SUR, A Program to Generate Error Covariance Files

F. C. Difilippo

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Neutron Physics Division

SUR, A PROGRAM TO GENERATE ERROR COVARIANCE FILES

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*On assignment from Comisión Nacional de Energía Atómica, Argentina.

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Abstract

Covariance matrices were calculated for the $^{238}\text{U}$, $^{241}\text{Pu}$, and $^{239}\text{Pu}$ fission cross sections and for the $^{238}\text{U}$, $^{240}\text{Pu}$, $^{241}\text{Pu}$, and $^{239}\text{Pu}$ capture cross sections. A computer program was written which uses the evaluated ENDF/B data files and the measured or evaluated (from other evaluations) cross sections for the calculation of the uncertainty files. An effort has been made to make the output of the program consistent with the ENDF/B error files format. A user's manual for the present code and references utilized in the covariance matrix calculations are given.
I. INTRODUCTION

The economic impact of nuclear data uncertainties in fast breeder as well as in thermal reactors has been the subject of many studies.\textsuperscript{1-5}

To evaluate the effect of group cross-section uncertainties in sensitivity calculations, the correlation both within the group structure and among different isotopes has to be calculated. Extensive discussions of this procedure are given in refs. 6-8.

II. CALCULATION OF RELATIVE COVARIANCE MATRICES

The relative covariance matrix elements are defined here as:

\[ \text{COV}(I,J) = \left\langle \left( \frac{X^\ell_i - X_i}{X_i} \right) \left( \frac{X^\ell_j - X_j}{X_j} \right) \right\rangle, \quad (1) \]

where \( X^\ell_i \) and \( X^\ell_j \) are the group average cross sections for the \( i^{th} \) and \( j^{th} \) energy groups, respectively, for the \( \ell^{th} \) data set. The cross sections \( X_i \) and \( X_j \) are the reference ("true") values, which by convention are taken to be the corresponding ENDF/B values. The bracket denotes a weighted average over the ensemble of data sets, having common data in the \( i^{th} \) and \( j^{th} \) groups, where weights, \( W_\ell \), have been assigned to each data set.

The ENDF/B-IV files, used as the reference data, were energy-weighted by a flat weighting function in producing the group-average cross sections. Details of calculations are given in Sect. III.
The present study of the error covariance matrix implies an "external" analysis of the data. Each data set, whether the results of a measurement or of an evaluation, is assigned an arbitrary weight and is compared with a reference line taken to be the ENDF/B-IV evaluation.

III. BRIEF DESCRIPTION OF THE PROGRAM

The calculations were done by the code SUR, which, in its present form, only handles error correlation for a given cross-section data set within a given energy range. A description of the main steps in the program follows.

Step 1: The program sets the energy limits of the group structure for several options: (1) constant lethargy interval, (2) decimal interval, or (3) a mixture of the first two.

Step 2: For the ratio measurements, the standard reference cross section was always the ENDF/B-IV evaluation.

Step 3: The measurements corresponding to the data set $\lambda$, inside a group $j$, are reduced to the mean energy of the group. This is implemented by approximating the shape of the cross section with a parabola determined by the evaluated cross sections in groups $j - 1$, $j$, $j + 1$. Then, all the measurements corresponding to the data set $\lambda$, inside group $j$, are averaged.
Step 4: Whenever there are not measurements in the \( \ell \)th set of data, inside group \( j \), the program makes a linear interpolation of data set, \( \ell \), values corresponding to the neighboring groups. Before implementing the interpolation, the program searches whether or not the data points for the interpolation procedure are within energy limits preset by the user. If not, the interpolation is not made.

Step 5: Calculation of \( \text{COV}(I,J) \) is made. This is done by the formula

\[
\text{COV}(I,J) = \frac{1}{RR} \sum_{K=1}^{NA} \left[ \frac{\sigma(K,I) - \sigma(I)}{\sigma(I)} \right] \left[ \frac{\sigma(K,J) - \sigma(J)}{\sigma(J)} \right] W(K),
\]

where

\[
RR = \sum_{K=1}^{NA'} W(K),
\]

\( \sigma(K,I), \sigma(K,J) = \text{measured or interpolated cross sections of data set} \ K, \text{in groups} \ I \text{and} \ J, \)
\( \sigma(I), \sigma(J) = \text{evaluated cross sections of groups} \ I \text{and} \ J, \)
\( W(K) = \text{weight of data set} \ K, \)
\( NA = \text{number of data sets with common, given or interpolated, measurement in groups} \ I \text{and} \ J, \)
\( NA' = \text{number of data sets with measured or interpolated cross sections in group} \ I \text{or} \ J, \text{ whichever is greater}. \)
If there are not common data sets in groups I and J, the covariance is set to zero. If there are not data inside a group, the standard deviation for that group is set to the average of the corresponding values in neighboring groups.

**Step 6:** The program also calculates the correlation matrix \([\text{COR}(I,J)]\) according to the formula

\[
\text{COR}(I,J) = \frac{\text{COV}(I,J)}{\sqrt{\text{COV}(I,I) \times \text{COV}(J,J)}}.
\]

### IV. DESCRIPTION OF THE INPUT-OUTPUT SPECIFICATIONS

**A. Input**

Card 1: NG,NAS,NAR,NL,IP,IP0,MAT,MT,IP,IP0,EMA,RLER,RLER,DELT,ECA,ID

[FORMAT(9I4,5E7.0,II)]

- **NG:** number of group;
- **NAS:** number of cross-section data sets included in the error file evaluation;
- **NAR:** number of ratio data sets included in the error file evaluation;
- **NL:** number of energy limits preset to make linear interpolation between measurements in a given data set;
- **IP:** option
  - = 0, the word FISSION is printed;
  - = 1, the word CAPTURE is printed;
  - = 3, the word ALFA is printed;
- **MAT:** material number according to ENDF/B specifications;
MT: reaction-type number according to ENDF/B specifications;

IP: option

- 0, part of the input is a cross-section ratio;
- ≠ 0, otherwise;

IP\(\emptyset\): = 1, the output includes punched cards of the covariance matrix according to ENDF/B format;
- ≠ 1, otherwise;

EMA: higher energy limit corresponding to group 1 (MeV) (group 1 is the highest energy group);

RLER: lethargy corresponding to the lower limit of group 1 (it is assumed that lethargy zero corresponds to 10 MeV);

RLET: group lethargy interval;

DELT: (MeV) increment corresponding to the first energy decade in the decimal group structure;

ECA: (MeV) higher energy limit of the decimal group structure; if all the groups are decimal, ECA must be greater than EMA; if all the groups are of constant lethargy ECA must be lower than the lower limit of the last group;

ID: ≠ 0, the output includes punched cards of the correlation matrix;
- = 0, otherwise.

**Cards 2:** NPE(\(l\), \(l = 1, NA; NA = NAS+NAR [FORMAT (1415)]\)

Number of experimental points of set \(l\).

**Cards 3:** FORMAT (7E10.0)

Cross sections corresponding to the data set \(l\).
Cards 4: FORMAT (7E10.0) (MeV)

Energies corresponding to the previous data set.

Cards 3 and Cards 4 must be repeated in a sequential order from \( \lambda = 1 \)
to \( \lambda = \text{NAS} \). Following these cards, one has to place a set of cards in
the same format but now for the ratio measurements (only present if
IP = 0).

Cards 5: ENDF/B evaluated cross section for group J \( (J = 1,\text{NC}) \)

[FORMAT(6E12.0)]

Cards 6: (Only present if IP = 0.) FORMAT (6E12.0), ENDF/B evaluated
cross sections for group J \( (J = 1,\text{NG}) \) of the reference standard
cross section corresponding to the ratio measurement. (It is
assumed that all ratio measurements in the input are relative
to the same cross section.)

Cards 7: FORMAT (7E10.0)

Weight corresponding to each data set \( \lambda \), \( (\lambda = 1,\text{NA}) \).

Cards 8: FORMAT (7E10.0). Energy limits for the interpolation procedure
(see step 4 in Sect. III). These limits are preset by the
user, based on his judgment on the validity of the interpolation scheme. The limits must be given in MeV and in decreasing
order \([\text{EL}(J), J = 1,\text{NL}]\).
B. Output

Printed output:

(1) All the measured cross sections are ordered and displayed according to authors and group limits.

(2) The evaluated and the measured cross sections (now reduced to the mean energy of the group interval) are ordered and displayed according to authors and group limits.

(3) The covariance matrix.

(4) The relative standard deviation.

(5) The information contained in each punched card corresponding to the covariance matrix in the ENDF/B format.

(6) The information contained in each punched card corresponding to the correlation matrix. The formats are the following:
First NG cards (three values in each card):
Lower energy limit (MeV) in group I, and the corresponding relative standard deviation in percent and reference cross sections (1X,E11.4,11X,E11.4,F11.4)
The rest of the cards:
COR(I,J), for each I, J varies from 1 to NG format 7E10.4.
These cards are suitable for a three-dimensional plot of the correlation matrix.

(7) The correlation matrix is printed as can be seen in Appendix B.

Punched card:

With the option (IPO = 1), the covariance matrix is punched out according to the ENDF/B format.
The correlation matrix output is punched out, under option.

V. LISTING OF THE PROGRAM AND SAMPLE PROBLEM

Data for the sample problem: [COV(I,J) for the $^{240}$Pu capture cross section].

\[\begin{align*} 
NG &= 45; \quad NAS = 4; \quad NAR = 0; \quad NL = 2; \quad IOP = 1; \quad MAT = 1265; \quad MT = 102; 
IP &= 1; \quad IPO = 1; \quad EMA = 10.; \quad RLER = 0.; \quad RLET = 0.; \quad DELT = 1. 
ECA &= 11.; \quad ID = 1 
NPE(\ell = 1,4) &= 29;6;36;36 
EL(J = 1,2) &= 11., .0001 
\end{align*}\]
**FTN L.G.E.Y.**

C **LISTING OF THE PROGRAM SUR**

C THIS PROGRAM CALCULATES THE COVARIANCE AND CORRELATION MATRICES OF
C CROSS SECTIONS, THE COVARIANCE MATRIX FILE IS PUNCHED ACCORDING TO THE
C COV/FR FORMAT. THE CORRELATION MATRIX IN A FORMAT SUITABLE FOR 3-D PLOT
C
C DIMENSION SFE28(120),SFE25(120),SFM28(35,150),E(35,150),E(35),NPE
C 1(35),EV(120),SFM(35,120),NM(120),COV(120,120),NMA(35,120),EL(120).
C 2(35),AUX(120,120),TITLE(18),STA(100)
C
C DIMENSION NDER(28)
C DC 125 I=1,15
C DC 125 J=1,15
C SFM28(I,J)=C.

C DATA INPUT
C READ 1,NG,NAS,NAR,NL,IP,MAC,MT,IF,IPC,EMA,RER,LER,DEL,EC,TD
C 1 FORMAT(9I4,S7.0,1)
C GC=EG0. CALL EX1
C NA=NAS+NAS
C READ 2,(NPE(I),I=1,NA)
C 2 FORMAT(14(I5))
C C J=1,NA.
C READ 4, (SFM28(I,J),J=1,JM)
C 3 READ 4, (E(I,J),J=1,1M)
C A FORMAT(LOE=0)
C READ 6, (SFE28(I,J),I=1,NG)
C IF(IP,NE,0) GO TO 253
C READ 6, (SFE28(I,J),I=1,NG)
C 253 READ 4, (EL(I),I=1,NL)
C READ 400, (TITLE(I),I=1,18)
C 400 FORMAT(I8A)

C RATIO MEASUREMENT ARE REDUCED TO ABSOLUTE ONES, AND LOCATED IN THE SAME
C LOCATION, THEN WE LOOSE THE RATIOS, EV(I) ARE THE LIMITS OF GROUP I.
C EV(I)=EMA
C DEL=DEL
C NE=NG+1
C DC 243 I=1,NE
C IF(EC(I,GT,EMA) GO TO 245
C EV(I)=10, E*EXP(-RER)
C IF(EV(I,GT,EC(I)) GO TO 244
C EV(I)=EC(I)-DEL
C IF(I,NE,0) GC TO 243
C 245 CONTINUE
C IF(ABS(EV(I-2),EV(I-1)-2.),LT,1.E-03) DEL=DELT,1
C EV(I)=EV(I-1)-DELT
C GC TO 243
C 244 RER=RER+RER
C K=1
C 243 CONTINUE
C IF(IP,NE,0) GC TO 254
C NA=NE(I)
C DC 8 I=1,NA
C JM=PE(I)
C DC 8 J=1,JM
C K=1
C 9 CONTINUE
C IF(I,J)=E,EV(K),AND,E(J,J),GT,EV(K+1)) GC TO 10
C K=K+1
C IF(K,NE,AE) GC TO 8
C GO TO 10
C 10 IF(K,NE,1) GC TO 85
C IF(K,NE,NG) GO TO 286
C EKI=(EV(K)+EV(K+1))/2.
C EK2=(EV(K)+EV(K+1))/2.
C EK3=(EV(K)+EV(K-1))/2.
C AC=SFE25(K+1)-SFE25(K)/(EK1*EK2+EK3)-SFE25(K+1)-SFE25(K)
C EK1=(SFE25(K+1)-SFE25(K))/(EK1*EK2+EK3)
C EK2=(SFE25(K+1)-SFE25(K))/(EK1*EK2+EK3)
C CC=SFE25(K+1)-AC*EK1*EK2
C SF25=AC*E1+2*AC*E1+CC
C GO TO 87
C 846 EK=(EV(K+1)+EV(K+1))/2.
C EKI=(EV(K+1)+EV(K+1))/2.
C SF25=SFE25(K+1)-SFE25(K)/(EK1*EK1+E(J,J)-EK)
C GO TO 87
C 845 E1=(EV(1)+EV(2))/2.
C E2=(EV(2)+EV(1))/2.
C PE=(SFE25(I)-SFE25(I))/(E1-E2)
C SF25=SFE25(E1*4PC+I,J)-E2
C 85 SF28(I,J)=SFM28(I,J)*SF25
C 8 CONTINUE
C OUTPUT OF MEASURED DATA
C 274 PRINT 11
C 11 FORMAT(1H11,6H GROUP,3X,20H ENERGY LIMITS (EV) 8X,16H MEASURED VAL
C LUES//)
C DC 12 J=1,NG
C IF(IP,NE,0) PRINT 13,J,EV(J),EV(J+1)
C IF(IP,NE,0) PRINT 93,J,EL(J),EL(J+1)
C IF(IP,NE,0) PRINT 325,J,EV(J),EV(J+1)
13 FORMAT(16,3X,1PE11.4,3X,1PE11.4,3X,7H AUTHOR,3X,7H ENERGY,7X,11H S
11GFISSION,7H WEIGHT)
13 FORMAT(16,3X,1PE11.4,3X,1PE11.4,3X,7H AUTHOR,3X,7H ENERGY,7X,11H S
11GCAPTURE,7H WEIGHT)
325 FORMAT(16,3X,1PE11.4,3X,1PE11.4,3X,7H AUTHOR,3X,7H ENERGY,7X,11H
ALFA,7H WEIGHT)

14 CONTINUE.
17 IF(J.EQ.0) PRINT 17
12 CONTINUE
C THE MEASUREMENT CF AUTHOR I INSIDE GROUP J IS REDUCED TO THE MEAN ENERGY OF
C THE GROUP AND THEN AVERAGED. THE RESULTS ARE LOCATED IN SFM(I,J)
DO 16 J=1,12C
16 CONTINUE.

DO 18 I=1,35
18 SFM(I,J)=0.
DO 19 I=1,NA
19 K=K+1.
100 J=K.
IF(EV(J).LT.EV(J+1)) GO TO 110
EJ=(EV(J)+EV(J+1))/2.
110 CONTINUE.
IF(J.EQ.1) GO TO 194
EJ2=(EV(J)+EV(J+1))/2.
AC=(SFE28(J)+SFE28(J+1))/((EJ1-EJ2)*(EJ2-EJ3))-(SFE28(J+1)-SFE28(J,
111)/((EJ1-EJ3)*(EJ2-EJ3))
CC=SFE28(J)+AC*EJ1*EJ2*AC.
R=2*SFM28(J)+AC*EJ1*EJ2*AC.
AC=R*K+AC.
BC=AC*K.
CC=AC*CC.
SFM(I,J)=SF28(I,J)+AC*EJ2**2+BC*EJ2+CC.
RR=RR+1.
GO TO 20.
355 EJ=(EV(J+1)+EV(J))/2.
356 EJ2=(EV(J)+EV(J+1))/2.
PE=(SFE28(J)+SFE28(J))/((EJ1-EJ2)*(EJ2-EJ3))
RR=RR+1.
GO TO 20.

19 CONTINUE
C NUMBER OF REAL MEASUREMENTS NM(J) INTO EACH GROUP
DO 21 J=1,NG
21 CONTINUE
C TO GSF GROUP AND AUTHORS IN WHICH THERE ARE NO MEASUREMENT ARE MARKED
DO 457 J=1,NG
457 CONTINUE
C ASSIGNATION OF MEASUREMENTS TO GROUP J BY INTERPOLATION IN
C (IF POSSIBLE)
CC=NM(I,J)*GT.0.
IF(SFM(I,J).LT.EO.G) NMAR(I,J)=NM(I,J)+1
21 CONTINUE.
C assignation of measurement of author I in group J by interpolation
C (if possible)
CC=NM(I,J)*GT.0.
IF(SFM(I,J).LT.EO.G) NMAR(I,J)=0
455 CONTINUE.
C ASSIGNATION OF MEASUREMENTS TO GROUP J BY INTERPOLATION IN
C (IF POSSIBLE)
L=1
111 CONTINUE
IF(EV(J).GT.EL(L) AND EV(J).GT.EL(L+1)) GO TO 112
L=L+1.
GO TO 111.
112 KAR=J-1.
113 CONTINUE.
IF(SFM(I,KAR).NE.0) GO TO 114.
KAR=KAR-1.
114 CONTINUE.
IF(EV(KAR).LT.EL(L)) GO TO 113.
GO TO 110.
115 CONTINUE.
IF(SFM(I,KAR).NE.0) GO TO 116.
KAR=KAR+1.
116 CONTINUE.
IF(EV(KAR).LT.EL(L)) GO TO 115.
GO TO 110.
119 CONTINUE.

116 IF(EV(KAB+1),LT.,EL(L+1)) GO TO 110
   EAR=(EV(KAR)+EV(KAR+1))/2.
   EAR=(EV(KAB)+EV(KAB+1))/2.
   EJ=(EV(J)+EV(J+1))/2.
   IF(SFM(I,KAR),EQ.O.) OR.(SFMM1(I,KAB),EQ.O.) GO TO 110
   IF(SFM(I,1,J),EQ.O.) GO TO 110
   SFM(I+1,J)=(SFMM1(I,KAB)-SFMM(I,KAR))/((EAR-EAB)*(EJ-EAR))
   NM(J)=NM(J)+1
110 CONTINUE
C CALCULATION OF THE DIAGONAL TERMS OF COV(I,J)
DC 22 I=1,NG
DC 22 J=1,NG
22 COV(I,J)=0.
DC 22 I=1,NG
IF(NMJ(J),EQ.O.) GO TO 23
23 CONTINUE
IF(COV(KAR,KAB),EQ.O.) GO TO 30
DC 22 J=1,NG
DC 22 I=1,NG
DO 23 I=1,NG
DO 23 J=1,NG
COV(I,J)=COV(I,J)+CM(I)*CM(J)*SFM(I,J)
23 CONTINUE
DO 30 J=1,NG
DO 30 I=1,NG
DO 30 J=1,NG
DO 30 I=1,NG
30 CONTINUE
C OUTPUT OF DATA
PRINT 35
35 FORMAT(1H1,6H GROUP,3H, 10H EVALUATED, 3X,60H MEASURES AND INTERPOLATED VALUES RECEIVED TO THE MESH ENERGY//)
36 DO I=1,NG
36 CONTINUE
40 PRINT 40
40 FORMAT(16X,1PE11.4,13X,1PE11.4,13X,1PE11.4,13X,1PE11.4)
41 CONTINUE
C OUTPUT OF DATA
PRINT 49
49 FORMAT(1H1)
49 CONTINUE
C PRINT 37
37 FORMAT(1H1,6H GROUP,3X,10H EVALUATED, 3X,60H MEASURES AND INTERPOLATED VALUES RECEIVED TO THE MESH ENERGY//)
38 DO I=1,NG
38 CONTINUE
42 PRINT 42
42 FORMAT(16X,1PE11.4,13X,1PE11.4,13X,1PE11.4,13X,1PE11.4)
43 CONTINUE
C PRINT 39
39 FORMAT(1H1,6H GROUP,3X,10H EVALUATED, 3X,60H MEASURES AND INTERPOLATED VALUES RECEIVED TO THE MESH ENERGY//)
40 DO I=1,NG
40 CONTINUE
44 PRINT 44
44 FORMAT(1H1,6H GROUP,3X,10H EVALUATED, 3X,60H MEASURES AND INTERPOLATED VALUES RECEIVED TO THE MESH ENERGY//)
45 PRINT 45
45 FORMAT(1H1,6H GROUP,3X,10H EVALUATED, 3X,60H MEASURES AND INTERPOLATED VALUES RECEIVED TO THE MESH ENERGY//)
46 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
PRINT 49
49 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
PRINT 49
49 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
PRINT 49
49 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
PRINT 49
49 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
PRINT 49
49 CONTINUE
C THE ORDER IN THE GROUPS ARE INVERTED
12

\[ M = M(1/2) \]

DO 212 1 = 1, M

EV = EV(1)

EV(1) = EV(NG(1) + 1 - 1)

212  \[ M = M(1/2) \]

DO 213 1 = 1, M

SFT = SFE28(1)

SFE28(1) = SFE28(NG(1) + 1 - 1)

IF (EV(NG(1) + 1) = 20000000)

EV(NG(1) + 1) = 0.000

EV(NG(1) + 1) = EV(NG(1) - 0.000)

EV(NG(1) + 1) = EV(NG(1) + 1)

213 DC 214 = 1, NG

DC 214 J = 1, NG

AUXNG + 1, NG + 1 = J

AUXH(NG + 1, J) = 0.

CONTINUE

46 FORMAT(1H1, 2H RELATIVE ERROR FROM GROUP 1 TO 13)

CONTINUE

47 CONTINUE

PRINT 211

48 FORMAT(10F16.5)

211  \[ FORMAT(1H1, 2H, 63H CARDS OUTPUT... \]

PRINT 40, NG

CONTINUE

46 FORMAT(1H1, 2H, 63H CARDS OUTPUT... \]

PRINT 40, NG

CONTINUE

GO TO 230

222 CONTINUE

220, EV(I) = AUX(I) + 1, EV(I + 1) AUX(I + 1, J), EV(I + 2) = AUX(I + 2, J), MAT

1, IIA, MT

IF (IP(I) = 1) PUNCH 218, EV(I), AUX(I + 1, J), EV(I + 1) AUX(I + 1, J), EV(I + 2) = AUX(I + 2, J), MAT

1, IIA, MT

220 FORMAT(6E11.4, 14, 12, 13)

IF (NG2 = NG2 + 1)

GO TO 221

221 CONTINUE

220, EV(I) = AUX(I + 1, J), EV(I + 1) AUX(I + 1, J), MAT

1, IIA, MT

IF (IP(I) = 1) PUNCH 224, EV(I) AUX(I + 1, J), EV(I + 1) AUX(I + 1, J), MAT

1, IIA, MT

GO TO 223

223 PRINT 225, EV(I) AUX(I + 1, J), MAT, IIA, MT

225 FORMAT(14, 14, 12, 13)

230 CONTINUE

230 CONTINUE

IF (ID = NE = 0) PUNCH 305, TITLE, NG

309 FORMAT(18A/15)

PRINT 310

310 FORMAT(1H1, 4H CORRELATION MATRIX CARDS FOR THE DRAWING//)

GCC 300, 35, 35

START = 100, SORT = (AUX(I + 1),

ENE = 000001, EV(I)

PRINT 301 NE = ST

IF (ID = NE = 0) PUNCH 305, EN = ST, SFE28(1)

301 FORMAT(18A/15)

CONTINUE

300 CONTINUE

ENE = EV(I), ID = NE = 0

DO 301 I = 1, NG

DO 301 J = 1, NG

301 CDV(I + 1, J) = CDV(I + 1, J) / CDV(I + 1, J) / AUX(J, J)

GO TO 302, 221

302 CONTINUE

302 CONTINUE

301 ID = NE = 0, SORT = (AUX(I + 1),

IF (ID = NE = 0) PUNCH 303, CDV(I + 1, J), J = 1, NG

303 FORMAT(1H1, 18A/15)

CONTINUE

300 CONTINUE

DO 301 I = 1, NG

301 STA(I) = 100, SORT = (AUX(I + 1),

PRINT 402, TITLE

402 FORMAT(1H1, 18A/15)

CONTINUE

300 CONTINUE

DO 301 R = 1, 22

305 NDER = 9 = R

DC 400, 221

CONTINUE
400 LABEL(L) = L
L = 1
401 LM = LM + 27
   IF(LM .GT. NG) LM = NG
   PRINT 405, (LABEL(L), L = LM)
405 FORMAT(25H0, 1 ELG(KEV), RSD, CCRR100, /14X3HCT, 1X10I4, 1X10I4, 1X10I4, 1IX10I4)
   PRINT 430
   430 FORMAT (IH )
   DD 421 I = LM .NG
   ENDCTEV(1) /1000.
   DC 405 L = LM
   TEMP = CDV(I, L) /100.
409 LABEL(L) = TEMP
410 PRINT 405, I, EN(KEV), STA(I), (LABEL(L), L = LM)
   IL = IL + 1
   IF(IL .GT. 28) GO TO 421
   EDER(IL) = 4H
   PRINT 420, EDER
420 FORMAT (IH, 17X10A4, 1X10A4, 1X8A4)
   EDER(IL) = 4H
421 CONTINUE
   ENE = EV(KE) /1000.
   PRINT 406, KE, ENE
   LM = LM + 1
   IF(LM .LE. NG) GO TO 401
40C CONTINUE
   GC TO 897
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RELATIVE ERROR FROM GROUP 1 TO 4

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CARDS OUTPUT. WARNING THE ORDER IN THE GROUPS ARE NOW INVERTED.

COV(I,J) CARDS IN THE ENDF/B FORM.

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CARDS OUTPUT, WARNING THE ORDER IN THE GROUPS ARE NOW INVERTED.

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CORRELATION MATRIX CARDS FOR THE DRAWING

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0.3004E+03  0.2136E+01
0.4004E+03  0.2470E+01
0.5004E+03  0.9568E+01
0.6004E+03  0.1052E+02
0.7004E+03  0.3145E+02
0.8004E+03  0.1700E+02
0.9004E+03  0.3360E+02
1.0004E+03  0.1152E+03
1.1004E+03  0.2108E+03
1.2004E+03  0.4153E+03
1.3004E+03  0.2684E+03
1.4004E+03  0.1047E+03
1.5004E+03  0.1487E+03
1.6004E+03  0.2482E+03
1.7004E+03  0.1237E+03
1.8004E+03  0.3678E+03
1.9004E+03  0.1915E+03
2.0004E+03  0.1809E+03
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2.8004E+03  0.3082E+03
2.9004E+03  0.2924E+03
3.0004E+03  0.1191E+03
3.1004E+03  0.3147E+03
3.2004E+03  0.2436E+03
3.3004E+03  0.3147E+03
3.4004E+03  0.2924E+03
3.5004E+03  0.1191E+03
3.6004E+03  0.3147E+03
3.7004E+03  0.2436E+03
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3.9004E+03  0.2924E+03
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5.0004E+03  0.1191E+03
```

VI. THE THREE-DIMENSIONAL CORRELATION MATRIX PLOT

As noted, part of the card output of the program can be used to generate a three-dimensional plot of the correlation matrix. This can be seen in Fig. 1, where this plot is shown for the $^{238}\text{U}$ fission cross section.

Several conclusions can be deduced from this plot:

(1) A lot of structure can be seen. This corresponds to the fact that the cross section was analyzed with very much detail.

(2) The standard deviation shows large uncertainties in the low-energy region. This reflects the lack of data in this region.

(3) Positive correlation corresponds to differences in magnitude but not in shape; negative correlation corresponds to differences in shape. Then, differences in shape in the low-energy range can be detected. This reflects the fact that in this zone the cross section rises so fast that differences in cross-section values correspond to a large difference in shape.

(4) The recent measurement of Behrens et al. correlates all the analyzed energy intervals.$^9$
REFERENCES


APPENDIX A. LIST OF REFERENCES USED IN THE CALCULATION OF THE COVARIANCE MATRICES

238U Fission: In this case the covariance $[\text{COV}(I,J)]$ was calculated for 36 groups from 20 MeV to 550.24 keV in a 0.1 lethergy unit interval. The following set of references was used:

   One measurement at 14 MeV. Original data.

   Two measurements at 14.1 and 15 MeV. Original data.


   One measurement at 13.6 MeV. Original data.

   One measurement at 14.6 MeV. Original data.

   Eight measurements at 13.74-14.75 MeV. Original data.

   One measurement at 14.6 MeV. Original data.

   Thirty eight measurements at 1.3-6.92 MeV. Data renormalized to 0.5176b at 4.50 MeV.
Four measurements at 8.8-13.86 MeV. Renormalized to 1.109 b at 13.86 MeV.

Fourteen measurements at 12.7-19.4 MeV. Renormalized to 1.125 b at 14 MeV.

Fifteen measurements at 10.6-20.4 MeV. Renormalized to 1.125 b at 14 MeV.

Thirty six measurements at 5.1-22.5 MeV. Renormalized to 1.125 b at 14 MeV.


The following are ratio measurements relative to the $^{235}$U fission cross section. They were reduced to $^{238}$U fission data utilizing the $^{235}$U fission cross-section ENDF/B-IV evaluation.

One measurement at 14 MeV.

One measurement at 2.5 MeV.

Eighty eight measurements at 0.573-2.995 MeV, measurement multiplied by 0.95.
    One measurement at 14.1 MeV.

    Twenty measurements at 2.95-8.30 MeV.

    One measurement at 14.6 MeV.

    One measurement at 2.5 MeV.

    Fourteen measurements at 1.5-5 MeV.

    Three measurements at 2.25-14.1 MeV.

    Sixteen measurements at 1.68-8.07 MeV.

    Three measurements at 2-3 MeV.

    Twenty one measurements at 0.898-5.33 MeV.

26. Behrens, J. W., et al., Conf. of Nuclear Cross Sections and
    White source, 30.23-0.1077 MeV.

$^{238}$U Capture. In this case the covariance [COV(I,J)] was calculated for
91 groups for energies ranging from 10 MeV to 100 eV. From 10 MeV down
to 4.095 keV, 0.1 lethargy unit intervals were used. The energy range
between 4.095 keV and 100 eV was divided in decimal intervals. The following set of references was used:

   Eleven measurements at 29-840 keV. Original data.

   Seven measurements at 400 keV-4.05 MeV. Data revised by Davey in ref. 19.

   Two measurements at 220-850 keV. Original data.

   One measurement at 25 keV. Original data.

   One measurement at 195 keV. Original data.

   Thirteen measurements at 2.55-217 keV. Data revised by Davey in ref. 19.

   Seven measurements at 0.175-1 MeV. Data revised by Davey in ref. 19.

   Two measurements at 30-65 keV. Original data.

Eight measurements at 18-300 keV. Data revised by Davey in ref. 19.


Two measurements at 30-64 keV. Data revised by Davey in ref. 19.


Sixteen measurements at 8.8-54.7 keV. Data according to a recent evaluation of $\sigma$(Ta) in ref. 19.


Eleven measurements at 15-180 keV. Corrected by non-$1/v^{10}$B behavior and normalized to the Belanova (ref. 13) value. Data from Sowerby (ref. 20).


One measurement at 22.8 keV as corrected by Miller et al. in Nucl. Sci. Eng. 35: 295 (1969).


Nine measurements at 24-503 keV. Original data.


White source, time of flight; 0.50-100 keV. Results average in decimal intervals. Date revised in 1970 (ref. 20).


White source, time of flight; 1-100 keV. Results average in decimal intervals, 100-752 keV point results. Original data.


White source, time of flight; 0.100-100 keV. Results average over decimal intervals. Original data.
   Evaluation.

   Evaluation.

   Evaluation.

   Ten measurements at 24-145 keV. Original data.

   Two measurements at 132-160 keV. Original data.

   One measurement at 24 keV. Original data.

   Ten measurements at 3.3-35 keV. Original data.

   Four measurements at 157-624 keV. Original data.

   Eleven measurements at 200-1750 keV. Original data.


The following are ratio measurements relative to the $^{235}$U fission cross section. They were reduced to $^{238}$U capture data utilizing the $^{235}$U fission cross-section ENDF/B-IV evaluation.
    Thirteen measurements at 0.005-5.9 MeV. Original data.
    Thirteen measurements at 0.127-7.6 MeV. Original data.
    See also ref. 10.
    Two measurements at 30-64 keV. Original data.
    Thirteen measurements at 30 keV-1.4 MeV. Original data.
    Evaluation.

\(^{239}\text{Pu} \text{Capture}: \) In this case the covariance \([\text{COV}(I,J)]\) was calculated
for 36 groups for energies ranging from 1 MeV to 100 eV. The energy
range was divided in decimal intervals. The following set of references
was used:

    IAEA.


$^{239}$Pu Fission: In this case the covariance [COV(I,J)] was calculated for 45 groups for energies ranging from 10 MeV to 100 eV. The energy range was divided in decimal intervals. The following set of references was used:


\[ ^{240}\text{Pu and }^{241}\text{Pu Capture.} \ ^{241}\text{Pu Fission: In this case the covariance was calculated for 45 groups for energies ranging from 10 MeV to 100 eV.} \]

The following sets of references were used:

\[ ^{240}\text{Pu Capture Cross Section} \]


100 eV to 300 keV with weight of 9 on the variance.


6 to 30 keV with weight of 9 on the variance.


1 keV to 10 MeV with weight of 1 on the variance (model calculation).


1 keV to 10 MeV with weight of 1 on the variance (model calculation).
241Pu Capture Cross Section

   100 eV to 200 keV with weight of 9 on the variance.

   100 eV to 10 MeV with weight of 1 on the variance (model calculation).

   80 keV to 10 MeV with weight of 1 on the variance (model calculation).

241Pu Fission Cross Section (all references with weight of 1 on the variance)

1. Weston, L. W., and Todd, J. H., same reference as with 241Pu capture.
   100 eV to 200 keV.

   100 eV to 10 keV.


   100 eV to 2 keV.
   200 keV to 10 MeV.

   20 keV to 1 MeV.

   40 keV to 6 MeV.

   300 keV to 2 MeV.
APPENDIX B. STANDARD DEVIATION AND CORRELATION MATRICES CORRESPONDING TO DIFFERENT CROSS SECTIONS
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**Notes:**
- ELO(KEV): ELO values in KEV.
- RSD: RSD values.
- CONN: Connection values.
- 101A: 101A values.
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**PU241 CAPTURE 45 GROUPS**

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