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COVARIANCE MATRICES IN EVALUATED NUCLEAR DATA

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COVARIANCE MATRICES IN EVALUATED NUCLEAR DATA

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ABSTRACT

The implications of nuclear data uncertainties for reactor calculations are shown. The origin of the formalism of the concepts of variance, covariance and correlation is analysed, by intuitive definitions. These concepts are also expressed with the help of the statistical theory. The format of the covariance data for ENDF/B is explained and formulae to obtain multigroup covariances are given.

I. INTRODUCTION

The purpose of the present study is to provide the researcher interested in uncertainties with practical guidance on the importance and significance of covariance data and their processing for multigroup calculations.

The study is divided into five sections.

Section I is a general introduction to the subject.

Section II shows the origin of the formalism by means of intuitive definitions of the concepts of variance, covariance and correlation. These concepts are illustrated in the case of a scalar and a vector quantity. It is also explained how the covariance matrix is obtained for an experimental cross-section measurement and in the case where the cross-section is obtained from a ratio. The same concepts which are introduced in Section II are expressed by means of the statistical theory in Section III.

The definitions are clarified and the format of data for ENDF/B-V files 31, 32 and 33 is explained in Section IV.

Section V explains the multigroup processing of uncertainty data specified in Section IV.

Nuclear data play a basic role in power reactor design and operational calculations. Uncertainties in these data propagate, giving rise to deviations in the final reactor parameters. It is therefore necessary to provide for some margin of possible error in reactor parameters so as to be able to ensure, for example, reactor behaviour as regards control and fuel burnup with sufficient accuracy for purposes of cost estimates.

Provision for such a margin of error involves an increase in reactor cost. This cost increase can be lowered if the uncertainties in the basic data are reduced.

Unfortunately, there are very few studies which analyse the consequences of nuclear data uncertainties. The paper of Greebler and co-workers [1] for fast reactors is a little old and needs updating.

Becker and Harris [2] recently made an analysis of the effects of nuclear data uncertainties on the fuel cost of a light-water reactor. Confirmation of these results by a similar study would be highly useful.

There are also some preliminary studies on the influence of uncertainties in cross-sections on fusion reactors [3,4].

C.R. Weisbin's [5] work makes a general survey of the current (1981) nuclear data uncertainties and of data requirements for nuclear power programmes.

I.1. Uncertainties, costs and required accuracies

Table I, taken from Ref. [1], shows the relationship between uncertainties in some data and their implications for a fast reactor (LMFBR) fuel cycle.

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The total cost of uncertainties in Table I amounts to 0.13 mill/kW(e)h or US \$900 000 [1] for 1970. (This value varies from country to country and with time). By reducing the uncertainties as is shown in the last column of Table I, it was aimed to bring down the extra cost to 0.03 mill/kW(e)h.

Table II, taken from Ref. [2], refers to a water-moderated thermal reactor.

It will be seen that in Table II the costs are calculated in United States dollars for the year 1985.

It is logically desirable to minimize the costs given in Tables I and II. Minimization of these costs imposes conditions on the maximum tolerable inaccuracy in the integral parameters of a reactor. As an example, we can look at Table III taken from Ref. [5].

The uncertainties in the basic nuclear data became so significant that it was necessary to include them with nuclear data in ENDF/B evaluations. These uncertainties, after processing, can be used together with sensitivity coefficients for computing error propagation in reactor parameters such as K_{eff} , conversion ratio etc. so that adjustments can be made.

II. ORIGIN OF THE FORMALISM

A very important aspect of reactor parameter calculation and analysis is the degree of reliability of the results obtained and its adequacy for the solution of a given problem.

Although the concepts of "experimental error" and "error propagation method" are well known, they seem to have been applied very little to reactor physics.

Considering that vast amounts of nuclear data are needed for reactor calculation, it appears almost impossible to apply the error propagation theory. Until recently, the quantity of data was so large from the standpoint of computation that it was not practical to perform the error propagation. However, with the development of the theory of sensitivity during the last decade it has been demonstrated that the partial derivatives appearing in the error theory can be obtained by simpler calculations like flux and adjoint flux which are solutions of the transport equation of the problem under study.

From this point of view reactor analysts have tried to obtain estimates of errors in the input nuclear data used in calculations. So far they have employed approximate estimates obtained by themselves. Aware of this problem, a group of specialists in the area called the Cross Section Evaluating Working Group decided some years ago to attempt to include these errors with the data in ENDF/B evaluations.

Although the present version of ENDF/B-V already contains a fair amount of data on these errors, the progress has been slow. This was due in part to the fact that the subject was new in the field of evaluations but basically because it was necessary to communicate an aspect of uncertainties which were not considered normally if there was correlation between different errors.

For reactor calculations it is important to know when and how an uncertainty affects several nuclear data. Since the amount of data involved is large, the uncertainties affecting data individually tend to be compensated while those affecting several data in the same manner tend to be additive. Some reactor calculation results are a function of relative values; in this case, the uncertainties tend to cancel each other out.

It is therefore necessary to describe the uncertainties in detail, specifying whether they are or are not common to several data ("covariances of evaluated data").

The greatest problem which evaluators have faced in generating covariances is that experimentalists do not supply sufficient information. An example of how experimentalists ought to proceed is provided by Ref. [6].

II.1.1. Concept of correlation

We consider an experiment in which quantities X and Z are measured.

Let ϵ_{i} i = 1, 2, 3...N n_{i} i = 1, 2, 3...N

be the set of two different errors for each quantity.

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With these values there may occur situations (a), (b), and (d) shown in Fig. 1.

The covariance between ε and n [7,8] is defined as

$$\sigma = E \left[(\varepsilon_{\tau}\mu_{\varepsilon}) (\eta-\mu_{\eta}) \right] = \lim_{N \to \infty} \sum_{i=1}^{N} (\varepsilon_{i}\mu_{\varepsilon}) (\eta_{i}-\mu_{\eta}) (A)$$

where μ_{ε} and μ_{η} are the expected values or the most probable value of ε and η . For example, in Fig. 1 in case (d) where ε and η are not correlated, the sum of the products $(\varepsilon_i - \mu_{\varepsilon}) (\eta_i - \mu_{\eta})$ can be positive or negative. There will be compensation and $\sigma_{\varepsilon} = 0$.

In case (a) in Fig. 1 $(\epsilon_i - \mu_{\epsilon})$ and $(n_i - \mu_{\eta})$ are always positive and it can be demonstrated that $\sigma_{\epsilon\eta} = \sigma_{\epsilon\eta} \sigma_{\epsilon\eta}$ is the highest value of covariance between two random variables. It is customary to define as the correlation factor

$$C_{e\eta} = \frac{\sigma_{e\eta}}{\sigma_{e\eta}}$$
, obviously $-1 \le C_{e\eta} \le +1$

(Value -1 indicates that the relationship between ϵ and η is inverse). II.2. Curvilinear co-ordinates and metric coefficients

Let P be a point with Cartesian co-ordinates (Y_1, Y_2, Y_3) and curvilinear co-ordinates (X_1, X_2, X_3) , the following being the functional relationship between the two systems:

$$x_{1} = x_{1}(Y_{1}, Y_{2}, Y_{3}) \quad x_{2} = x_{2} (Y_{1}, Y_{2}, Y_{3}) \quad x_{3} = x_{3} (Y_{1}, Y_{2}, Y_{3}) \quad (II-1)$$

We suppose that there is one-to-one correspondence between the points of each system and that there exists a continuous derivative in region R. It should also be possible to obtain the inverse relationship in this region.

 $Y_1 = Y_1(X_1, X_2, X_3)$ $Y_2 = Y_2(X_1, X_2, X_3)$ $Y_3 = Y_3(X_1, X_2, X_3)$ (II-2)



We consider a curve C in region R. Let dL be an infinitesimal length of the curve at a point p. Let \vec{r} be the positional vector to point P. So we can write:

In Cartesian co-ordinates:

$$\vec{r} = \vec{i}_{1}Y_{1} + \vec{i}_{2}Y_{2} + \vec{i}_{3}Y_{3}$$
(II-3)
$$d\vec{r} = \vec{i}_{1}dY_{1} + \vec{i}_{2}dY_{2} + \vec{i}_{3}dY_{3}$$
(II-4)
$$(dL)^{2} = d\vec{r} \cdot d\vec{r} = \sum_{i=1}^{3} (dY_{i})^{2}$$
(II-5)

In curvilinear co-ordinates
$$d\vec{r} = \vec{a}_1 dx_1 + \vec{a}_2 dx_2 + \vec{a}_3 dx_3$$
 (II-6)
where the basis vectors $\vec{a}_i = \frac{d\vec{r}}{dx_i}$ e $\vec{a}_i = S_i \vec{u}_i$ i = 1,2,3 (II-7)

(i the unit vector in the directon of \dot{a}_{i})

$$(dL)^{2} = d\vec{r}. d\vec{r} \sum_{i=1}^{3} \sum_{i=1}^{3} (\vec{a}_{i}.\vec{a}_{j}) dx_{i} dx_{j}$$
 (II-8)

We define

 $G_{ij} = \stackrel{\rightarrow}{a}_{i} \cdot \stackrel{\rightarrow}{a}_{j}$ (II-9) $(dL)^{2} = \sum_{i=1}^{3} \sum_{j=1}^{3} G_{ij} dx_{i} dx_{j}$

(II - 10)

therefore

G is symmetrical $G_{ij} = G_{ji}$ and is called the metric coefficient. Equation (II-9) can be written in the matrix form

$$(dL)^{2} = \begin{bmatrix} dx_{1} & dx_{2} & dx_{3} \end{bmatrix} \cdot \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \cdot \begin{bmatrix} dx_{1} \\ dx_{2} \\ dx_{3} \end{bmatrix}$$
(II-11)

$$\vec{G}$$
 being the matrix of elements G_{ij}
 $(dL)^2 = (d\vec{x})^T \cdot \vec{G} \cdot (d\vec{x})$, (II-12)

or taking into account (II-7)

$$(dL)^{2} = d\vec{r} \cdot d\vec{r} = \sum_{i=1}^{3} \sum_{i=1}^{3} (\hat{u}_{i} \cdot \hat{u}_{j}) S_{i} S_{j} dx_{i} dx_{j} \cdot (II-13)$$

By definition $C_{ij} = \mu_i \cdot \mu_j$, and the corresponding matrix is denoted by \overline{C} , elements C_{ij} of which satisfy

$$-1 \leq C_{ij} \leq +1$$
 $C_{ii} = 1$ $C_{ij} = C_{ji}$ (II-14)

and therefore

$$(dL)^{2} = \sum_{i=1}^{J} \sum_{i=1}^{J} C_{ij} S_{i} S_{j} dx_{i} dx_{j},$$
 (II-15)

or $(dL)^2 = (\overline{S} \cdot d\overline{x})^T \cdot \overline{C} \cdot (\overline{S} \cdot d\overline{x})$

$$\overline{\mathbf{s}} = \begin{bmatrix} \mathbf{s}_1 & \mathbf{0} \\ \mathbf{s}_2 \\ \mathbf{0} & \mathbf{s}_3 \end{bmatrix}$$

will be called sensitivity matrix

 $\vec{c} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}$

will be called correlation matrix for this system of curvilinear coordinates.

The infinitesimal length dL of a curve can therefore be calculated if the sensitivity matrix and the correlation matrix are known. The analogy of this formalism with the problem of error propagation is as follows: the curvilinear co-ordinates correspond to the parameters and the points on the curve to experimental values for different values of the parameters. The distance between two very close points will correspond to an uncertainty in the experimental value due to errors in the parameters (values of curvilinear co-ordinates). This uncertainty in the experimental value can be calculated if we know the sensitivity of the experimental value (point on the curve), the experimental parameters (i.e. the sensitivity matrix) and the correlation between the parameters (correlation matrix).

The covariance matrix is defined as

 $dx_{i} dx_{j} (i, j = 1, 2, 3).$

$$M_{ij} = C_{ij} dx_i dx_j$$
If $\vec{I} = \begin{bmatrix} 1\\ 1\\ 1 \end{bmatrix}$

Ιf

(II - 16)

(II - 17)

 (II_{-18})

(II-20)

(II - 19)

Equation (II-15) can be written as

 $(dL)^2 = (\overline{S}, \overline{I}) \quad . \quad \overline{M} \quad . \quad (\overline{S} \quad \overline{I}) \quad .$

The diagonal elements of C are always equal to one. For Cartesian co-ordinates the off-diagonal elements are zero. A system of Cartesian co-ordinates is a system of orthogonal co-ordinates, i.e. variables $Y_1 Y_2 Y_3$ can vary independently of each other. A system of curvilinear co-ordinates may or may not be orthogonal. If vectors a_i at a particular point p are not orthogonal (they are not <u>1</u>), a small displacement dx_i will also mean a change in another x_j for which coefficient C_{ij} is different from zero. If we apply this formalism to the theory of errors, we shall see that the errors in any two parameters are correlated provided there is locally a non-orthogonal relationship between the two parameters.

II.3. Error analyses for a scalar quantity

Let V be a quantity which is to be measured and suppose that it is a smooth function of n parameters $x_1 x_2 \cdots x_n$. By smooth function we mean that we expect the function and its derivatives to be continuous.

$$V = V (x_1, x_2, \dots, x_n) = V (\vec{x})$$

Let E_V be the uncertainty (error) in V resulting from uncertainties E_{x_1} of parameters \bar{X} . Applying (II-16)

$$E_v^2 = (\vec{S} \cdot \vec{E}_x)^T \cdot \vec{C} \cdot (\vec{S} \cdot \vec{E}_x)$$
 (II-23)



or applying (II-21)

$$E_{v}^{2} = (\vec{S} \cdot \vec{I})^{T} \cdot \vec{M}_{x} \cdot (\vec{S} \cdot \vec{I}) \cdot (II-25)$$
where
$$M_{x_{ij}} = C_{x_{ij}} E_{x_{i}} E_{x_{j}} (II-26)$$

(II - 21)

 (II_{-22})

(II - 24)

II.4 Interpretation of the covariance matrix

Sometimes it is preferable to work with \vec{E}_x and \vec{C}_x instead of \vec{M}_x since the elements of \vec{E}_x give explicit errors in the parameters and C_x gives an indication of the degree of correlation between them. M_x is more difficult to understand. We look at one explanation:

 (II_{-27})

(II - 29)

Let us define the differential of a vector

$$d\vec{v} = \sum_{i=1}^{m} \left(\frac{\partial v}{\partial x_i} \right) \quad d\vec{x}_i$$

If symbol < \cdots > is used to indicate an expectation value

 $M_{x_{ij}} = \langle dx_i \cdot dx_j \rangle$



defining

applying (II-25), we get

 $\langle d\vec{v} \cdot d\vec{v} \rangle = E_v^2$ (II-29A)

Equation (II-29) is used often as the definition of the covariance matrix. II.5. How to obtain the covariance matrix in an experimental measurement

The first step would be to catalogue all sources of error in parameters x and to decide what type of correlation exists between them.

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These errors should be expressed in units of these parameters so that we would have a table of the form:



Quantity e_{il} is the magnitude of the uncertainty in x_i due to the effect "l" (some e_{il} will be = 0). The elements of the covariance matrix are calculated as:

$$M_{x_{ij}} = \sum_{\ell=1}^{L} b_{ij_{\ell}} C_{i_{\ell}} C_{j_{\ell}} (i, j = 1....m) . \qquad (II-30)$$

b are correlation parameters which relate the components of error for x and y. They have the following properties:

$$b_{ii} = 1$$
 (i = 1,2...,m $\ell = 1,2...,L$),
 ℓ
and $-1 \leq b_{ij} \leq +1$ (i \neq j and $\ell = 1,..L$).
 ℓ

When the errors in x_i and x_j due to effect "2" are totally uncorrelated, $b_{ij} = 0$. When the error in x_i and x_j due to effect "2" are totally correlated in the positive sense, $b_{ij} = +1$; if totally anti-correlated $b_{ij} = -1$. Since the experimentalist does not obtain the covariance matrix, he should supply sufficient information for the evaluator to determine b_{ij} and to generate the covariance matrix.

Example:

Error in the ratio of two cross-sections. We know σ_1 and σ_2 and we want to find the error in the ratio σ_1/σ_2 .

$$R = R (\sigma_1, \sigma_2) = \sigma_1/\sigma_2$$

It is known that each cross-section has an uncorrelated error of 1% and a correlated error of 2%. This correlation exists because the two cross-sections were measured with respect to the same standard. It is therefore said that they are correlated positively. We set up the covariance matrix

Parameters	Uncorrelated components	Correlated components	Total error
σ	0,010 ₁	0.020 ₁	$\left[(0.01\sigma_1)^2 + (0.02\sigma_1)^2 \right] \frac{1}{2}$
σ ₂	0.01 ₉	0.020 ₂	$\left[(0.01\sigma_2)^2 + (0.02\sigma_2)^2 \right]^{1/3}$

We want to find E_R . For this purpose, we apply 24 instead of 26 because it will be easier to understand the propagation of the errors of the cross-sections

 $E_{R}^{2} = (\vec{S} \cdot \vec{E})^{T} \cdot \vec{C} \cdot (\vec{S} \cdot \vec{E})$

(II-23)

The sensitivity matrix is given by

$$\overline{S} = \begin{bmatrix} \frac{\partial R}{\partial \sigma_1} & 0\\ 0 & -\frac{\partial R}{\partial \sigma_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sigma_2} & 0\\ 0 & -\frac{\sigma_1}{\sigma_2^2} \end{bmatrix} ; e \overrightarrow{E} = \begin{bmatrix} E_{\sigma_1}\\ B_{\sigma_1}\\ B_{\sigma_2} \end{bmatrix}$$
(II-31A)

It remains to find C_{ij}. We recall that because of (16) C_{ij} = C_{ji} and C_{ii} = 1.

We point out that that $C_{12} = C_{21}$, and that because of (II-26)

$$C_{12} = \frac{M_{12}}{E_{\sigma_1} E_{\sigma_2}}$$
(II-32)

Because of (II-30) we have

We put

$$E_{\sigma_1}^2 = \left[(0.01\sigma_1)^2 + (0.02\sigma_1)^2 \right] e E_{\sigma_2}^2 = \left[(0.01\sigma_2)^2 + (0.02\sigma_1)^2 \right]^{1/2},$$
(II-32B)

therefore $C_{12} = 0.8$.

By multiplying, we have

$$E_{R}^{2} = \left(\frac{1}{\sigma_{2}}\right)^{2} E_{\sigma_{1}}^{2} + \left(\frac{-\sigma_{1}}{\sigma_{2}^{2}}\right)^{2} E_{\sigma_{2}} + 2 (0.8) \left(\frac{1}{\sigma_{2}}\right) \left(\frac{-\sigma_{1}}{\sigma_{2}^{2}}\right) E_{\sigma_{1}} E_{\sigma_{2}}$$

$$\left(\frac{E_{r}}{R}\right)^{2} = \left(\frac{E\sigma_{1}}{\sigma_{1}}\right) + \left(\frac{E_{\sigma_{2}}}{\sigma_{2}}\right)^{2} - 2. \quad (0.8) \left(\frac{E_{\sigma_{1}}}{\sigma_{1}}\right) \left(\frac{E_{\sigma_{2}}}{\sigma_{2}}\right). \quad (II-33)$$

Since $\frac{E_{\sigma_1}}{\sigma_1} \cong \frac{E_{\sigma_2}}{\sigma_2} \cong 0.02236$, we have $\left(\frac{E_r}{R}\right) \cong 0.0141$.

If the last term (i.e. the correlation term) in the equation were ignored, we would have

 $\left(\begin{array}{c} \frac{E}{r} \\ \frac{R}{r} \end{array}\right) \cong 0.03162 .$

In the case under study, inclusion of the correlation gave a smaller error because the ratio of the two cross-sections σ_1 and σ_2 is related and an element of the sensitivity matrix is negative.

If the relationship is the product of two cross-sections, the matrix elements will be positive and the last term in relation (33) will have a positive sign and the correlation will increase the error.

The expression for M_{12} is positive, indicating that there is a positive correlation between the errors in σ_1 and σ_2 , i.e. if σ_1 is too large, σ_2 also is too large.

If there is an anticorrelation, i.e. when one increases, the other decreases, M_{12} will have a negative sign. Care should be taken to distinguish the sign due to the type of correlation and that due to the sign of the sensitivity matrix.

II.6 Error analysis in the case of a vector

In the preceding section we saw how to obtain the error of one quantity dependent on several experimental parameters. However, it is sometimes necessary to obtain the error of several quantities dependent on several experimental parameters. We assume that m quantities $V_1 V_2 \dots V_m$ will be obtained from m parameters and that the relationship between them is defined by m continuous and differentiable functions represented by the vector equation $\vec{V} = \vec{V}(\vec{x})$.

The errors in parameters \dot{x} are represented by vector \vec{E}_x and \vec{C}_x is the correlation matrix for these errors. So the elements of the covariance matrix \vec{M}_y for values V are given by the expression

 $M_{v_{j,j}} = \left[\vec{s}_{i} \cdot \vec{E}_{x} \right]^{T} \cdot \vec{c}_{x} \cdot \left[\vec{s}_{j} \cdot \vec{E}_{x} \right] \qquad \left[i, j = 1, m \right] \quad (II-33A)$

The dimensions of the matrices are

$$\begin{array}{c} \overline{M}_{v} \longrightarrow m \times m \\ \overline{C}_{x} \longrightarrow n \times n \\ \overline{E}_{x} \longrightarrow n \end{array} \tag{II-33B}$$

We now have m sensitivity matrices of dimension m x n

$$\vec{s}_{i} = \begin{bmatrix} \partial V_{i} / \partial x_{1} \\ & \ddots & \partial V_{i} / \partial x_{k} \\ 0 & & \ddots & \partial V_{i} / \partial x_{n} \end{bmatrix} (i = 1, m) , \quad (II-34)$$

and the error in component i of V is given by

$$E_{vi} = \begin{bmatrix} M_{v_{ii}} \end{bmatrix}^{1/2} \qquad \qquad \qquad \begin{bmatrix} i = 1, m \end{bmatrix}, \qquad (II-35)$$

and the matrix of correlation between Vi and Vj by

$$C_{v_{ij}} = M_{v_{ij}} \begin{bmatrix} E_{v_i} & E_{v_j} \end{bmatrix} \qquad [i,j=1,m] \qquad (II-36)$$

Example

Let us consider two foils of different materials exposed to the same neutron flux. The activity of the foils is measured with the same detector and the cross-sections are calculated by the following formulae:



 $\sigma_1 = Y_1 / (F N_1)$

$$\sigma_2 = Y_2 / (F N_2)$$

Y = Yield or production rate
N = Number of atoms
F = Flux

(II-37)

Foil	Error in Y		Érror in N		Error in F	
	Uncorr.	Corr.	Uncorr.	Corr.		
1	3%	2%	0.5%	1%	4%	
2	5%	2%	0.7%	1%	4%	

The errors of the parameters are given in the following table:

A correlation exists between Y1 and Y2 and between N1 and N2. The error in the flux is fully correlated in the two foils because the flux is the same. The correlation between Y1 and Y2 could be due to the fact that the calibration factor for the efficiency of the two detectors is the same. The correlation between N1 and N2 was due to the use of the same balance.

There are five experimental parameters to be considered, namely $\sigma_1 = \sigma_1 (Y_1, Y_2, N_1, N_2, F)$, (11-39)

 $\sigma_2 = \sigma_2 (Y_1, Y_2, N_1, N_2, F)$, (II-40)with Y2 , N2 dummy variables in (39) and N1, N1 dummy variables in (40), we can write in terms of sub-matrices

Y₂ N₁ **,** 5 $\dot{\mathbf{x}}$ N (II-41) N 2 F E_{Yl} E_{Y2} E_{NI} E_{N2} Ē Ĕx (II_{-42})



Similarly for the correlation matrix we have:



and the sensitivity matrices are



$$\bar{s}_{2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & (\partial \sigma_{2} / \partial Y_{2}) \\ 0 & (\partial \sigma_{2} / \partial Y_{2}) \\ 0 & 0 & (\partial \sigma_{2} / \partial N_{2}) \\ 0 & (\partial \sigma_{2} / \partial F) \end{bmatrix} = \begin{bmatrix} \bar{s}_{2Y} & 0 \\ \bar{s}_{2N} \\ 0 & 2s \end{bmatrix} (II-47)$$

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Calculating the derivatives we have

$$(\partial \sigma_i / \partial Y_i) = 1/(FN_i) = \sigma_i / Y_i$$
 (i = 1, 2), (II-48)
 $(\partial \sigma_i / \partial N_i) = -Y_i / (FN_i^2) = -\sigma_i / N_i$ (i = 1, 2), (II-49)

$$S_{iF} = (\partial \sigma_i / \partial F) = -Y_i / (N_i F^2) = -\sigma_i / F$$
 (i = 1, 2) . (II-50)

The elements of the covariance matrix will be

$$M_{\sigma i j} = (\vec{s}_{i} \cdot \vec{E}_{x})^{T} \cdot \vec{c}_{x} \cdot (\vec{s}_{j} \cdot \vec{E}_{x})$$
 (i, j = 1, 2), (II-51)

$$M_{\sigma i j} = (\vec{s}_{iY} \cdot \vec{E}_{Y})^{T} \cdot \vec{c}_{YY} \cdot (\vec{s}_{jY} \cdot \vec{E}_{Y})$$

+ $(s_{iN} \cdot \vec{E}_{N})^{T} \cdot c_{NN} \cdot (\vec{s}_{jN} \cdot \vec{E}_{N})$ (II-52)

$$+ S_{iF} S_{jF} E_{F^{2}}$$
(i, j = 1, 2) .

$$M_{\sigma 11} = \sigma_{1}^{2} \left[\left(\frac{E_{Y1}}{Y1} \right)^{2} + \left(\frac{E_{N1}}{N_{1}} \right)^{2} + \left(\frac{E_{F}}{F} \right)^{2} \right],$$
(II-53)

$$M_{\sigma 12} = M_{\sigma 21} = \sigma_{1}^{\sigma} \sigma_{2} \left[C_{YY12} \left(\frac{E_{Y1}}{Y_{1}} \right) \left(\frac{E_{Y2}}{Y_{2}} \right) + C_{NN12} \left(\frac{E_{N1}}{N_{1}} \right) \left(\frac{E_{N2}}{N_{2}} \right) \left(\frac{E_{F}}{F} \right)^{2} \right],$$

(11-54)

$$M_{\sigma 22} = \sigma_2^2 \left[\left(\frac{E_{Y2}}{Y_2} \right)^2 + \left(\frac{E_{N2}}{N_2} \right)^2 + \left(\frac{E_F}{F} \right)^2 \right] .$$

or

(II-55)

The components of \vec{E}_x are: $\vec{E}_y \begin{pmatrix} E_{y1}^2 = (0.03 \ Y_1)^2 + (0.02 \ Y_1)^2 \\ E_{y2}^2 = (0.05 \ Y_2)^2 + (0.02 \ Y_2)^2 \\ (II-56) \end{pmatrix}$ (II-56)

$$\vec{E}_{N} \begin{cases} E_{N1}^{2} = (0.005 N_{1}) + (0.01 N_{1}), \\ E_{N2}^{2} = (0.007 N_{2})^{2} + (0.01 N_{2})^{2}, \\ E_{F}^{2} = M_{FF}^{2} = (0.04 F)^{2}. \end{cases}$$
(II-58)

In order to find Mo12 with the help of Eq. (54) we have to determine C_{YY12} and C_{NN12} , and for this purpose it is necessary to generate the covariance matrices M_{YY} and M_{NN} . In the explicit form they are:

$$\bar{M}_{YY} = \begin{bmatrix} E_{Y1}^{2} & (0.02 \ Y_{1}) \ (0.02 \ Y_{2}) \\ (0.02 \ Y_{1}) \ (0.02 \ Y_{2}) \\ (0.02 \ Y_{1}) \ (0.02 \ Y_{2}) \\ E_{Y2}^{2} \end{bmatrix} (II-59)$$
and
$$M_{NN} = \begin{bmatrix} E_{N1}^{2} & (0.01 \ N_{1}) \ (0.01 \ N_{2}) \\ (0.01 \ N_{1}) \ (0.01 \ N_{2}) \\ E_{N2}^{2} \end{bmatrix} (II-60)$$

$$\frac{E_{N12}^{2} & E_{N12}^{2} \\ E_{Y12}^{2} = C_{YY21} = M_{Y12} \ / \ (E_{Y1} \ E_{Y2}) = 0.2060 , \qquad (II-61)$$

$$C_{NN12} = C_{NN12} = M_{NN12} \ / \ (E_{N1} \ E_{N2}) = 0.7327 . \qquad (II-62)$$
It follows that
$$(E_{\sigma1}/\sigma_{1}) = (M_{\sigma11})^{1/2}/\sigma_{1} = 0.055 , \qquad (II-63)$$

$$(E_{\sigma2}/\sigma_{2}) = (M_{\sigma22})^{1/2}/\sigma_{2} = 0.068 . \qquad (II-64)$$

and the correlation coefficient connecting these two terms is

$$C_{\sigma 12} = C_{\sigma 21} = M_{\sigma 12} / (E_{\sigma 1} E_{\sigma 2}) \approx 0.56$$
 (II-64A)

i.e. the errors of (II-63) and (II-64) are correlated to within ~56% II.7 Combination of the standard error with the error of a ratio

A typical problem in the area of nuclear data is as follows: we measure a set of ratios of an unknown or little known cross-section to a set of standard cross-sections. The errors and correlations for the ratios can be derived if we know the experimental parameters, as was described in the preceding sections. The information on covariances for the standard cross-sections is available in the ENDF/B files. Suppose we want to obtain the cross-sections from the measurements of ratios Ri to the standard cross-section σ_i , i.e.

$$\sigma_i = R_i S_i$$

In vector notation we have

 $\vec{\sigma} = \vec{\sigma}(\vec{R},\vec{S})$.

Assuming that \vec{E}_R , \vec{C}_R , \vec{E}_S and \vec{C}_S are known we define

(i = 1, ..., n).



We are assuming that there is no correlation between R and S so that the diagonal elements of \vec{C}_{\downarrow} are = 0

(i,j = 1...n), (II-69)

 $M_{\sigma_{jj}} = \left(\overline{S}_{i} \cdot \overline{E}_{x} \right)^{T} \overline{C}_{x} \left(\overline{S}_{j} \cdot \overline{E}_{x} \right)$

(II-66)

(II-68)

(II - 67)

(II**-**65)

where s_{Ri} ō ŝ, (i = 1, n)(II**-**70) ਙ s∶ ō 0 s Ri $(\partial \sigma_i / \partial R_i)$ (i = 1, n)(II-71) 0 0 (20,/25) (i = 1, n)₹_{Si} (II_{-72}) 0 $(\partial \sigma_i / \partial R_i) = S_i = \sigma_i / R_i$ (i = 1, n)(II**-**73) $(\partial \sigma_i / \partial S_i) = R_i = \sigma_i / S_i$ (i = 1, n) $(\partial \sigma_i / \partial R_i) = S_i = \sigma_i / R_i$ (i = 1, n) $(\partial \sigma_i / \partial S_i) = R_i = \sigma_i / S_i$ (i = 1, n)

Equation (II-69) is transformed into

$$M_{\sigma ij} = (\vec{S}_{Ri} \cdot \vec{E}_{R})^{T} \cdot \vec{C}_{R} \cdot (\vec{S}_{Rj} \cdot \vec{E}_{R})$$

$$+ (\vec{S}_{Si} \cdot \vec{E}_{S})^{T} \cdot \vec{C}_{S} \cdot (\vec{S}_{Sj} \cdot \vec{E}_{S}) \quad (i, j = 1, n) \quad . \qquad (II-74)$$

We again see that if there is no correlation between R and S the problem is divided into two parts and becomes simpler

$$M_{\sigma i j} = \sigma_{i} \sigma_{j} \left[C_{R i j} \left(\frac{E_{R j}}{R_{i}} \right) \left(\frac{E_{R j}}{R_{j}} \right) + C_{S i j} \left(\frac{E_{S i}}{S_{i}} \right) \left(\frac{E_{S j}}{S_{j}} \right) \right] (i, j = 1, n),$$
(II-75)

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and hence we can calculate the error in the cross-section and its corresponding correlation matrix

$$E_{\sigma i} = (M_{\sigma i i})^{1/2} = \sigma_{i} \left[\left(\frac{E_{Ri}}{R_{i}} \right)^{2} + \left(\frac{E_{Si}}{S_{i}} \right)^{2} \right]^{1/2} \quad (i = 1, n) (II-75A)$$

$$C_{\sigma i j} = M_{\sigma i j} / (E_{\sigma i} E_{\sigma j}) \quad (i, j = 1, n) \quad .$$

We refer the reader to report [9] for further clarification of the topics treated here.

III. COVARIANCES OF EXPERIMENTAL DATA WITH THE APPLICATION OF STATISTICAL MATHEMATICS

In the foregoing sections we attempted to explain the concepts of variance, covariance and correlation, by means of analytical geometry and vector calculation. Such an approach is more intuitive and less abstract and hence more suitable as an introduction to the subject.

In the following sections the same concepts are defined again with the use of the formalism of statistical mathematics. This approach is more abstract but also more precise and suitable for representation of data in the ENDF/B files.

The "real value" of a physical quantity is in fact never known; all that the experimentalist can do is to determine quantities which are as close as possible to the real value.

Each experimental value should be taken as an estimate of the "real value" and be therefore accompanied by an uncertainty expressing the accuracy of the experimental value.

The uncertainty can be defined by statistical theory (we shall later see how).

III.1 Definitions

Let ϕ (x) be the probability density function of the random variable X. The expected value is defined as

 $\langle x \rangle = \mu = \int_{-\infty}^{+\infty} x \phi(x) dx.$

(III-1)

Symbol < > is used here to indicate the expected value and Eq. (III-1) represents the <u>first moment</u>. The <u>second moment</u> is defined as

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \phi(x) dx$$
,

 $dx = x-\mu$ being the value of the deviation between x and the expected value μ .

Variance is defined as the expected value of the square of dx.

(III-2)

Var (x)	= < dx dx	$> = < x^2$	`>	- <×>	2.	(III - 3)
Standard	deviation =	$\sqrt{Var(x)}$		•		(111-4)

It will be noted that no assumption was made about the form of the probability density function; in particular it was not assumed that "x" had a normal distribution (Gaussian form). The given equations are valid if the integrals exist, i.e. if they have finite values.

(a) Probability density function of several variables

Although the definitions which follow are valid for several variables, we shall use only two variables in order to simplify the consideration. Let x and y be two dependent variables and $\phi(x,y)$ their probability function. The first and second moments are defined as before

$$\langle x \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{\infty} y \phi(x,y) dx dy,$$

$$\langle y \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y \phi(x,y) dx dy,$$

(III-5)

and

Var $(x) = \langle dx dx \rangle$, Var $(y) = \langle dy dy \rangle$, (III-6) and the <u>covariance</u> of x with y

Cov.
$$(x,y) = \langle dx dy \rangle = \langle xy \rangle - \langle x \rangle \langle y \rangle$$
. (III-7)

Correlation coefficient

$$Corr (x,y) = \frac{Cor(x,y)}{\sqrt{var(x)} \sqrt{var(y)}} \frac{\langle dx dy \rangle}{\sqrt{dx dx} \sqrt{dy dy}} , \quad (III-8)$$

where the following inequality holds good:

$$-1 \leq Corr (x,y) \leq +1$$

If x and y are independent,

$$\phi(x,y) = \phi_1(x) \phi_2(y)$$
, (III-9)

then

$$\langle x y \rangle = \int_{-\infty}^{\infty} x \phi_1(x) dx \int_{-\infty}^{\infty} y \phi_2(y) dy = \langle x \rangle \langle y \rangle$$
, (III-9A)

and substituting in III-7 we obtain

$$\langle dx dy \rangle = 0$$
 . (III-10)

This means that if the covariance of two independent variables is = 0, the reciprocal is not valid (unless the density function has a normal distribution).

(b) Linear function

For a linear function,

$$f = \sum_{i} a_{i} x_{i} ,$$

the expected value is given by the sum of the expected values of all the variables

$$\langle f \rangle = \sum_{i} a_{i} \langle x_{i} \rangle$$
, (III-11)

and the variance is therefore

$$\operatorname{Var}(f) = \langle \operatorname{df} \operatorname{df} \rangle = \sum_{i} \sum_{j} a_{i} a_{j} \langle \operatorname{dx}_{i} \operatorname{dx}_{j} \rangle, \quad (\text{III-12})$$

(III-10A)

Eq. (12) can be written as

$$\langle df df \rangle = \sum_{i} a_{i}^{2} \langle dx_{i} dx_{i} \rangle + \sum_{i} \sum_{\substack{i \ i \neq j}} a_{i} a_{j} \langle dx_{i} dx_{j} \rangle$$
$$= \sum_{i} a_{i}^{2} Var(x_{i}) + \sum_{\substack{i \ i \neq j}} \sum_{j} a_{i} a_{j} Cov (x_{i}x_{j})$$
(III-13)

$$\langle dx_i dx_j \rangle = \langle dx_j dx_i \rangle$$
 (III-13A)

we can also write

$$Var(f) = \sum_{i} a_{i}^{2} Var(x_{i}) + 2 \sum_{i} \sum_{j} a_{i}a_{j} Cov(x_{i}x_{j})$$
 (III-14)

The first term represents the classical rule of error propagation for independent variables and the second term takes into account that the variables are interdependent.

(c) Non-linear functions
$$\langle x_i \rangle = \mu_i$$

If it is possible to represent the function by a first-order Taylor expansion

$$f(x_{i}) = f(u_{i}) + \sum_{i} \frac{\partial f}{\partial x_{i}} | (x_{i} - x_{j}), \qquad (III-16)$$

we define

$$a_{i} = \frac{\partial f}{\partial x_{i}} \bigg|_{\mu} , \qquad (III-17)$$

then

$$f(x_{i}) - f(u_{i}) + \sum_{j} a_{i} (x_{i} - u_{i})$$
,

and the expectation value is given by

$$\langle f(x_i) \rangle - f(\mu_i) = \overline{f}$$

(III-19)

(III-18)

with

$$dx_i = x_i - \mu_j$$
 (III-19A)
(d) Application to cross-sections

A function (cross-section) is often represented by a product or a ratio of cross-sections $\dot{}$

$$f(x_i) = \pi_i x_i$$
 ou $(f(x_i) = \frac{1}{\pi_i} x_i)$. (III-22)

Therefore the coefficient is

$$\mathbf{a}_{\mathbf{i}} = (\overset{+}{-}) \quad \frac{\overline{f}}{\mu_{\mathbf{i}}} \tag{III-22A}$$

In this case, it is convenient to introduce the relative variances (denoted by the symbol δ instead of d)

Rel. Var(f) =
$$\langle \delta f \delta f \rangle$$
 = $\langle \frac{df}{f} \frac{df}{f} \rangle$ (III-23)

and III-21 is transformed into

$$\langle \delta f \ \delta f \rangle = \sum_{i} \langle \delta x_{i} \ \delta x_{i} \rangle + \sum_{i} \sum_{j} b_{i} b_{j} \ \langle \delta x_{i} \ \delta x_{j} \rangle$$

$$b_{i} = \begin{cases} +1 \ \text{for a product} \\ -1 \ \text{for a ratio} \end{cases}$$

It will be noted that:

Equations III-21 and III-24 are valid provided that the expansion in a first-order Taylor series is valid,
 i.e. (III-24A),

$$\langle dx_i dx_i \rangle \ll \mu_i^2$$

(III-24A)

(ii)

The first term of Eqs (III-21) and (III-24) is always positive (quadratic form of the classical formula of "error propagation"). The sign of the second term depends on the sign of a_i and b_i .

Therefore,

$$df = f - \overline{f} = \sum_{j} a_{j} dx_{j} , \qquad (III-20)$$

$$Var (f) = \langle df df \rangle = \sum_{i} a_{i}^{2} \langle dx_{i} dx_{j} \rangle + \qquad (III-21)$$

$$\sum_{i} \sum_{\substack{j \\ (i \neq j)}} a_{i} a_{j} \langle dx_{i} dx_{j} \rangle .$$

This means that the problem was linearized with coefficients a given by Eq. (III-17).

III.2. Estimate of the parameters of the probability density function

In general, in physics if one wants to know the value of a quantity, it is measured several times and thus a set of values is obtained

$$X_{i}, i = 1...n$$

This set is called a population or a sample and is associated with a probability density function. This function is characterized by two parameters - <u>expected value</u> of the quantity and <u>variance</u>, which define an interval within which this quantity will lie. To obtain estimates of these parameters, we seek the average of the sample

$$\bar{X} = \frac{1}{n}$$
 $\sum_{i=1}^{n}$ X_{i} , (III-22)

and the variance of the sample

$$S = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2$$
, (III-23)

 \overline{X} and S can be regarded as the best estimate of μ and var (x), respectively. Frequently attempt is made to differentiate between "statistical" error and "systematic" error. The only real difference between the two is that the former can really be estimated from the laws of the probability

theory III-22 and III-23, while the latter is generally due to lack of information to correct the results supplied by the measurement apparatus. In nuclear physics experiments, generally the statistical component of uncertainty (counting uncertainty) can be kept small and the "systematic component" appears dominant.

IV. DEFINITIONS USED IN ENDF/B AND FORMAT OF DATA

Let X_i and Y_j be two variables which represent the crosssection for a reaction of type X and energy i and a reaction of type Y and energy j. The covariance matrix (or the absolute covariance matrix) can be written as

$$Cov(X_i, Y_j) = \langle (X_i - \hat{X}_i) | (Y_j - \hat{Y}_j) \rangle$$

Where the symbol < > denotes the expectation value and the symbol ^ the average value. Using IV-1 we can then define the relative covariance matrix as

Rel. Cov(X_i,Y_j) =
$$\frac{Cov(X_j,Y_j)}{X_i Y_j}$$

the standard deviation as

St.dev.
$$(X_i) = Cov(X_i, X_i)$$

and the relative standard deviation

Rel.st.dev.
$$(X_i) = \frac{\text{St.dev}(X_i)}{X_i}$$
 (IV-4)

The correlation matrix also can be defined as

$$\operatorname{Corr}(X_{i}, Y_{j}) = \frac{\operatorname{Cov}(X_{i}, Y_{j})}{(\operatorname{St.dev}(X_{i}))(\operatorname{St.dev}(Y_{j})),}$$
(IV-5)

or

$$Corr(X_{i}, Y_{j}) = \frac{Rel.Cov(X_{i}, Y_{j})}{(Rel.st.dev.(X_{i}))(Rel.st.dev.(Y_{j}))}.$$
 (IV-6)

(IV-2)

(IV-3)

(IV-1)

The correlation matrix gives the degree of correlation between X, and Y, and its absolute value should be ≤ 1

$$\operatorname{Corr}(X_{i}, Y_{j}) \mid \leq 1$$
.

When corr. $(X_i, Y_i) = 0$, variables X_i and Y_i are said to be totally uncorrelated. When corr. $(X_i, Y_i) = +1$ or -1, the variables are said to be totally correlated or totally anticorrelated, respectively.

(IV-7)

It should be noted that the terms covariance and uncertainty are used without distinction as synonyms.

IV.1 Format of covariance data in ENDF/B-V.

The ENDF/B microscopic data are grouped in the files in accordance with their types. For example, file 1 contains microscopic data for v (average number of neutrons per fission), file 2 the resonance parameters and file 3 the microscopic background cross-sections. The number of the covariance file is determined by adding 30 to the file number of the respective microscopic data. For example, file 31 contains the uncertainties for v, file 32 the uncertainties of the resonance parameters and file 33 those of the background cross-sections. For the time being these are the only covariance files of ENDF/B-V (in future they are to be extended to other files).

Files 31 and 33 have the same structure which is as follows. Each file is divided into <u>sections</u>, <u>sub-sections</u> and <u>sub-sub-sections</u>. One section refers specifically to the uncertainty in a type of reaction or to a specific MT, i.e. a section related to a total cross-section MT = 1 only describes the uncertainties referring to the total crosssection.

A sub-section describes only a covariance matrix and a sub-subsection several independent components of the covariance matrix.

There are two types of sub-sub-sections: type "NI" and type "NC". The former is used for explicit description of the components of the covariance matrix of the sub-section.

The latter type is used to indicate that some or all components of the covariance matrix have already been described in a different subsection, the idea being to avoid duplication of description of NI type sections described already. (a) Sub-sub-sections of type NI

There are six different classes of possible NI sub-sub-sections, depending on the correlation which may be a function of energy.

The correlation class is indicated by a control variable LB. The six possible classes of correlation are:

$$Cov(X_{i},Y_{j}) = \sum_{k,k} P_{j;k}^{i;k} F_{xy,k} F_{xy,k}^{i} Y_{j}, \qquad (IV-10)$$

LB = 3

The relative component correlated over interval E_n and E_1

$$Cov(X_{i},Y_{j}) = \sum_{k,l} P_{j;l}^{i;k} F_{x,k}F_{y,l}X_{i}Y_{j},$$

LB = 4

The relative component correlated over all intervals ${\rm E}_1$ within each interval ${\rm E}_n$

$$Cov(X_{i},Y_{j}) = \sum_{k,l,l} P_{j;k,l}^{i;k,l}, F_{k} F_{xy,l}F_{xy,l}, X_{i} Y_{j}, \qquad (IV-12)$$

LB = 5

The relative component of the covariance matrix

$$Cov(X_{i},Y_{j}) = \sum_{k,k}^{\Sigma} p_{j;k}^{i;k} F_{xy,k,k} X_{i}Y_{j}$$
 (IV-13)

 X_{i} and Y_{i} were already defined. Functions F are uncertainties which are tabulated directly in ENDF/B. Operator P is defined as

$$P_{j;m,n,...}^{i;k,\ell,...} = S_{i}^{k} S_{i}^{\ell} \dots S_{j}^{m} S_{j}^{n} \dots,$$
(IV-13A)
where $S_{i}^{k} = 1$ se $E_{k} \leq E_{i} \leq E_{k+1}$,

(IV-13B)

(IV-11)

and
$$S_{i}^{k} = 0$$
 se $E_{k} > E_{i} > E_{k+1}$

(IV-13C)

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Sub-sub-sections of type NC

A sub-sub-section of type NC is used to describe the covariance matrices in energy intervals where the cross-section was obtained from another cross-section.

- 31

Sub-sub-sections of type NC can be divided into two categories:

(i)

Those having a control variable LTY = 0, which means that in interval E_1 , E_2 these cross-sections were obtained as a linear combination of other reactions having the same MAT number but a different MT number, i.e.

MAT C. X(E) M. XXE) = MT

(IV - 14)

 ${\rm C}_{\rm i}$ are constant in interval ${\rm E}_{\rm 1}$ ${\rm E}_{\rm 2}$ and NCI denotes the number of sub-sub-sections "NC",

(ii)

The other category of sub-sub-section is that where the crosssection was obtained as a ratio and has a control variable LTY = 1, 2, 3. Evaluation of cross-sections based on ratios is used widely in ENDF/B and is the principal source of correlation. Let X_{MT}^{MAT} be the cross-section obtained in interval E_1 and E_2 from the ratio as the "standard"- cross-section MATR : MAT therefore X (E) = R(E) X (E), where R(E) is MT MTR X

the energy-dependent ratio.

LTY = 1 is used in a sub-section of X_{MT}^{MAT} to indicate that the latter is a ratio to

XMATR MTR

LTY = 2 is used to indicate a correlation between X_{MT}^{MAT} and X_{MTR}^{MATR} LTY = 3 is used in the reference material to indicate a correlation between

X^{MATR} MTR and XMAT

*/ Here"standard" cross-section is used in the sense that its covariance matrix is represented only by an NI type sub-sub-section.



MAT, 33, 0/b, b; b, b; b, b SEND

- (a) Heading of a section with covariance data for a reaction of type MT of material MAT.
- (b) NL is the number of sub-sub-sections which occur for different MAT 1, MT 1.
- (c) NC = Number of NC sub-sub-sections of the NC type. The first pair of records is an example for LTY = 0 and the second pair an example for LTY = 1 or 2. Cases LTY = 0 and LTY = 1 occur only when (MAT, MT) = (MAT1, MT1).
- (d) This sub-sub-section will be in sub-section (MAT, MT; MAT, MT) with LTY = 1 and in sub-sub-section (MAT, MT; MATS, MTS) with LTY = 2. In file 33 of the standard cross-section there will be a sub-sub-section with (MAT, MT; MATS, MTS) with LTY = 2.
- (e) There are NI of these sub-sub-sections. If a sub-sub-section with LTY = 1 exists, there will be at least one sub-sub-section of type NI giving the relative covariance of the ratio as the "standard" cross-section.

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(g)

Format for sub-sub-sections of type NI with LB = 0-4. For LB = 0-2 and LT = 0 there will only be the series of values E_k , F_k . For LB = 3 or 4, LT is the number of pairs E_2 , F_2 . NE energies E_n define a grid for a square matrix of relative covariances with elements F_{kk} . NT-NE is the number of given covariance elements. If LS = 0, the matrix can be asymmetric and NT = NE + (NE - 1)². If LS = 1, the matrix is symmetrical and the elements of the "upper half" are given by rows beginning with the diagonal and NE = NE (NE + 1)/2.

Covariances of v

The covariances for v (average number of neutrons per fission) are represented in file 31. The format is identical with that of file 33. It may be recalled in file 1, \overline{v} (MT = 452) \overline{v}_d (MT = 455) and \overline{v}_p (MT = 456) satisfy the relation \overline{v} (E) = \overline{v}_d (E) + \overline{v}_p (E).

Thus, if one of these quantities is derived from another, it is possible to use sub-sub-sections of type NC with LTY = 0 to describe the covariance matrix.

Covariances of the resolved-resonance parameters

In file 32 covariance data are available for the following resolved-resonance parameters:

Resonance energy (ER), total angular moment of resonance J, neutron width $\Gamma_n(GN)$, radiation width $\Gamma_\sigma(GG)$ and fission width $\Gamma_e(GF)$.

File 32 is used to express the uncertainties in resonance parameters. This type of data is available only for a few resonances of particular importance. Long range uncertainties which affect more than one resonance are treated in file 33.

For more details about the format the reader may refer to report [10].

COVARIANCE MATRICES IN A MULTIGROUP FORM

We first define the different energy grids used in the calculation.

<u>Cross-section grid</u> is the multigroup structure in which the cross-sections were processed.

<u>User's grid</u> is the structure in which the user desires to obtain covariances.

Evaluation grid is the grid in which the evaluator expresses the uncertainties.

Super grid is the combination of the user's grid with the evaluation grid and is needed for processing covariances due to ratio measurements (Eq. IV-15).

<u>User's super grid</u> is the combination of the user's grid with the limits of covariance intervals of cross-sections obtained as the sum of other cross-sections (Eq. IV-14). This grid is necessary for processing covariances which are linear combinations of other covariances.

In order to calculate the covariances in the user's grid, we need to know the flux and cross-sections in the super grid. For this purpose, we have to interpolate. The most convenient method is the one used by J.D. Smith III (Ref. [11]).

V.1. Multigroup covariances for sub-sub-sections of type NI

Assuming that no correlation exists between the flux and the cross-section of interest, we calculate the multigroup covariance matrices by the following formulae [12]:

LB = 0,

·V.

$$C_{ov}(X_{G}, Y_{H}) = \frac{\sum_{k \in G, H} F_{xy, k} \phi_{G, k} \phi_{H, k}}{\phi_{G} \phi_{H}}$$

LB = 1,

$$Cov(X_{G}, Y_{H}) = \frac{\sum_{k \in G, H} F_{xy, k} \phi_{G, k} G_{, k} \phi_{H, k} Y_{H, k}}{\phi_{G} \phi_{H}}$$

(V-2)

(V-1)

$$LB = 2,$$

$$Cov(X_{G}, Y_{H}) = \frac{\left(\sum_{k \in G} F_{xy,k}^{\phi}G_{,k}X_{H,k}\right) \left(\sum_{k' \in H} F_{xy,k'}^{\phi}H_{,k'}Y_{H,k'}\right)}{\varphi_{G}^{\phi}H}$$

$$LB = 3$$

$$Cov(X_{G}, Y_{H}) = \frac{\left(\sum_{k \in G} F_{x,k}^{\phi}G_{,k}X_{G,k}\right) \left(\sum_{L \downarrow H} F_{y, \downarrow}^{\phi}H_{,L}Y_{H,L}\right)}{\varphi_{G}^{\phi}H}$$

$$(V-3)$$

$$LB = 4$$

$$Cov(X_{G}, Y_{H}) = \frac{\sum_{k \in G, H} F_{k \in G} F_{x y, L} \circ G_{L} G_{L}}{\sum_{k \in G, H} F_{k \in G} F_{k \in G} F_{k \in G}} (V-5)$$

$$LB = 5,$$

$$Cov(X_{G}, Y_{H}) = \frac{d\varepsilon G, k' \varepsilon H}{d\varepsilon G, k' \varepsilon H}$$

$$(V-6)$$

where Cov (X_{G}, Y_{H}) = multigroup covariance between cross-section X of group G and cross-section Y of group G and cross-section Y of group H,

 ϕ_{G} = multigroup flux in group G,

 $X_{G,K}$ = multigroup cross-section for reaction X in the groups of the super grid (subscript G belongs to the evaluation grid of uncertainties and subscript K to the user's grid),

 $\phi_{G,k}$ = multigroup flux in the super grid,

F = covariance matrix components taken directly from the ENDF/B covariance files.

Sub-sub-sections of type NI form the basis for the construction of the NC type sub-sub-section and should therefore be processed first.

Multigroup covariances of type NC

LTY = 0

Let X be a cross-section obtained by means of linear combination of n other cross-sections Y.

$$X_{G} = \sum_{m=1}^{n} C_{m} Y_{G}^{m}$$

G is the subscript for group and C are constants generally +1 or -1.

(V-7)

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The uncertainty in X is expressed by

$$dx_{G} = \sum_{m=1}^{n} C_{m} dY_{G}^{m}$$
(V-8)

and the covariances between $X_{\mbox{\footnotesize G}}$ and $X_{\mbox{\footnotesize H}}$ and between $X_{\mbox{\footnotesize G}}$ and $Y_{\mbox{\footnotesize H}}$ are expressed by [11].

$$Cov (X_{G}, X_{H}) = \sum_{m=1}^{n} \sum_{m=1}^{n} C_{m} C_{m}, Cov (Y_{m,G}, Y_{m'H})$$
(V-9)

$$Cov (X_{G}, Y_{H}^{m}) = \sum_{m=1}^{n} C_{m} Cov (Y_{G}^{m'}, Y_{H}^{m})$$
(V-10)

$$LTY = 1, 2, 3$$

Let
$$R_G$$
 be the measured ratio of cross-sections X_G/Z_G
 $X_G = R_GZ_G$ (V-11)
The uncertainty in X_G is
 $dX_G = dR_G Z_G + R_G dZ_G$ (V-12)
from where [11]

Rel Cov
$$(X_G, X_H)$$
 = Rel Cov (R_G, R_H) + Rel Cov (Z_G, Z_H) (V-13)
and

Rel Cov
$$(X_{G}, Z_{H}) = \text{Rel Cov } (Z_{G}, Z_{H})$$

(V-14)

The multigroup covariances due to uncertainties in resolvedresonance parameters are calculated in the form shown in Ref. [11] and added to the covariances of file 33.

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VI. APPLICATIONS

At present evaluations of covariance data for dosimetry reactions are available in ENDF/B-V. As was noted in Section IV, these data are tabulated in files 32 and 33.

The ERROR module of the NJOY code [13] was implemented at the Institute of Advanced Studies. This module processes covariance files 32 and 33 and provides multigroup covariance matrices in accordance with Eqs (V-1) to (V-6).

Multigroup covariance matrices were obtained for some dosimetry reactions with the use of NJOY.

It is intended to study the propagation of these matrices in the calculation of the integral dosimetry parameters.

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<u>Fig. 1</u>.

Different degrees of correlation: (a) Perfect linear correlation; (b) moderate linear correlation; (c) non-linear correlation; (d) without correlation.

Table	I.	Data uncertainties up to 1970 and recommende	d
	-	accuracy goals for 1975	

••••••••••••••••••••••••••••••••••••••	Uncertain	ty (±1) (a)	Cost Uncertainty (tmill/KW(e)h)(b)	
Neutron Energy Range	Present (c)	<u>1975 Goal</u>	Present	1975 Coal
238 U a(n,y) 100 eV to 1 HeV	10	2	0,065	0.013
238 U g(n,f) 1 to 10 May	6:	3	0.013	0,006
238 U g(n,n') 100 keV to 10 MeV	20	5	0.025	0.008
239 Pu g(a,y) 0.1 to 500 keV	20	. 3	0.045	0,007
239 Pu g(n,f) 0.1 keV to 10 HeV	. 10	2	0,034	0.007
239 _{Pu} v >0.1 keV	2	0.5	0,050	0.013
239_{Pu} $\overline{E_{\chi}(2)} > 0.1 \text{ keV}$	10	1	0.033	0.006
240 Pu d(a,f) >1 keV	20	10	0.008	0,004
240 Pu σ(n,γ) 0.1 keV to: 1. HeV	30	10	0.004	0,001.
241 7u.σ(n,f) >0.1 keV	25	10:	0,007	0.003
Fiss. Prod. o(n,y) >0.1 keV	40 .	10.	0.038	0.010
Fe,Ni,Cr d(n,y) >0.1 keV Combined Data Uncertainties	30	10:	0.041 0.13 (4)	0,010 0,03 (4)

(a) Each data is assumed to be correlated over the energy range indicated.

(b) For a 1000 NW(e) reactor based on cost assumptions stated in Ref. [1] and estimated 90% confidence limits in data uncertainties.

(c) See Ref. [1].

(d) Statistical combination assuming separately listed data uncertainties are not correlated.

Nuclear Data (2200 m/s)	% Uncertainty in data	With recycling	BWR Without recycling	With recycling	PWR Without recycling
ci-252 v	0.24	332,540	438,970	384,720	558,790
2u-239 (α,γ)	1.22	233,810	309,980	277,312	406,450
-≥u239 v	0.28	-165,380	-219,780	-195,170	-285,570
ແ=235 ນີ້	0.21	-129,170	-171,540	-146,100	-213,500
2÷235 (¤,γ)	1.12	102,680	120,260	. 112,78	139,850
?u≈241 (a,y)	3.00	89,060	111,080	10-,1-3	143,700
Pu-239 (a,i)	0.34	- 77,480	-108,260	- 90,3-1	-137,790
Xe-135 (a, y)	7.50	55,660	83,300	71,332	81,710
Pu-241 (s,f)	1.00	- 41,040	- 56,930	- 47,133	- 69,970
Pu-241 V	0.34	- 40,370	- 53,820	- 43,123	- 70,640
C-235 (a,f)	0.22	- 37,170	- 58,850	- 40,173	- 67,260
8 (a,7)	0.60	32,740	46,930	27,111	43,600
1-238 (n,γ)	0.74	10,660	51,710	13,:22	58,550
Zr (n,1)	1.60	13,270	18,510	5,370	12,920
C-236 (a,y)	6.00	7,860	8,330	5,712	6,460
?=-147 (n,y)	2.92	3,820	4,050	, , 	6,290
B (n, y)	0,26	•	-	2,312	6,300
?u-240 (n,7)	0.50	1,090	2,780	2,2	5,390
Pu-242 (a, y)	5.00	2,180	2,310	÷:-	1,080
Cost		43,653,000	46,281,000	47,353,120	53,821,000

Table II. Implications of nuclear data uncertainties for a thermal reactor full cycle for a load, in 1985 US dollars

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	Uncertainty %	Uncertainty %	
Parameter	1982	Goal	
Keff	0.7	0.6	
Peak power/ Average power	4.7	3	
Control rod worth	5	3	
Doppler coefficient	10	10	• •
Sodium void. reactivity	20	17	

Table III. Uncertainties in the design parameters of a fast reactor (USA)

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