

MATERIAL=9999 REACTION= 3---NONELASTIC

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	3.0000+00	4.2426+01
2	1.0000+07	1.0000+06	3.0000+00	3.2404+01
3	1.0000+06	1.0000+05	3.0000+00	2.2361+01
4	1.0000+05	1.0000+04	3.0000+00	2.4449+00
5	1.0000+04	1.0000-05	3.0000+00	2.2361+00

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 3

ROW	COLUMN				
	1	2	3	4	5
1	1000	982	949	0	0
2	982	1000	966	0	0
3	949	966	1000	0	0
4	0	0	0	1000	996
5	0	0	0	996	1000

MATERIAL=9999 REACTION= 4---TOTAL N,NPRIME

GROUP	E HIGH	E LOW	X-ION	STD.DEV.(%)
1	2.0000+07	1.0000+07	2.0000+00	2.9155+01
2	1.0000+07	1.0000+06	1.0000+00	6.0000+01
3	1.0000+06	1.0000+05	0.0000	0.0000
4	1.0000+05	1.0000+04	0.0000	0.0000
5	1.0000+04	1.0000-05	0.0000	0.0000

** CORRELATION MATRIX(*1000) ** MAT=9999 MT= 4

ROW	COLUMN				
	1	2	3	4	5
1	1000	286	0	0	0
2	286	1000	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0
5	0	0	0	0	0

MATERIAL 1=9999 REACTION 1= 1 , MATERIAL 2=9999 REACTION 2= 2

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	4.0000+00	1.0000+00	1.0000+01	1.3342+02
2	1.0000+07	1.0000+06	4.0000+00	1.0000+00	5.0000+00	9.9247+01
3	1.0000+06	1.0000+05	4.0000+00	1.0000+00	5.0000+00	7.0000+01
4	1.0000+05	1.0000+04	4.0000+00	1.0000+00	3.1004+00	1.0000+01
5	1.0000+04	1.0000-05	4.0000+00	1.0000+00	2.0917+00	5.0000+00

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 1 , ROW--MAT2=9999 MT2= 2

ROW	COLUMN				
	1	2	3	4	5
1	300	0	0	0	0
2	0	202	202	0	0
3	0	286	286	0	0
4	0	0	0	806	598
5	0	0	0	806	598

MATERIAL 1=9999 REACTION 1= 1 , MATERIAL 2=9999 REACTION 2= 18

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	4.0000+00	1.0000+00	1.0000+01	3.7417+00
2	1.0000+07	1.0000+06	4.0000+00	1.0000+00	5.0000+00	3.7417+00
3	1.0000+06	1.0000+05	4.0000+00	1.0000+00	5.0000+00	3.3166+00
4	1.0000+05	1.0000+04	4.0000+00	1.0000+00	3.1004+00	5.0000+00
5	1.0000+04	1.0000-05	4.0000+00	1.0000+00	2.0917+00	5.0000+00

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 1 , ROW--MAT2=9999 MT2= 18

ROW	COLUMN				
	1	2	3	4	5
1	0	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	403	598
5	0	0	0	403	598

MATERIAL 1=9999 REACTION 1= 1 , MATERIAL 2=9999 REACTION 2= 102

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	4.0000+00	0.0000	1.0000+01	0.0000
2	1.0000+07	1.0000+06	4.0000+00	1.0000+00	5.0000+00	6.6933+00
3	1.0000+06	1.0000+05	4.0000+00	1.0000+00	5.0000+00	5.8566+00
4	1.0000+05	1.0000+04	4.0000+00	1.0000+00	3.1004+00	5.3666+00
5	1.0000+04	1.0000-05	4.0000+00	1.0000+00	2.0917+00	4.4721+00

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 1 , ROW--MAT2=9999 MT2= 102

ROW	COLUMN				
	1	2	3	4	5
1	0	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	433	535
5	0	0	0	433	535

MATERIAL 1=9999 REACTION 1= 2 , MATERIAL 2=9999 REACTION 2= 3

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	1.0000+00	3.0000+00	1.3342+02	4.2426+01
2	1.0000+07	1.0000+06	1.0000+00	3.0000+00	9.9247+01	3.2404+01
3	1.0000+06	1.0000+05	1.0000+00	3.0000+00	7.0000+01	2.2361+01
4	1.0000+05	1.0000+04	1.0000+00	3.0000+00	1.0000+01	2.4449+00
5	1.0000+04	1.0000-05	1.0000+00	3.0000+00	5.0000+00	2.2361+00

** CORRELATION MATRIX(*1000) **

COLUMN--MAT1=9999 MT1= 2 , ROW--MAT2=9999 MT2= 3

COLUMN		1	2	3	4	5
ROW		1	2	3	4	5
1		-954	-962	-909	0	0
2		-937	-979	-926	0	0
3		-905	-946	-958	0	0
4		0	0	0	0	0
5		0	0	0	0	0

MATERIAL 1=9999 REACTION 1= 3 , MATERIAL 2=9999 REACTION 2= 18

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	3.0000+00	1.0000+00	4.2426+01	3.7417+00
2	1.0000+07	1.0000+06	3.0000+00	1.0000+00	3.2404+01	3.7417+00
3	1.0000+06	1.0000+05	3.0000+00	1.0000+00	2.2361+01	3.3166+00
4	1.0000+05	1.0000+04	3.0000+00	1.0000+00	2.4449+00	5.0000+00
5	1.0000+04	1.0000-05	3.0000+00	1.0000+00	2.2361+00	5.0000+00

** CORRELATION MATRIX(*1000) **

COLUMN--MAT1=9999 MT1= 3 , ROW--MAT2=9999 MT2= 18

COLUMN		1	2	3	4	5
ROW		1	2	3	4	5
1		0	0	0	0	0
2		0	0	0	0	0
3		0	0	0	0	0
4		0	0	0	682	745
5		0	0	0	682	745

MATERIAL 1=9999 REACTION 1= 3 , MATERIAL 2=9999 REACTION 2= 102

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	3.0000+00	0.0000	4.2426+01	0.0000
2	1.0000+07	1.0000+06	3.0000+00	1.0000+00	3.2404+01	6.6933+00
3	1.0000+06	1.0000+05	3.0000+00	1.0000+00	2.2361+01	5.8566+00
4	1.0000+05	1.0000+04	3.0000+00	1.0000+00	2.4449+00	5.3666+00
5	1.0000+04	1.0000-05	3.0000+00	1.0000+00	2.2361+00	4.4721+00

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 3 , ROW--MAT2=9999 MT2= 102

		COLUMN				
		1	2	3	4	5
ROW		-----				
1		0	0	0	0	0
2		0	0	0	0	0
3		0	0	0	0	0
4		0	0	0	732	667
5		0	0	0	732	667

MATERIAL 1=9999 REACTION 1= 4 , MATERIAL 2=9999 REACTION 2= 16

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	2.0000+00	1.0000+00	2.9155+01	3.0000+01
2	1.0000+07	1.0000+06	1.0000+00	0.0000	6.0000+01	0.0000
3	1.0000+06	1.0000+05	0.0000	0.0000	0.0000	0.0000
4	1.0000+05	1.0000+04	0.0000	0.0000	0.0000	0.0000
5	1.0000+04	1.0000-05	0.0000	0.0000	0.0000	0.0000

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 4 , ROW--MAT2=9999 MT2= 16

		COLUMN				
		1	2	3	4	5
ROW		-----				
1		514	0	0	0	0
2		0	0	0	0	0
3		0	0	0	0	0
4		0	0	0	0	0
5		0	0	0	0	0

MATERIAL 1=9999 REACTION 1= 4 , MATERIAL 2=9999 REACTION 2= 51

GROUP	E HIGH	E LOW	X-ION(1)	X-ION(2)	S.D.(1)	S.D.(2)
1	2.0000+07	1.0000+07	2.0000+00	1.0000+00	2.9155+01	5.0000+01
2	1.0000+07	1.0000+06	1.0000+00	1.0000+00	6.0000+01	6.0000+01
3	1.0000+06	1.0000+05	0.0000	0.0000	0.0000	0.0000
4	1.0000+05	1.0000+04	0.0000	0.0000	0.0000	0.0000
5	1.0000+04	1.0000-05	0.0000	0.0000	0.0000	0.0000

** CORRELATION MATRIX(*1000) **
 COLUMN--MAT1=9999 MT1= 4 , ROW--MAT2=9999 MT2= 51

		COLUMN				
		1	2	3	4	5
ROW		-----				
1		857	333	0	0	0
2		286	1000	0	0	0
3		0	0	0	0	0
4		0	0	0	0	0
5		0	0	0	0	0

***** PUFF PROCESSING COMPLETED *****