International Atomic Energy Agency

EXFOR Formats for Partial Uncertainties and Covariances

IAEA Nuclear Data Section
N. Otsuka

Why Covariance?

Let us consider a quantity $Q(\sigma^a, \sigma^b)$.

Error propagation from σ^a and σ^b to Q:

$$(\Delta Q)^2 = \left(\frac{\partial Q}{\partial \sigma^a}\right)^2 \underline{(\Delta \sigma^a)^2} + \left(\frac{\partial Q}{\partial \sigma^b}\right)^2 \underline{(\Delta \sigma^b)^2} + \left(\frac{\partial Q}{\partial \sigma^a}\right) \underline{V^{ab}} \left(\frac{\partial Q}{\partial \sigma^b}\right)$$

Total uncertainty ofσ^a

Total uncertainty ofσ^b

Covariance between σ^a and σ^b

Not only total uncertainty, but also <u>covariance</u> may play an important role in error propagation.

Derivation of Experimental Covariance

Cross section derived from parameter a,b,c,…: $\sigma^i = \sigma^i (a,b,c,\ldots)$

If the cross section is expressed by the product of a, b, c, ….
(no correlation among a, b, c,…), its uncertainty and covariance are

Total uncertainty
(%)

$$\left(\frac{\Delta\sigma_i}{\sigma_i}\right)^2 = \left(\frac{\Delta a_i}{a_i}\right)^2 + \left(\frac{\Delta b_i}{b_i}\right)^2 + \left(\frac{\Delta c_i}{c_i}\right)^2 + \ldots \text{ (partial uncertainty)}$$

Total covariance
($\%^2$)

$$V_\sigma{}^2 = V_a{}^2 + V_b{}^2 + V_c{}^2 + \ldots \text{(partial covariance)}$$

(if no correlation among a, b, c, …)

Experimental Information on Uncertainty

- **Set of partial covariances (PC)**
  Best information, rarely available

- **Set of partial uncertainties (PU)**
  Often available, Useful to guess PC and TC.

- **Total covariance (TC)**
  Useful information, rarely available

- **Total uncertainty (TU)**
  Always available, “better than nothing”

TU $$\left(\frac{\Delta\sigma_i}{\sigma_i}\right)^2 = \left(\frac{\Delta a_i}{a_i}\right)^2 + \left(\frac{\Delta b_i}{b_i}\right)^2 + \left(\frac{\Delta c_i}{c_i}\right)^2 + \ldots$$ **PU**

TC $$V_\sigma{}^2 = V_a{}^2 + V_b{}^2 + V_c{}^2 + \ldots$$ **PC**

Partial Uncertainties

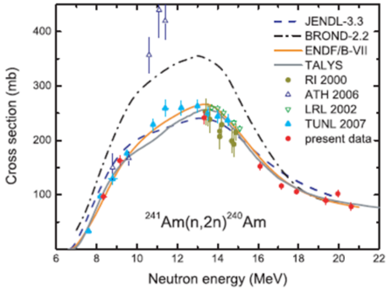
- **Often available from articles and authors.**
- **People reporting *total uncertainties* should be able to provide its partial uncertainties.**
- **We can guess a partial covariance V_a from partial uncertainties**

Example of parameter a between two energy i and j

$$V_{a,ij} = \left(\frac{\Delta a_i}{a_i} \right) c_{a,ij} \left(\frac{\Delta a_j}{a_j} \right)$$

$C_{a,ij}$ =0 Uncorrelated (Short energy range correlation; SERC)
=1 Fully correlated (Long energy range correlation; LERC)
<1 In general (Medium energy range correlation; MERC)

Example of Partial Uncertainties



C. Sage, V. Semkova et al.,
Phys. Rev. C81(2010)064604 (EXFOR 23114)

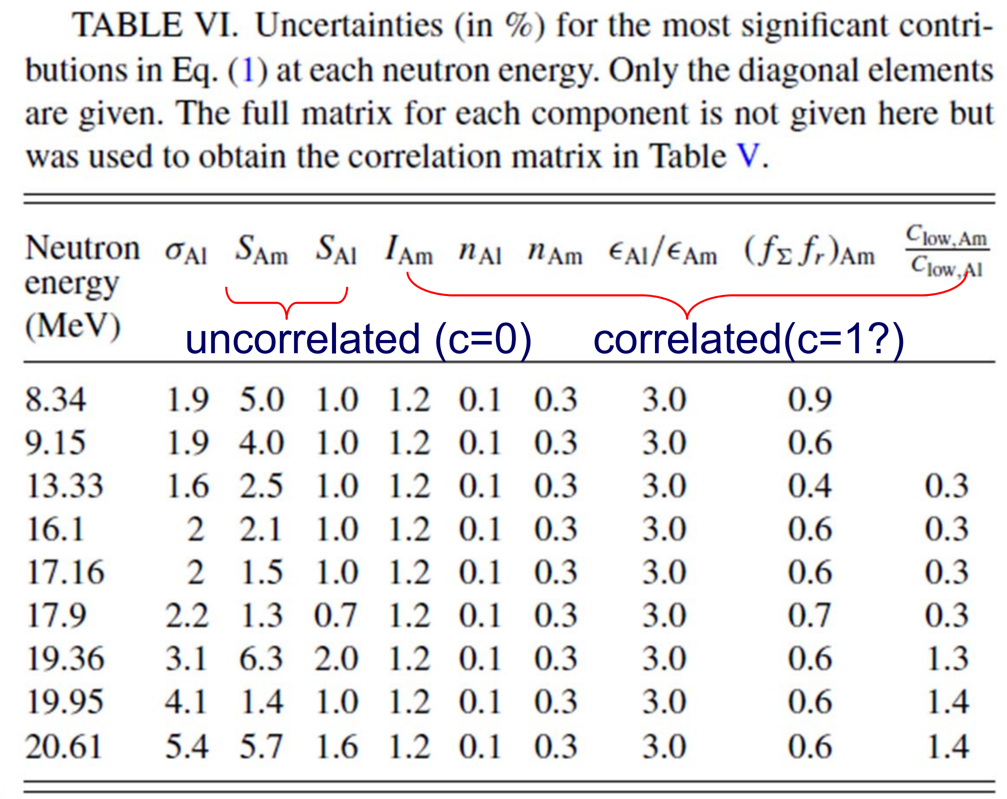


TABLE VI. Uncertainties (in %) for the most significant contributions in Eq. (1) at each neutron energy. Only the diagonal elements are given. The full matrix for each component is not given here but was used to obtain the correlation matrix in Table V.

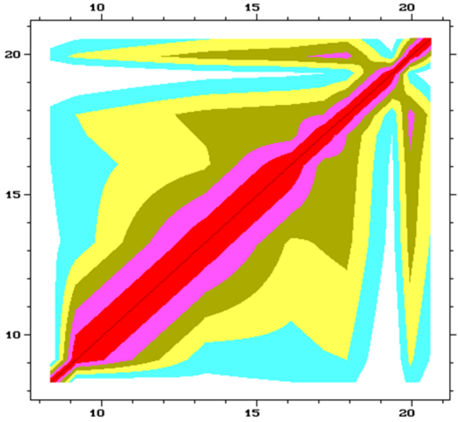
Neutron energy (MeV)	$\sigma_{\rm Al}$	$S_{\rm Am}$	$S_{\rm Al}$	$I_{\rm Am}$	$n_{\rm Al}$	$n_{\rm Am}$	$\epsilon_{\rm Al}/\epsilon_{\rm Am}$	$(f_\Sigma f_r)_{\rm Am}$	$\frac{C_{\rm low,Am}}{C_{\rm low,Al}}$
		uncorrelated (c=0)		correlated(c=1?)					
8.34	1.9	5.0	1.0	1.2	0.1	0.3	3.0	0.9	
9.15	1.9	4.0	1.0	1.2	0.1	0.3	3.0	0.6	
13.33	1.6	2.5	1.0	1.2	0.1	0.3	3.0	0.4	0.3
16.1	2	2.1	1.0	1.2	0.1	0.3	3.0	0.6	0.3
17.16	2	1.5	1.0	1.2	0.1	0.3	3.0	0.6	0.3
17.9	2.2	1.3	0.7	1.2	0.1	0.3	3.0	0.7	0.3
19.36	3.1	6.3	2.0	1.2	0.1	0.3	3.0	0.6	1.3
19.95	4.1	1.4	1.0	1.2	0.1	0.3	3.0	0.6	1.4
20.61	5.4	5.7	1.6	1.2	0.1	0.3	3.0	0.6	1.4

How can evaluators guess the total covariance as the sum of partial covariances?

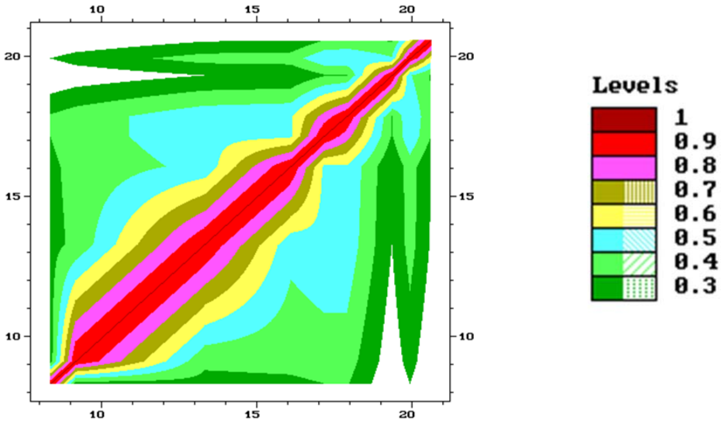
$$V_{ij} = \sum_a \left(\frac{\Delta a_i}{a_i}\right) c_{a,ij} \left(\frac{\Delta a_j}{a_j}\right)$$

Evaluation of Covariance from EXFOR

Full correlation
estimated by an evaluator
(c=1 assumed)



Correlation by authors



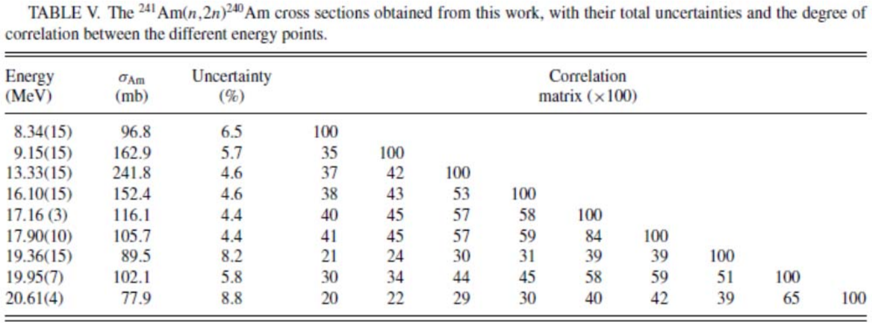


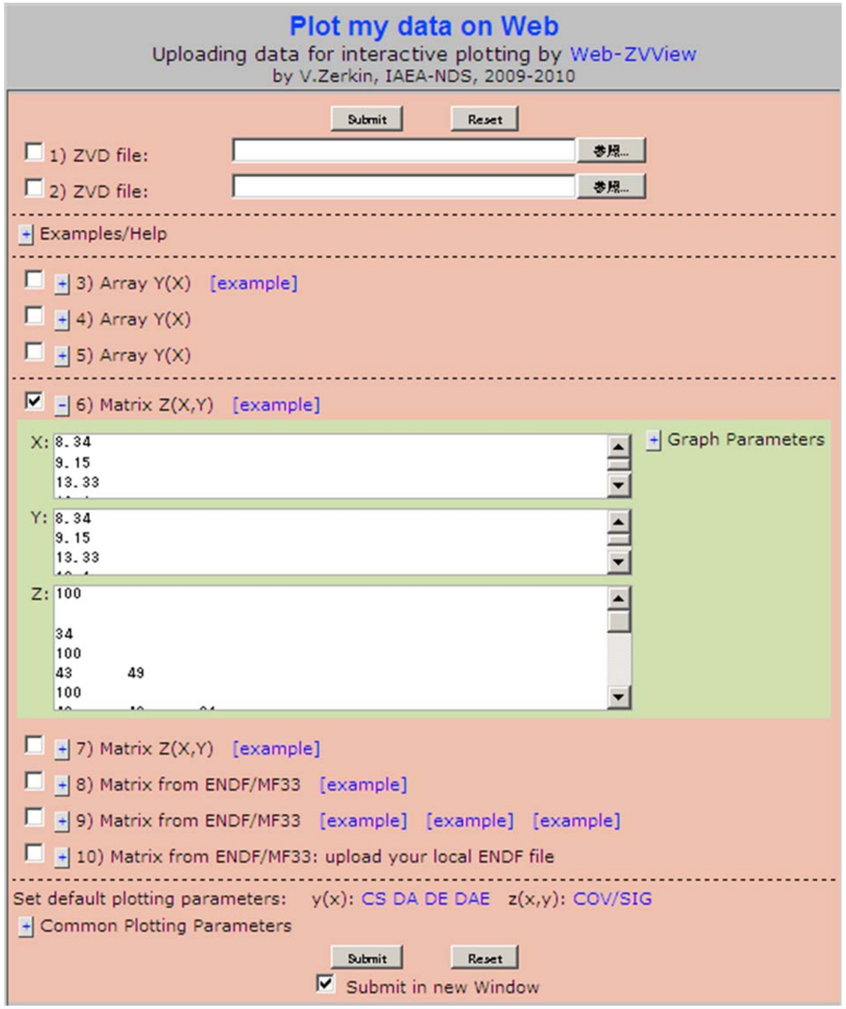
TABLE V. The ^{241}Am(n,2n)^{240}Am cross sections obtained from this work, with their total uncertainties and the degree of correlation between the different energy points.

Energy (MeV)	σ_{Am} (mb)	Uncertainty (%)	Correlation matrix (×100)								
8.34(15)	96.8	6.5	100								
9.15(15)	162.9	5.7	35	100							
13.33(15)	241.8	4.6	37	42	100						
16.10(15)	152.4	4.6	38	43	53	100					
17.16 (3)	116.1	4.4	40	45	57	58	100				
17.90(10)	105.7	4.4	41	45	57	59	84	100			
19.36(15)	89.5	8.2	21	24	30	31	39	39	100		
19.95(7)	102.1	5.8	30	34	44	45	58	59	51	100	
20.61(4)	77.9	8.8	20	22	29	30	40	42	39	65	100

Correlation properties are important to construct more realistic covariance.

ZVView for Covariance Plot

http://www-nds.iaea.org/exfor/myplot.htm



Plot my data on Web

Uploading data for interactive plotting by Web-ZVView

by V.Zerkin, IAEA-NDS, 2009-2010

☐ 1) ZVD file: 参照...

☐ 2) ZVD file: 参照...

+ Examples/Help

☐ + 3) Array Y(X) [example]

☐ + 4) Array Y(X)

☐ + 5) Array Y(X)

☑ - 6) Matrix Z(X,Y) [example]

X: 8.34
9.15
13.33

Y: 8.34
9.15
13.33

Z: 100

34
100
43 49
100

+ Graph Parameters

☐ + 7) Matrix Z(X,Y) [example]

☐ + 8) Matrix from ENDF/MF33 [example]

☐ + 9) Matrix from ENDF/MF33 [example] [example] [example]

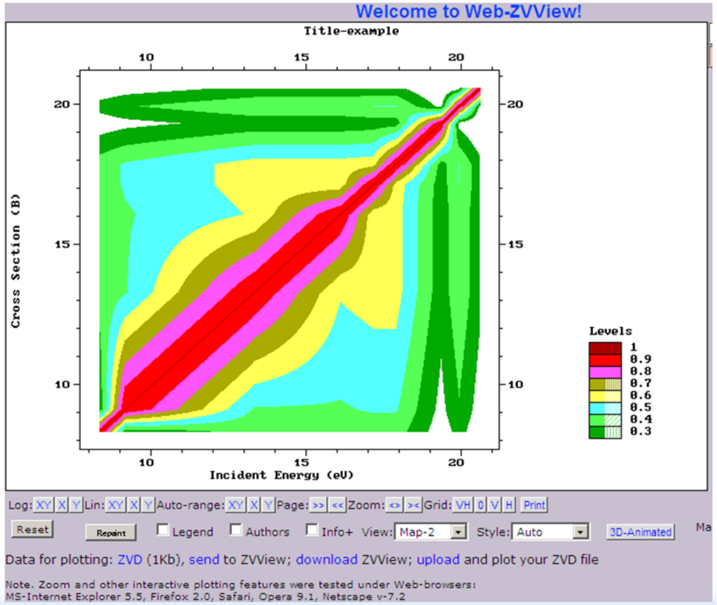
☐ + 10) Matrix from ENDF/MF33: upload your local ENDF file

Set default plotting parameters: y(x): CS DA DE DAE z(x,y): COV/SIG

+ Common Plotting Parameters

☑ Submit in new Window

Very helpful to plot plotting of matrices



Welcome to Web-ZVView!

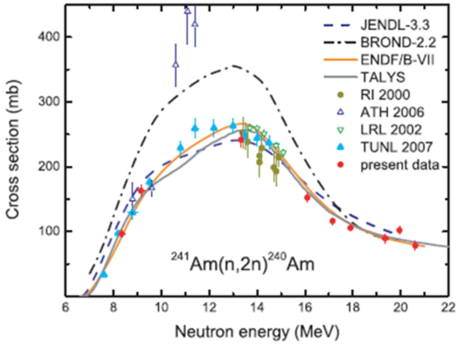
Data for plotting: ZVD (1Kb), send to ZVView; download ZVView; upload and plot your ZVD file

Note. Zoom and other interactive plotting features were tested under Web-browsers:
MS-Internet Explorer 5.5, Firefox 2.0, Safari, Opera 9.1, Netscape v-7.2

Partial Covariance for Renormalization

$$\sigma_{Am} = \underline{\sigma_{Al}} \frac{S_{Am}}{S_{Al}} \frac{[I\varepsilon f_{\Sigma} f_{r} n\Phi_{0}]_{Al}}{[I\varepsilon f_{\Sigma} f_{r} n\Phi_{0}]_{Am}} \prod_{k} \frac{C_{k,Am}}{C_{k,Al}}$$

$$V_{\sigma \mathrm{Am}}{}^{2} = \underline{V_{\sigma \mathrm{Al}}}{}^{2} + V_{I\mathrm{Al}}{}^{2} + V_{\varepsilon \mathrm{Al}}{}^{2} + \ldots$$

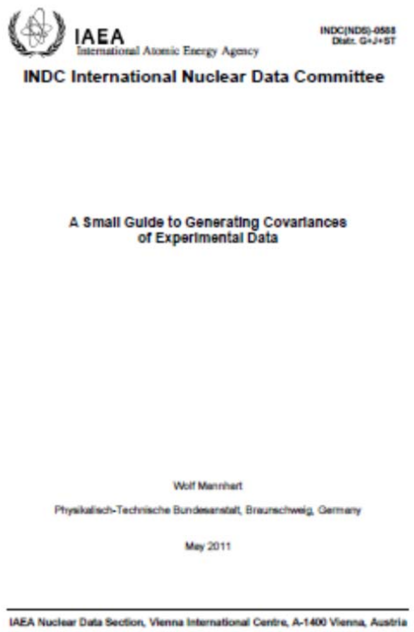


- **We should be able to renormalize the cross section when a better ^{27}Al(n,α) monitor reaction is available.**

- **Not only ^{243}Am(n,2n) cross section, but its uncertainty and covariance should be able to revise.**

  → **Not only full covariance, but also partial covariance must be available for future data renormalization.**
  (Sage gives partial covariances in his theesis!
  Should be kept in EXFOR.)

Details of Uncertainties than Covariances?



IAEA
International Atomic Energy Agency

INDC(NDS)-0588
Distr. G+J+ST

INDC International Nuclear Data Committee

**A Small Guide to Generating Covariances
of Experimental Data**

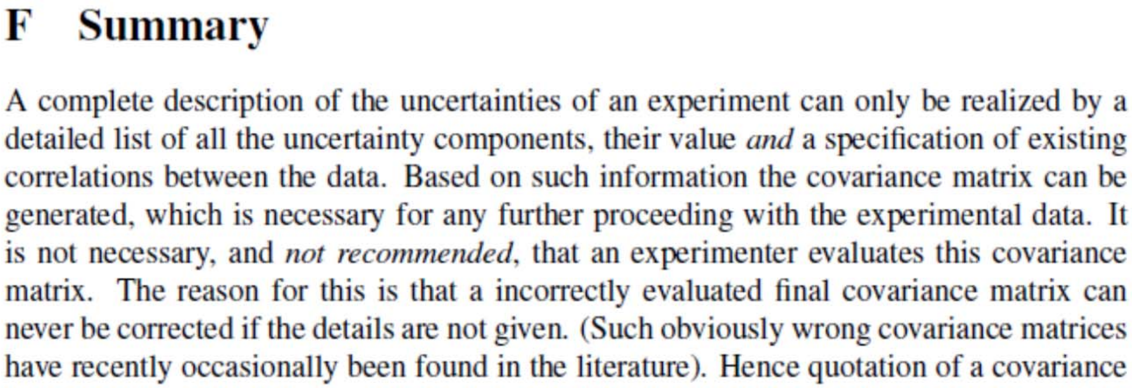
Wolf Mannhart

Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

May 2011

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

W. Mannhart,
“A Small Guide to
Generating Covariances
of Experimental Data”
INDC(NDS)-0588, in print



F Summary

A complete description of the uncertainties of an experiment can only be realized by a detailed list of all the uncertainty components, their value *and* a specification of existing correlations between the data. Based on such information the covariance matrix can be generated, which is necessary for any further proceeding with the experimental data. It is not necessary, and *not recommended*, that an experimenter evaluates this covariance matrix. The reason for this is that a incorrectly evaluated final covariance matrix can never be corrected if the details are not given. (Such obviously wrong covariance matrices have recently occasionally been found in the literature). Hence quotation of a covariance

… Detailed list of all the uncertainty components, their value and a specification of existing correlations rather than the covariance matrix....

… A incorrectly evaluated final covariance matrix can never be corrected if the details are not given…

We should be able to follow error propagation by authors.
Partial uncertainties and partial covariances are important!

Requirement for Experimental Data Library

- We should be able to compile partial correlation properties (c=0, =1, or = general matrix) with their partial uncertainties when they are provided from experimentalists.
- It should be designed for computer programs which read full correlation properties and construct covariance and renormalize cross sections.
- Unnecessary complication (e.g., formalism for theoretically interesting, but not experimentally available information) should not be introduced.

New ERR-ANALYS and COVARIANCE

```
ERR-ANALYS (ERR-T) Total uncertainty
           (ERR-S) Total uncorrelated uncertainty
           (MONIT-ERR,,,P) Monitor uncertainty
           (ERR-1,,,U) 1st uncertainty (uncorrelated)
           (ERR-2,,,F) 2nd uncertainty (full-correlated)
…
COVARIANCE (EN,MEV)
            8.34 9.15 13.33 16.11 …
           (COR,ERR-T,PER-CENT)
            100
             35 100
             37 42 100
             38 43 53 100
            …
           (COR,MONIT-ERR,PER-CENT)
            100
             43 100
              0   0 100
              0   0   6  100
```

Partial matrix is given when c≠0, 1.

Number of matrix columns are always equal to N1 of ENDDATA.

F	Fully correlated (c=1)
U	Uncorrelated (c=0)
P	Partly correlated (c is coded)
C	Correlated (details unknown)
	No information on correlation

Well Done!!
(Vladimir Poroynaev)

Covariance in EXFOR Library

40 EXFOR entries giving matrices in free text.

1. Energy-energy correlation and only energy is the independent variable (9)
2. Reaction-reaction correlation and the energy is a constant or spectrum averaged (9)
3. Leg. coef. - Leg. coef. (or angle-angle) correlation and no energy-energy correlation considered (16)
4. Other coefficients correlation (e.g. resonance parameter, strength function) (3)

Computer readable EXFOR covariance (General)

			x1	x2	x3	…
			y1	y2	y3	…
		…				
x1	y1		100	90	80	
x2	y2		90	100	90	
x3	y3		80	90	100	
…	…					…

```
COVARIANCE (x,UNIT)
            x1,x2,x3,...
           (y,UNIT)
            y1,y2,y3,...
           …
           (COR,ERR-T,PER-CENT)
            100
              43   100
                0     0   100
                0     0     6   100
            …
           (COR,ERR-1,PER-CENT)
            100
              43   100
                0     0   100
                0     0     6   100
           …
           …
```

Grid definition

Data structure:

- Grid (x, y, …)
- Matrix elements

Coding sample: Energy-Energy correlation

Example: Energy-energy correlation of cross section for one reaction

```
COVARIANCE (EN,MEV)
            8.34 9.15 13.33  16.1 17.16  17.9 19.36 19.95 20.61
           (COR,ERR-T,PER-CENT)
            100
             35   100
             37    42   100
             38    43    53   100
             40    45    57    58   100
             41    45    57    59    84   100
             21    24    30    31    39    39   100
             30    34    44    45    58    59    51   100
             20    22    29    30    40    42    39    65   100
           (COR,MONIT-ERR,PER-CENT)
            100
             43  100
              0    0  100
              0    0    6  100
              0    0    9   12  100
              0    0   11   12  100  100
              0    0   11   11   40   40  100
              0    0   11   11   40   40  100  100
            100    0   11   11   40   40  100  100  100
           (COR,ERR-2,PER-CENT)
            100
              0  100
              0  100  100
              0  100  100  100
              0    0    0    0  100
            100    0    0    0    0  100
              0    0    0    0  100    0  100
              0    0    0    0    0    0    0  100
            100    0    0    0    0  100    0    0  100
```

Grid definition (energy)

Total correlation

Correlation due to monitor

Correlation due to sample

Coding sample: Reac.-Reac. correlation

Example: Reaction-reaction correlation of cross section for one energy

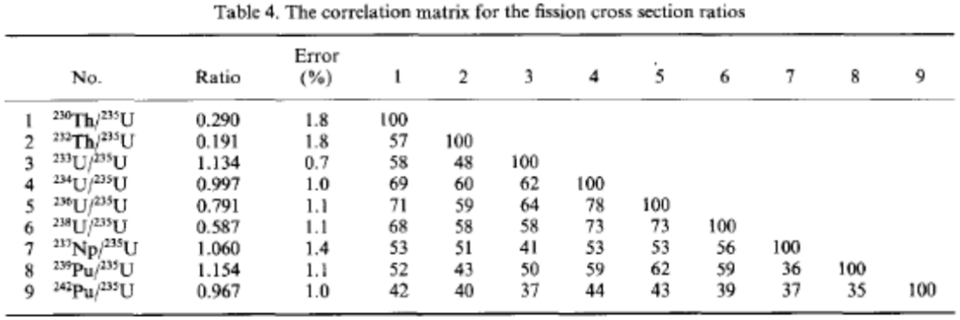


Table 4. The correlation matrix for the fission cross section ratios

No.		Ratio	Error (%)	1	2	3	4	5	6	7	8	9
1	^{230}Th/^{235}U	0.290	1.8	100								
2	^{232}Th/^{235}U	0.191	1.8	57	100							
3	^{233}U/^{235}U	1.134	0.7	58	48	100						
4	^{234}U/^{235}U	0.997	1.0	69	60	62	100					
5	^{236}U/^{235}U	0.791	1.1	71	59	64	78	100				
6	^{238}U/^{235}U	0.587	1.1	68	58	58	73	73	100			
7	^{237}Np/^{235}U	1.060	1.4	53	51	41	53	53	56	100		
8	^{239}Pu/^{235}U	1.154	1.1	52	43	50	59	62	59	36	100	
9	^{242}Pu/^{235}U	0.967	1.0	42	40	37	44	43	39	37	35	100

J.W.Meadows et al.,
Ann. Nucl.Energ.**15**(1988)421
(EXFOR 13134)

```
COVARIANCE (SUBENT) 9 elements
            1 2 3 4 5 6 7 8 9
           (EN,MEV) 9 elements
            14.74 14.74 14.74 14.74 14.74 14.74 14.74 14.74 14.74
           (COR,ERR-T,PER-CENT) 45 elements
            100
             57   100
             58    48   100
             69    60    62   100
             71    59    64    78   100
             68    58    58    73    73   100
             53    51    41    53    53    56   100
             52    43    50    59    62    59    36   100
             42    40    37    44    43    39    37    35   100
```

Grid definition (Subentry #)

Grid definition (Energy)

Total correlation

2 independent variables to define each grid:

Subentry # , Incident energy

Coding sample: Leg.-Leg. correlation

Example: Leg.coef.-Leg.coef. correlation

D.Schmidt et al., PTB-N-55(2007) (EXFOR 22973): ^{9}Be(n,el)^{9}Be at 4 energies

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=\frac{\sigma}{4\pi}\left[1+\sum_{l\geq 1}a_l(2l+1)P_l(\cos\theta)\right]$$

```
COVARIANCE (SUBENT) 9 elements
            2 4 4 4 4 4 4 4 4 4
           (EN,MEV) 9 elements
            7.10 7.10 7,10 8.09 8.09 8.09 9.09 9.09 9.09 9.97 9.97 9.97
           (NUMBER,NO-DIM) 9 elements of Legendre order.(0th to 2nd).
            0,1,2,0,1,2,0,1,2
           (COR,ERR-T,PER-CENT) 45 elements
             100
              12 100
               5  80 100
               0   0   0  100
               0   0   0   13 100
               0   0   0    7  82 100
               0   0   0    0   0   0  100
               0   0   0    0   0   0   13 100
               0   0   0    0   0   0    6  81 100
               0   0   0    0   0   0    0   0   0  100
               0   0   0    0   0   0    0   0   0   14 100
               0   0   0    0   0   0    0   0   0    8  84 100
```

7.1 MeV

8.09 MeV

9.09 MeV

9.97 MeV

Grid definition (Subentry #)

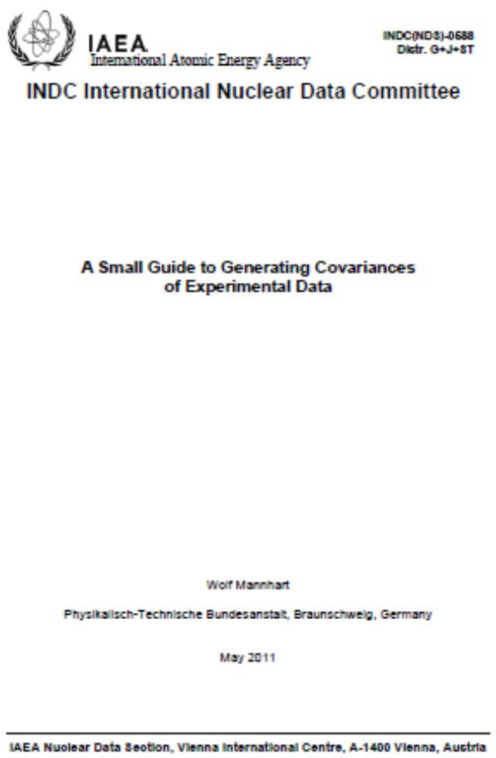
Grid definition (Energy)

Grid definition (Leg. order,≤2)

Total correlation
(No correlation between
energies)

3 independent variables to define each grid:
Subentry #, incident energy, Leg. order

New Publication (as a response to TM)



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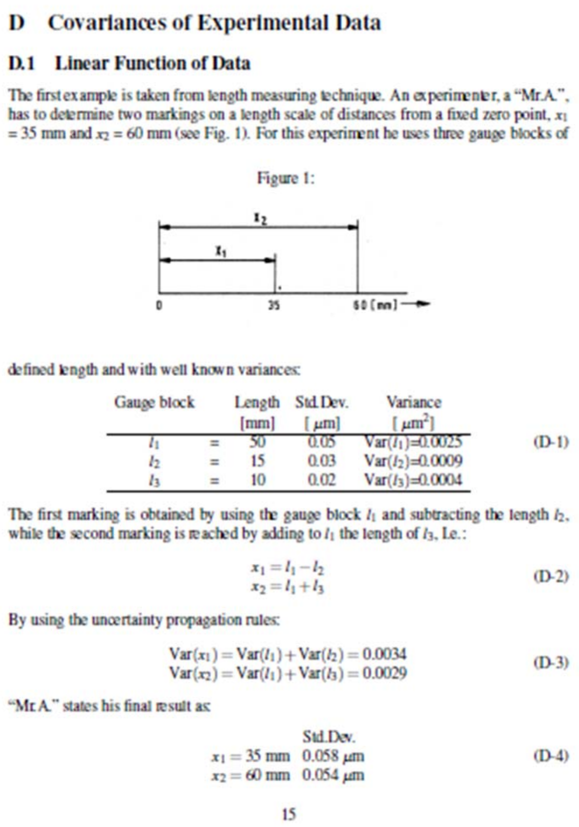

D Covariances of Experimental Data

D.1 Linear Function of Data

The first example is taken from length measuring technique. An experimenter, a "Mr.A.", has to determine two markings on a length scale of distances from a fixed zero point, x_1 = 35 mm and x_2 = 60 mm (see Fig. 1). For this experiment he uses three gauge blocks of defined length and with well known variances:

Figure 1:

Gauge block		Length [mm]	Std.Dev. [μm]	Variance [μm^2]
l_1	=	50	0.05	Var(l_1)=0.0025
l_2	=	15	0.03	Var(l_2)=0.0009
l_3	=	10	0.02	Var(l_3)=0.0004

(D-1)

The first marking is obtained by using the gauge block l_1 and subtracting the length l_2, while the second marking is reached by adding to l_1 the length of l_3, I.e.:

$$\begin{aligned} x_1 &= l_1 - l_2 \\ x_2 &= l_1 + l_3 \end{aligned} \qquad \text{(D-2)}$$

By using the uncertainty propagation rules:

$$\begin{aligned} \mathrm{Var}(x_1) &= \mathrm{Var}(l_1) + \mathrm{Var}(l_2) = 0.0034 \\ \mathrm{Var}(x_2) &= \mathrm{Var}(l_1) + \mathrm{Var}(l_3) = 0.0029 \end{aligned} \qquad \text{(D-3)}$$

"Mr.A." states his final result as:

$$\begin{array}{ll} & \text{Std.Dev.} \\ x_1 = 35 \text{ mm} & 0.058\ \mu\text{m} \\ x_2 = 60 \text{ mm} & 0.054\ \mu\text{m} \end{array} \qquad \text{(D-4)}$$

15

"A small guide to generating covariances of experimental data"
by Wolf Mannhart (PTB). INDC(NDS)-0588 (in press), 50 pages.
Send me an e-mail if you need a hard copy. Good for students!

Summary

- EXFOR should be able to accumulate **details of experimental uncertainty** information from authors. (See recom. from TM)
- Not only total uncertainty and total covariance, but also **partial uncertainties and partial covariances** should be kept when available.
- The new format should be **readable for computer programs** (construction of full covariance and renormalization of existing data etc.).
- Unnecessary **complication should be excluded**. But we should remember **key information available experimentalists must be kept**.
- More specific (more computer oriented) format may be designed by programmers. (**output format**, e.g., X4+, C4).
- Some proposals based on real EXFOR entries were presented. Revision of EXFOR Formats and LEXFOR entry is urged by users.