International Atomic Energy Agency

Uncertainty and Covariance in EXFOR

N. Otsuka, R. Capote, V. Zerkin
IAEA Nuclear Data Section

Contents

1. Compilation of experimental covariance for EXFOR (Otsuka)

2. Evaluation of nuclear reaction data covariance at NDS (Capote)

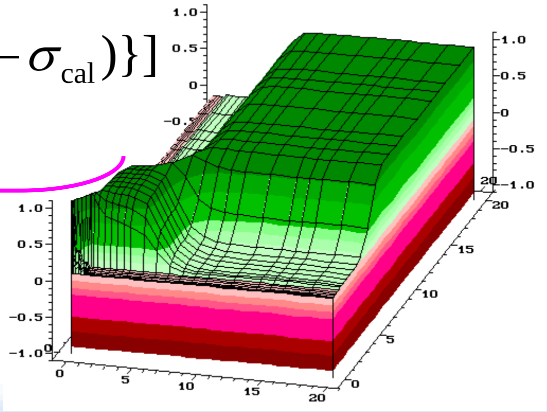
3. Web interface for covariance in ENDF Formats (Zerkin)

$$p(\vec{\sigma}) \sim \exp[\underbrace{-1/2\{(y-y_{\mathrm{exp}})^T V_{\mathrm{exp}}^{-1}(y-y_{\mathrm{exp}})}_{1} + (\sigma-\sigma_{\mathrm{cal}})^T V_{\mathrm{cal}}^{-1}(\sigma-\sigma_{\mathrm{cal}})\}]$$

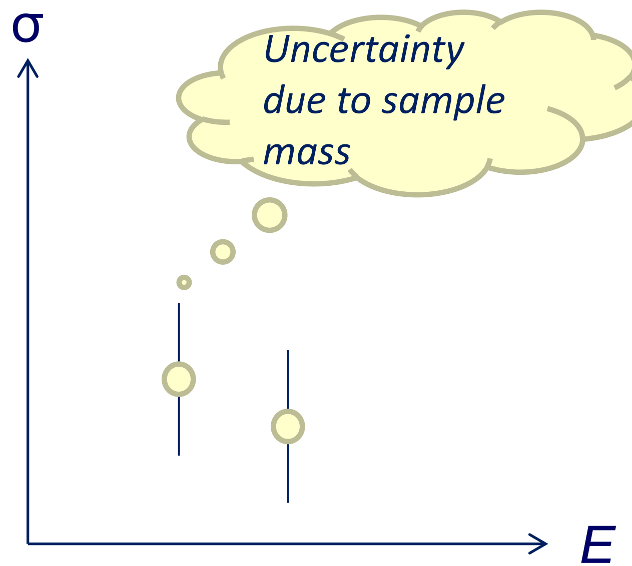
1

2

3

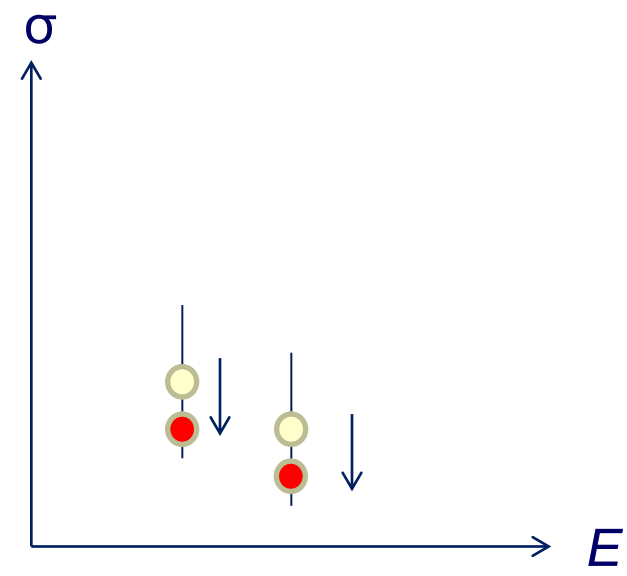


Example of Correlations



Two cross section points measured with same sample

If the *sample mass* is revised to higher value...



Two cross section points measured with same sample

No such a relation for uncorrelated source (e.g., counting statistics)

Uncertainty – for Future Use of EXFOR data

Let us consider a quantity *Q* which depends on the capture cross sections at two neutron energy points a and b:

$$Q\,(\sigma^{a}_{(n,\gamma)}, \sigma^{b}_{(n,\gamma)})\,.$$

Error propagation from σ to Q:

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

Total uncertainty of σ^a

Total uncertainty of σ^b

Covariance between σ^a and σ^b

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

Partial Uncertainty and Correlation Coefficient

$$V^{ab} = \sum_i \frac{\partial \sigma^a}{\partial x_i^a} V_i^{ab} \frac{\partial \sigma^b}{\partial x_i^b} = \sum_i \Delta\sigma_i^a c_i^{ab} \Delta\sigma_i^b$$

correlation coeff. $|c| \leq 1$

partial uncertainty due to *i*-th parameter

- In order to obtain the covariance V^{ab}, both partial uncertainties and correlation coefficients for each *i*-th component should be known.

- Partial uncertainties (or their ranges) are often reported. But correlation properties are rarely reported.

Example of Correlation Coefficient "c"

Example of correlation property in $^{67}Zn(n,\alpha)^{64}Ni$ cross section
(Guohui Zhang et al., Phys.Phys.C82(2010)054619)

$$\sigma_\alpha = \sigma_f \frac{N_\alpha}{N_f} \frac{N_{^{238}\mathrm{U}}}{N_{^{67}\mathrm{Zn}}}$$

reference cross section $^{238}U(n,f)$

count

\# of nuclei

TABLE I. Measured cross sections of the $^{67}Zn(n,\alpha_0)^{64}Ni$ and $^{67}Zn(n,\alpha)^{64}Ni$ reactions.

E_n (MeV)	σ_{exp} (mb)	
	$^{67}Zn(n,\alpha_0)$	$^{67}Zn(n,\alpha)$
4.0	2.0 ± 0.2	7.4 ± 0.9
5.0	1.4 ± 0.1	7.6 ± 0.9
6.0	0.81 ± 0.1	8.1 ± 0.9
6.0 [6]	0.86 ± 0.1	7.3 ± 1.1

E_i →

E_j ↓

	σ_f	N_α	N_f	N_{238U}	N_{67Zn}
σ_f	0<c<1	c=0	c=0	c=0	c=0
N_α	c=0	c=0	c=0	c=0	c=0
N_f	c=0	c=0	c=0	c=0	c=0
N_{238U}	c=0	c=0	c=0	c=1 (?)	c=0
N_{67Zn}	c=0	c=0	c=0	c=0	c=1 (?)

Impact of Covariance – Example

Two activation cross section ratios under ^{252}Cf(sf) PFNS

- W. Mannhart, *A Small Guide to Generating Covariances of Experimental Data*, INDC(NDS)-0588 (2010)

R_1=^{27}Al(n,p)/^{27}Al(n,α)

R_2=^{24}Mg(n,p)/^{115}In(n,n')

If we *ignore* covariance (e.g., treat all uncertainties as random uncertainties),

R_1=4.797±4.84%

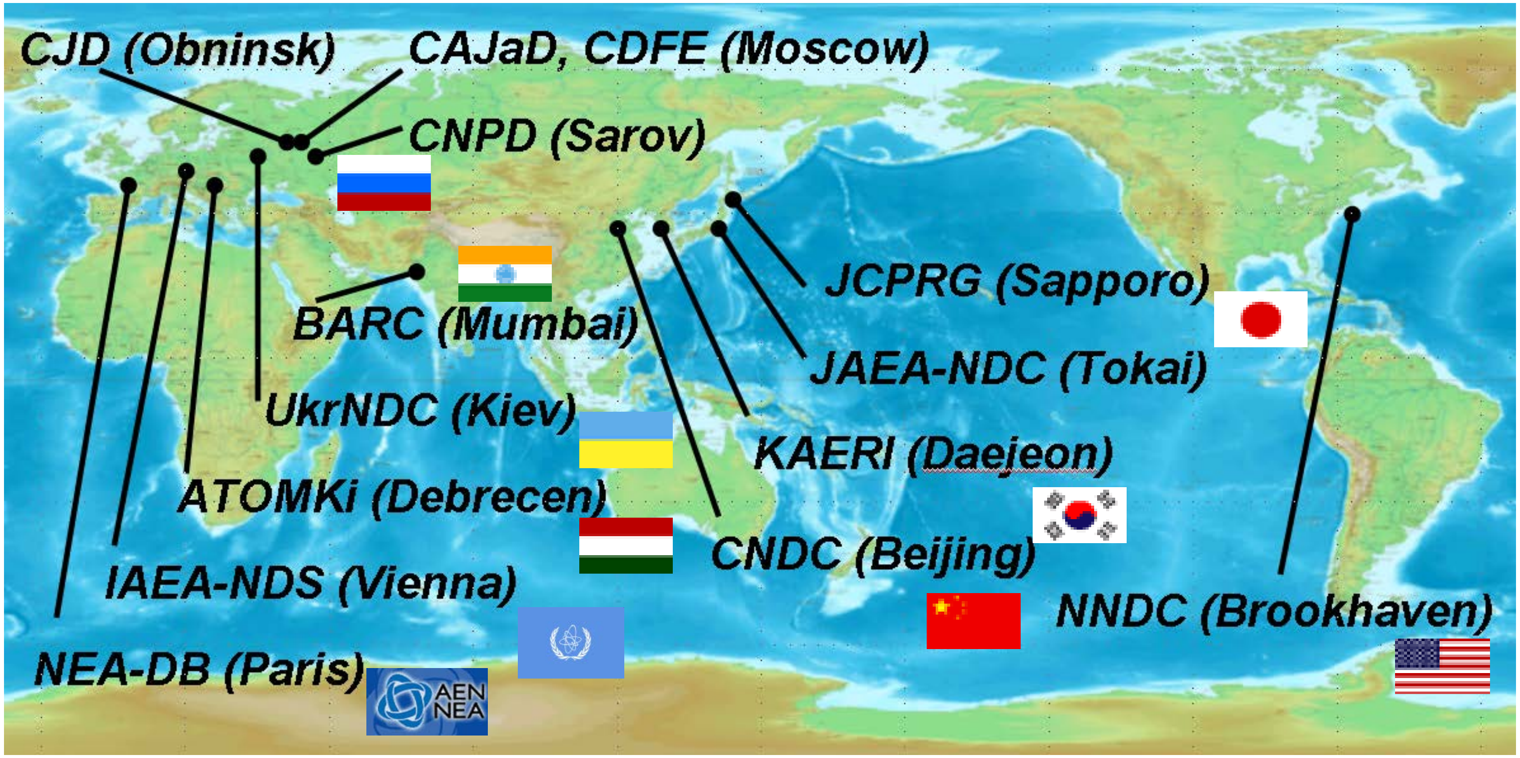
R_2=0.009651±5.67%

If we *consider* covariance,

R_1=4.797±3.35%

R_2=0.009651±4.36%

EXFOR – Experimental Data *Exchange*



14 centres from 8 countries and 2 international organisations
(China, Hungary, India, Japan, Korea, Russia, Ukraine, USA, NEA, IAEA)

Experimental data exchange coordinated by IAEA-NDS

Uncertainty in EXFOR – Brief History

F. G. Perey (ORNL) – Harwell Conference (Sept. 1978)

"We urge experimentalists to report the uncertainties in their measurements in such a fashion that the covariance matrix of their results can be generated."

"We hope that data compilers in the future will expand their data compilation formats such that this valuable information can be made available."

In reality, authors often report only "total uncertainty".

COVARIANCE MATRICES OF EXPERIMENTAL DATA*

F. G. Perey
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830 U.S.A.

ABSTRACT

A complete statement of the uncertainties in data is given by its covariance matrix. It is shown how the covariance matrix of data can be generated using the information available to obtain their standard deviations. Determination of resonance energies by the time-of-flight method is used as an example. The procedure for combining data when the covariance matrix is non-diagonal is given. The method is illustrated by means of examples taken from the recent literature to obtain an estimate of the energy of the first resonance in carbon and for five resonances of ^{238}U.

"Total uncertainty" is insufficient !!

5th NRDC Meeting (October 1980) – M. Bhat (NNDC) mentioned:

When evaluators go back to the original references, as they must, the needed information is not there. If the data centres required experimenters to supply the needed information, the data available to the evaluators would be more complete.

Data Centres (EXFOR compilers) are encouraged receive not only total uncertainty but also partial uncertainties from authors even if they are not reported in the articles.

Note: Authors providing the "total uncertainty" also should be able to provide partial uncertainties.

What we can keep in the current EXFOR Formats?

- Both total uncertainty and partial uncertainties

- Constant and energy dependent uncertainties

C. Sage et al., Phys. Rev. C81(2010)064604

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)	σ_{Al}	S_{Am}	S_{Al}	I_{Am}	n_{Al}	n_{Am}	$\epsilon_{Al}/\epsilon_{Am}$	$(f_\Sigma f_r)_{Am}$	$\frac{C_{low,Am}}{C_{low,Al}}$
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

```
COMMON
ERR-1       ERR-2
PER-CENT    PER-CENT
 1.2         0.1
ENDCOMMON
DATA
EN          DATA        ERR-T       ERR-S       ERR-3       ERR-4
MEV         MB          PER-CENT    PER-CENT    PER-CENT    PER-CENT
 8.34        96.8        6.5         5.0         1.9         0.9
 9.15       162.9        5.7         4.0         1.9         0.6
  …           …           …           …           …           …
```

From EXFOR uncertainty to covariance

A typical experimental covariance derivation from EXFOR (between two energy bin Ei and Ej)

$V_{ij} = \delta_{ij}\Delta_{sta}(E_i)\Delta_{sta}(E_j)$ (statistical uncertainty)

$+ \Sigma_k \Delta^k_{sys}(E_i)\Delta^k_{sys}(E_j)\, c^k_{ij}$ (k-th systematic uncertainty)

c^k : correlation matrix of k-th uncertainty

Partial uncertainties Δ and their correlation properties c are required for construction of experimental covariance.

Sometimes they are missing in EXFOR even they are reported in the original article…

Retroactive corrections of EXFOR entries

Example: EXFOR 22292.003

45Sc(n,2n)44Sc cross section

```
ERR-ANALYS (DATA-ERR) TOTAL ERRORS.
…
REACTION   (21-SC-45(N,2N)21-SC-44,,SIG)
DATA                   4          4
EN         EN-ERR     DATA       DATA-ERR
MEV        MEV        MB         MB
 1.1580E+01 1.7000E-01 2.0000E+00 8.0000E-01
 1.1970E+01 1.8000E-01 2.1000E+01 2.6000E+00
 1.2400E+01 1.8000E-01 5.2000E+01 6.1000E+00
 1.2850E+01 2.0000E-01 7.5000E+01 8.0000E+00
ENDDATA                6
```

M. Bostan et al., Phys. Rev. C49(1994)266

(More detailed reports on uncertainties)

TABLE II. Principal sources of errors and their magnitudes.

Source of uncertainty	Magnitude% Gamma counting $(n,2n)$	Magnitude% Gamma counting (n,α)	Magnitude% Beta counting (n,p)
Uncorrelated			
Sample weight	0.1	0.1	0.1
Irradiation time	0.1	0.1	0.1
Irradiation geometry and beam deviation	3	3	3
Error in peak area analysis	3	3	
Statistics of counting	3	3	3
Chemical yield[a]			3
Correction for activity induced by background neutrons (gas in/out, breakup)	1–3	5–20[b]	5–20[b]
Correlated			
Error in excitation function of monitor reaction	3–8	3–8	3–8
Efficiency of the detector (Self-absorption, geometry)	5	5–8	12
Decay data	1	1	1
Total	8–12	10–24	16–26

[a]Chemical separation was done only for the $^{45}Sc(n,p)^{45}Ca$ reaction product.

[b]This correction is high for low threshold reactions.

Retroactive correction is on-going.

EXFOR for experimental correlation

TABLE II. Principal sources of errors and their magnitudes.

Source of uncertainty	Magnitude% Gamma counting $(n,2n)$	Magnitude% Gamma counting (n,α)	Magnitude% Beta counting (n,p)
Uncorrelated			
Sample weight	0.1	0.1	0.1
Irradiation time	0.1	0.1	0.1
Irradiation geometry and beam deviation	3	3	3
Error in peak area analysis	3	3	
Statistics of counting	3	3	3
Chemical yield[a]			3
Correction for activity induced by background neutrons (gas in/out, breakup)	1–3	5–20[b]	5–20[b]
Correlated			
Error in excitation function of monitor reaction	3–8	3–8	3–8
Efficiency of the detector (Self-absorption, geometry)	5	5–8	12
Decay data	1	1	1
Total	8–12	10–24	16–26

[a]Chemical separation was done only for the ^{45}Sc$(n,p)^{45}$Ca reaction product.
[b]This correction is high for low threshold reactions.

$$V_{ij}=\delta_{ij}\Delta_{sta}(E_i)\Delta_{sta}(E_j) + \Sigma_k\Delta^k_{sys}(E_i)\Delta^k_{sys}(E_j)\, c^k_{ij}$$

Indication of correlation property in EXFOR is under discussion

U: Uncorrelated (Long range, $c_{ij}=\delta_{ij}$)
F: Fully correlated (Short range, $c_{ij}=1$)

(ERR-1,,,U) Sample weight
(ERR-2,,,U) Irradiation time
(ERR-3,,,F) Detector efficiency
...

Problem: Authors often do not know correlation properties.

EXFOR for experimental correlation (cont)

C. Sage et al., Phys.Rev.C81(2010)064604 – ^{243}Am(n,2n) cross section.

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)	σ_{Al}	S_{Am}	S_{Al}	I_{Am}	n_{Al}	n_{Am}	$\epsilon_{Al}/\epsilon_{Am}$	$(f_\Sigma f_r)_{Am}$	$\frac{C_{low,Am}}{C_{low,Al}}$
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

```
BIB
REACTION   (94-AM-241(N,2N)94-AM-240,,SIG)
...
ERR-ANALYS (ERR-T,,,P)      Total uncertainty
           (MONIT-ERR,,,P)  Monitor cross section
           (ERR-1,,,U)      Number of counts (Am)
           (ERR-2,,,U)      Number of counts (Al)
           (ERR-3,,,F)      Gamma intensity (Am)
           (ERR-4,,,U)      Sample mass (Al)
           (ERR-5,,,P)      Sample mass (Am)
           (ERR-6,,,F)      Efficiency ratio (Al/Am)
           (ERR-7,,,F)      Decay correction (Am)
           (ERR-8,,,U)      Secondary neutron correction (Am/
...
COMMON
ERR-3      ERR-4      ERR-5      ERR-6
PER-CENT   PER-CENT   PER-CENT   PER-CENT
 1.2        0.1        0.3        3.0
ENDCOMMON
DATA
EN         DATA       ERR-T      MONIT-ERR  ERR-1      ERR-2      ERR-7      ERR-8
MEV        MB         PER-CENT   PER-CENT   PER-CENT   PER-CENT   PER-CENT   PER-CENT
  8.34      96.8        6.5        1.9        5.0        1.0        0.9
  9.15     162.9        5.7        1.9        4.0        1.0        0.6
 13.33     241.8        4.6        1.6        2.5        1.0        0.4        0.3
 16.1      152.4        4.6        2.         2.1        1.0        0.6        0.3
 17.16     116.1        4.4        2.         1.5        1.0        0.6        0.3
 17.9      105.7        4.4        2.2        1.3        0.7        0.7        0.3
 19.36      89.5        8.2        3.1        6.3        2.0        0.6        1.3
 19.95     102.1        5.8        4.1        1.4        1.0        0.6        1.4
 20.61      77.9        8.8        5.4        5.7        1.6        0.6        1.4
ENDDATA
```

Correlation Property

U: uncorrelated

F: fully correlated

P: partly correlated

(for approval)

Partial uncertainty values

EXFOR for experimental correlation (cont)

Guohui Zhang et al., Phys.Phys.C82(2010)054619
– 67Zn(n,α)64Ni cross section (EXFOR 32689)

TABLE I. Measured cross sections of the ^{67}Zn(n, α_0)^{64}Ni and ^{67}Zn(n, α)^{64}Ni reactions.

E_n (MeV)	σ_{exp} (mb)	
	^{67}Zn(n, α_0)	^{67}Zn(n, α)
4.0	2.0 ± 0.2	7.4 ± 0.9
5.0	1.4 ± 0.1	7.6 ± 0.9
6.0	0.81 ± 0.1	8.1 ± 0.9
6.0 [6]	0.86 ± 0.1	7.3 ± 1.1

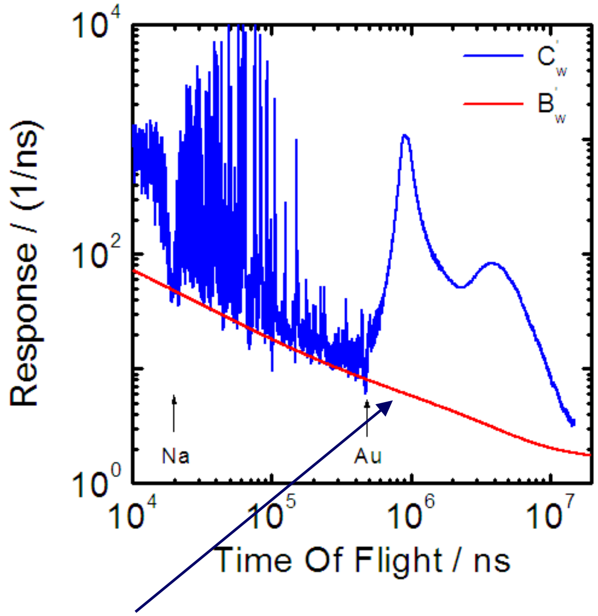
$$\sigma_\alpha = \sigma_f \frac{N_\alpha}{N_f} \frac{N_{^{238}U}}{N_{^{67}Zn}}$$

```
ERR-ANALYS (ERR-T) Total uncertainties
           (ERR-1,7.,11.)The uncertainty of alpha counts Na
           (ERR-2) The uncertainty of fission counts Nf
           (ERR-3) The uncertainty of the atomic number of 67Zn
           (ERR-4) The uncertainty of the atomic number of U238
           (MONIT-ERR) The uncertainty of 238U(n,f) cross-section…
ENDBIB              60
COMMON               4          3
ERR-2      ERR-3      ERR-4      MONIT-ERR
PER-CENT   PER-CENT   PER-CENT   PER-CENT
 2.5        1.5        1.3        1.
ENDCOMMON            3
ENDSUBENT           67
SUBENT        32689003   20110324
BIB                  1          1
REACTION   (30-ZN-67(N,A)28-NI-64,,SIG)
ENDBIB               1
NOCOMMON             0          0
DATA                 4          3
EN         DATA       ERR-T      MONIT
MEV        MB         MB         MB
4.0        7.4        0.9        554.40
5.0        7.6        0.9        546.71
6.0        8.1        0.9        610.79
ENDDATA              5
ENDSUBENT           11
```

- Alpha counting statistics must be given in energy dependent form.
- Counts Na and Nf are uncorrelated, but now it is not clear from the entry.
- Indication of correlation properties (**U**,**F**,**P**) is desired.

Covariance in resonance region
(Collaboration with P. Scillebeeckx et al. - IRMM)

Transmission=$(C_{in}-B_{in})/(C_{out}-B_{out})$
C: count, B: backgound



source of correlation

High resolution TOF experiment:
channel number n~10^4

V (n × n matrix**)** is too big for EXFOR!

Cholesky decomposition (by AGS package)

$$V = SS^T$$

(V: n × n matrix, S: n × k matrix, k~10)

S can be stored in to the EXFOR library.

n+^{113}Cd measured at GELINA
– EXFOR 23077 (released: 2 Sept. 2011)

Covariance in resonance region (cont)

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

The total cross section and resonance parameters for the 0.178 eV resonance of ^{113}Cd

S. Kopecky [a,*], I. Ivanov [a,1], M. Moxon [a,b], P. Schillebeeckx [a], P. Siegler [a], I. Sirakov [a,1]

[a] EC-JRC, Institute for Reference Materials and Measurements, Retieseweg 111, B-2440 Geel, Belgium
[b] Hyde Copse, Marcham, United Kingdom

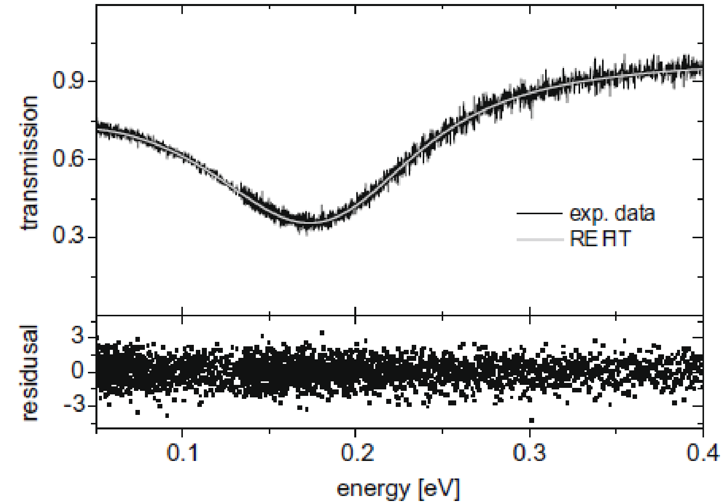


Fig. 2. Fit to sample 1, metallic sample with 30 μm thickness.

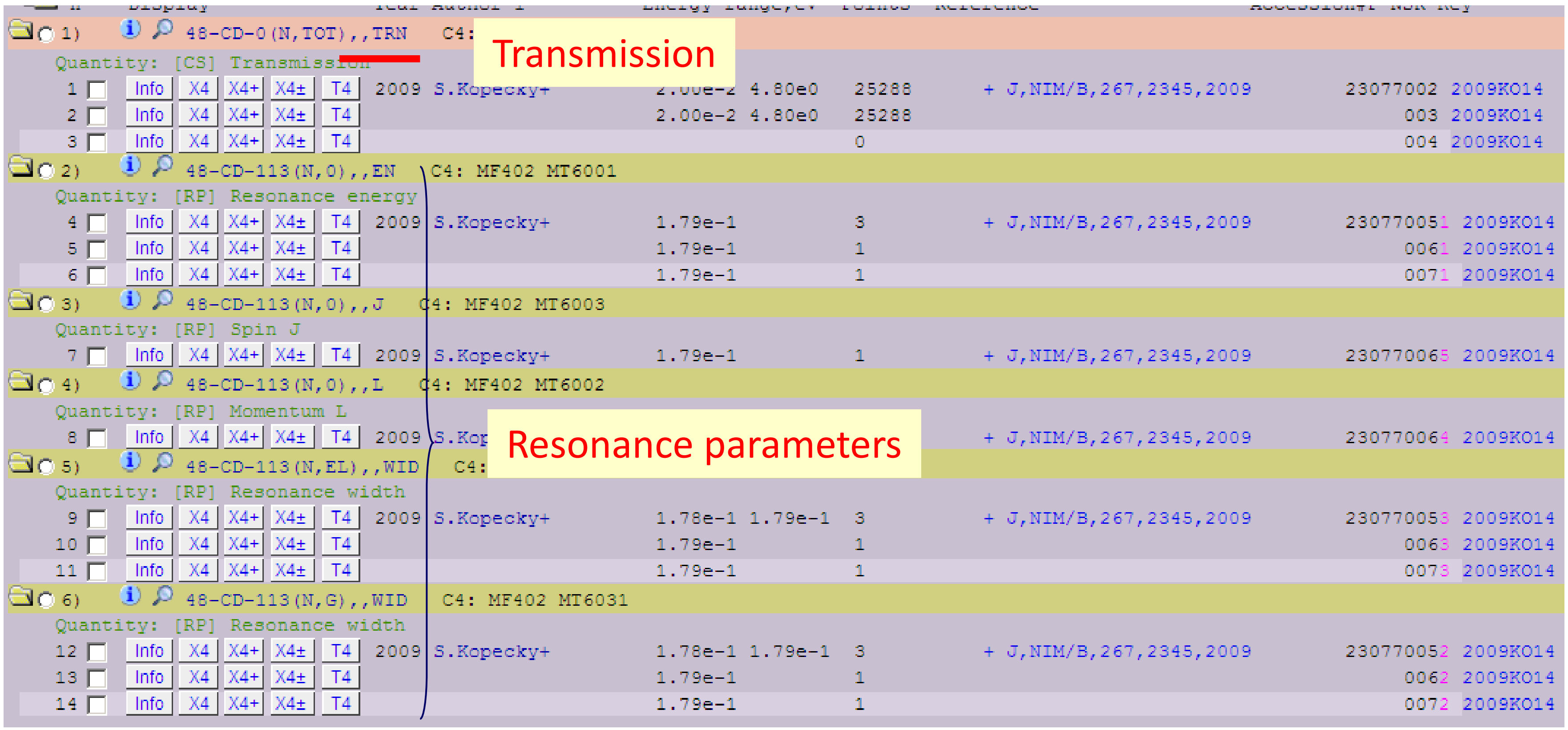
Table 1
Comparison of the resonance parameters of the 0.178 eV ^{113}Cd resonance found in the literature.

Experiment	Sample type	E_{res} (eV)	Γ_γ (meV)	Γ_n (meV)
Rainwater et al. [5]	Metal	0.176 ± 0.002	115 ± 2	0.620 ± 0.020
Brockhouse [6]	Metal	0.180 ± 0.003	113 ± 2	0.680 ± 0.020
Akyüz et al. [7]	Metal	0.181 ± 0.003	109 ± 3	0.645 ± 0.025
Widder and Brunner [8]	Powder	0.1776 ± 0.0006	114.3 ± 0.6	0.618 ± 0.003
Harz and Priesmeyer [9]	Various	0.1783 ± 0.0002	113.5 ± 0.5	0.650 ± 0.005

diff:5%

Covariance in resonance region (cont)

- n+^{113}Cd measured at GELINA
  - EXFOR 23077 subentries



#	Display	Year	Author 1	Energy range	Points	Reference	Accession#	NSR Key
1)	48-CD-0(N,TOT),,TRN C4:							
	Quantity: [CS] Transmission							
1	Info X4 X4+ X4± T4	2009	S.Kopecky+	2.00e-2 4.80e0	25288	+ J,NIM/B,267,2345,2009	23077002	2009KO14
2	Info X4 X4+ X4± T4			2.00e-2 4.80e0	25288		003	2009KO14
3	Info X4 X4+ X4± T4				0		004	2009KO14
2)	48-CD-113(N,0),,EN C4: MF402 MT6001							
	Quantity: [RP] Resonance energy							
4	Info X4 X4+ X4± T4	2009	S.Kopecky+	1.79e-1	3	+ J,NIM/B,267,2345,2009	230770051	2009KO14
5	Info X4 X4+ X4± T4			1.79e-1	1		0061	2009KO14
6	Info X4 X4+ X4± T4			1.79e-1	1		0071	2009KO14
3)	48-CD-113(N,0),,J C4: MF402 MT6003							
	Quantity: [RP] Spin J							
7	Info X4 X4+ X4± T4	2009	S.Kopecky+	1.79e-1	1	+ J,NIM/B,267,2345,2009	230770065	2009KO14
4)	48-CD-113(N,0),,L C4: MF402 MT6002							
	Quantity: [RP] Momentum L							
8	Info X4 X4+ X4± T4	2009	S.Kop			+ J,NIM/B,267,2345,2009	230770064	2009KO14
5)	48-CD-113(N,EL),,WID C4:							
	Quantity: [RP] Resonance width							
9	Info X4 X4+ X4± T4	2009	S.Kopecky+	1.78e-1 1.79e-1	3	+ J,NIM/B,267,2345,2009	230770053	2009KO14
10	Info X4 X4+ X4± T4			1.79e-1	1		0063	2009KO14
11	Info X4 X4+ X4± T4			1.79e-1	1		0073	2009KO14
6)	48-CD-113(N,G),,WID C4: MF402 MT6031							
	Quantity: [RP] Resonance width							
12	Info X4 X4+ X4± T4	2009	S.Kopecky+	1.78e-1 1.79e-1	3	+ J,NIM/B,267,2345,2009	230770052	2009KO14
13	Info X4 X4+ X4± T4			1.79e-1	1		0062	2009KO14
14	Info X4 X4+ X4± T4			1.79e-1	1		0072	2009KO14

Covariance in resonance region (cont)

EXFOR 23077.001

```
ENTRY            23077   20110128                                  23077000    1
SUBENT        23077001   20110128                                  23077001    1
BIB                 12         73                                  23077001    2
TITLE      The total cross section and resonance parameters for    23077001    3
            the 0.178 eV resonance of 113Cd                        23077001    4
AUTHOR     (S.Kopecky, I.Ivanov, M.Moxon, P.Schillebeeckx,         23077001    5
            P.Siegler, I.Sirakov)                                  23077001    6
INSTITUTE  (2ZZZGEL)                                               23077001    7
           (2UK UK) Hyde Copse, Marcham (M.Moxon)                  23077001    8
REFERENCE  (J,NIM/B,267,2345,2009)                                 23077001    9
           (W,KOPECKY,2009) EXFOR coding sheet prepared at Geel    23077001   10
REL-REF    (I,,J.M.Salome+,J,NIM/A,179,13,1981)                    23077001   11
            Details of GELINA facility                             23077001   12
           (I,,D.Tronc+,J,NIM/A,228,217,1985)                      23077001   13
            Details of GELINA facility                             23077001   14
           (I,,M.Flaska+,J,NIM/A,531,392,2004)                     23077001   15
            Details of neutron production                          23077001   16
FACILITY   (LINAC,2ZZZGEL) GELINA                                  23077001   17
INC-SOURCE Diameter of neutron beam = 40 mm                        23077001   18
           Time resolution of electron beam = 1 ns                 23077001   19
           (PHOTO) (g,n) on uranium target                         23077001   20
                   (2 containers, 100 x 100 mm, 40 mm thick)       23077001   21
           (THCOL) Water moderator                                 23077001   22
SAMPLE     (48-CD-113,NAT=0.1222) 12.22% +/- 0.04% is used.        23077001   23
            * Metal sample I                                       23077001   24
                Physical type:             Metal                   23077001   25
                Chemical composition:      Element (Cadmium)       23077001   26
                Purity of main element:    100%                    23077001   27
                Weight:                    1.2814 +/- 0.0001 g     23077001   28
                Weight per area:           0.02547 g/cm2           23077001   29
                Diameter:                  80.04 +/- 0.03 mm       23077001   30
                Thickness:                 0.030 mm (nominal)      23077001   31
                Thickness of main element: 1.3643E-04 atom/b       23077001   32
                Containment description:   No container            23077001   33
```

Covariance in resonance region (cont)

```
SUBENT        23077002   20110128   20110905   20110902        2226
BIB                  9         25
REACTION    (48-CD-0(N,TOT),,TRN)
            #(48-CD-0(N,TOT),,TRN)  Quantity: [CS] Transmission
            #          Process: [TOT] Total
SAMPLE       Metal sample I (0.03 mm)
INC-SPECT    EN gives neutron energy calculated with a flight
             path length of 26.464 m
MISC-COL    (MISC1)     Width of time-of-flight bin
            (MISC2)     Uncorrelated uncertainty squared
ERR-ANALYS  - Overall a normalisation uncertainty of 0.5% due to
              possible fluctuation of the beam monitor is excluded
              below and has to be added.
            - ERR-1 to ERR-4 gives "correlation vectors" in the
              AGS format.
            (ERR-T)  Total uncertainty (1 sigma)
            (ERR-S)  Uncorrelated uncertainty (1 sigma)
            (ERR-1)  Correlation dead time correction  (sample)
            (ERR-2)  Correlation background correction (sample)
            (ERR-3)  Correlation dead time correction  (open beam)
            (ERR-4)  Correlation background correction (open beam)
COVARIANCE  (CHLSK) Compiled in ERR-1 to ERR-4 in the AGS format
REL-REF     (N,,C.Bastian+,C,92BNL,,642,1992)
             Description of AGS format
            (N,,C.Bastian+,C,2006VANCOU,,(C013),2006)
             Description of AGS format
            (TA     Dat  received from S.Kopecky by e-mail
            (Al          ead by Stefan Kopecky (2011-01-28)
            (2(           . Received by e-mai    m S
                                     0
DATA                    12     25288          12
```

Transmission T
0.02 eV-4.8 eV,
25,288 data points
(EXFOR 23077.002)

<En> (eV)	TOF (nsec)			T	$\Delta_{tot}T$	$\Delta_{stat}T$		$\Delta_{sys,1}T$	$\Delta_{sys,2}T$	$\Delta_{sys,3}T$	
EN	TOF-MIN	TOF-MAX	MISC1	DATA	ERR-T	ERR-S	MISC2	ERR-1	ERR-2	ERR-3	ERR-4
EV	NSEC	NSEC	NSEC	NO-DIM	NO-DIM	NO-DIM	NO-DIM	NO-DIM	NO-DIM	NO-DIM	NO-DIM
4.7993	873301.2	873429.2	128.	1.1478	0.0665562	0.0665376	4.42725E-3	1.33447E-5	-9.12646E-4	-1.37145E-5	1.28552E-3
4.7979	873429.2	873557.2	128.	0.97025	0.0563176	0.0563021	3.16993E-3	1.09942E-5	-8.47529E-4	-1.1668E-5	1.00913E-3
4.79649	873557.2	873685.2	128.	1.04716	0.0601241	0.0601078	3.61295E-3	1.19256E-5	-8.59307E-4	-1.26779E-5	1.10425E-3
4.79509	873685.2	873813.2	128.	0.898725	0.0498278	0.0498155	2.48158E-3	1.02934E-5	-7.4616E-4	-1.13642E-5	8.22937E-4
4.79368	873813.2	873941.2	128.	1.03868	0.0579569	0.057942	3.35728E-3	1.21216E-5	-8.09122E-4	-1.30735E-5	1.03134E-3
4.79228	873941.2	874069.2	128.	1.05707	0.0591457	0.0591305	3.49642E-3	1.24728E-5	-8.1986E-4	-1.3079E-5	1.06353E-3
4.79088	874069.2	874197.2	128.	1.06048	0.0608753	0.0608588	3.70379E-3	1.23289E-5	-8.63242E-4	-1.28838E-5	1.12341E-3
4.78947	874197.2	874325.2	128.	1.06846	0.0605227	0.0605067	3.66106E-3	1.24478E-5	-8.43675E-4	-1.29684E-5	1.10621E-3

Uncertainties than covariance in EXFOR?

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 (2010)

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…

Publication of experimental full covariance must be reported with their derivation from partial uncertainties.

Evaluation with model covariances
(Roberto Capote)

Basic equation of evaluation σ from experiments and calculations

$$p(\vec{\sigma}) \sim \exp[-1/2\{(y-y_{\exp})^T V_{\exp}^{-1}(y-y_{\exp})+(\sigma-\sigma_{\mathrm{cal}})^T V_{\mathrm{cal}}^{-1}(\sigma-\sigma_{\mathrm{cal}})\}] = \exp[(-1/2)S]$$

$$\text{maximum of entropy} \Leftrightarrow \text{minimum of S}$$

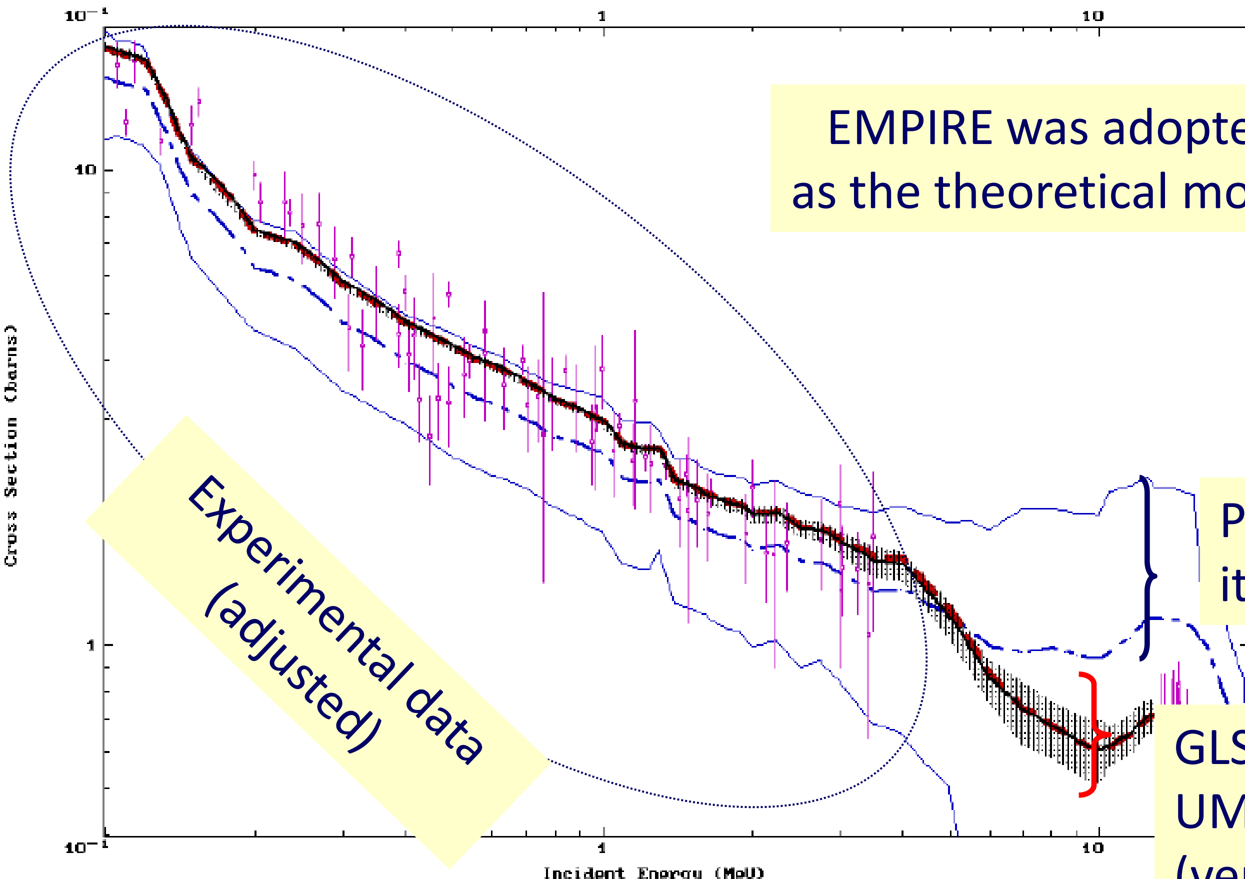
How we can obtain evaluated mean values and covariances?

- GLSQ (Generalized least-squares analysis – deterministic)
Generalized least-square fit where model covariance is defined as a *prior*; uses sensitivity matrices.

- Stochastic methods (e.g., Unified Monte Carlo approach)
Repetition of model calculations with random sets of input parameters combined with stochastic samples from experimental ***pdf***

- Hybrid methods (e.g., random model + GANDR least-squares fit)
Repetition of model calculations with random sets of input parameters, combined with generalized least-squares fit to include experiments

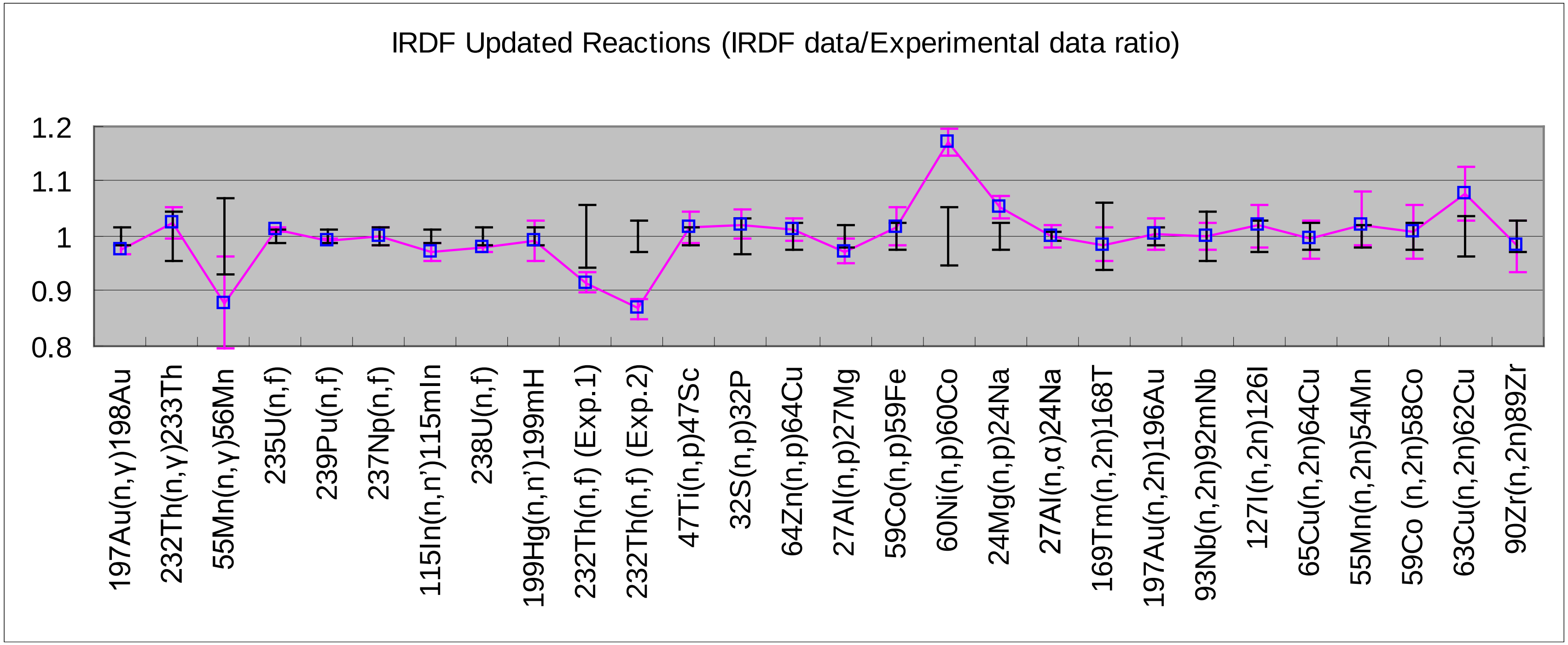
GLSQ v.s. UMC
$^{55}Mn(n,\gamma)^{56}Mn$ cross section



EMPIRE was adopted
as the theoretical model

GLSQ: Generalized least squares approach
UMC: Unified Monte-Carlo

Covariance matrix validation ^{252}Cf SPA XSs



(to be released as an updated IRDF Library at the end of 2011)

Evaluated data and uncertainty (both covariances in evaluated cross sections and ^{252}Cf reference neutron field are considered).

Experimental data uncertainty

Web tool for covariance visualization

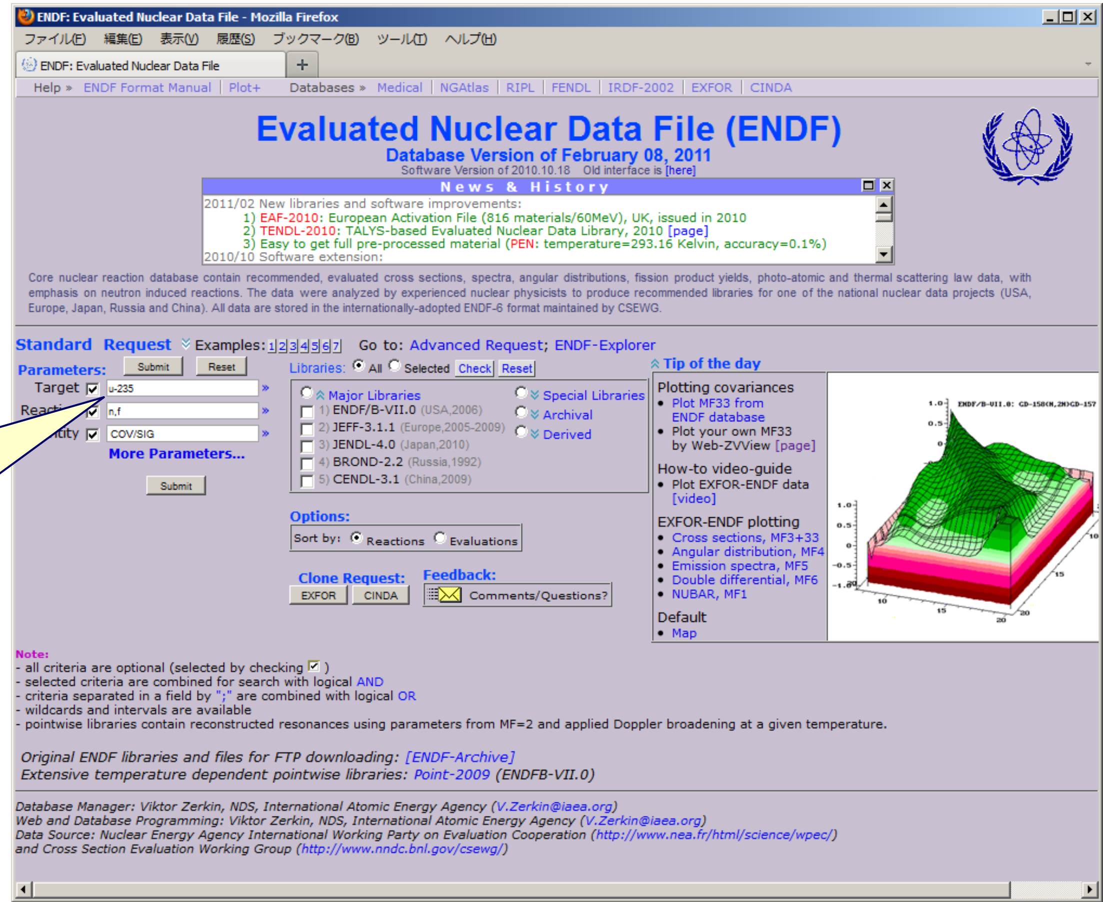
(Viktor Zerkin)

Creation of 2D or 3D plot from covariance matrices in nuclear data files are not a simple task.

→

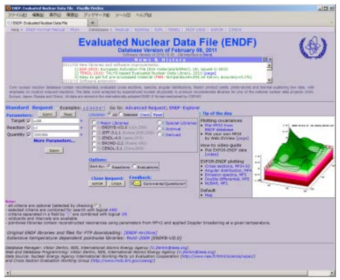
Web tool to plot covariance information

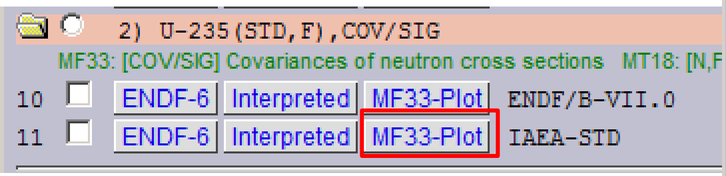
Target: U-235
Reaction: n,f
Quantity: COV/SIG
…
Then "Submit"

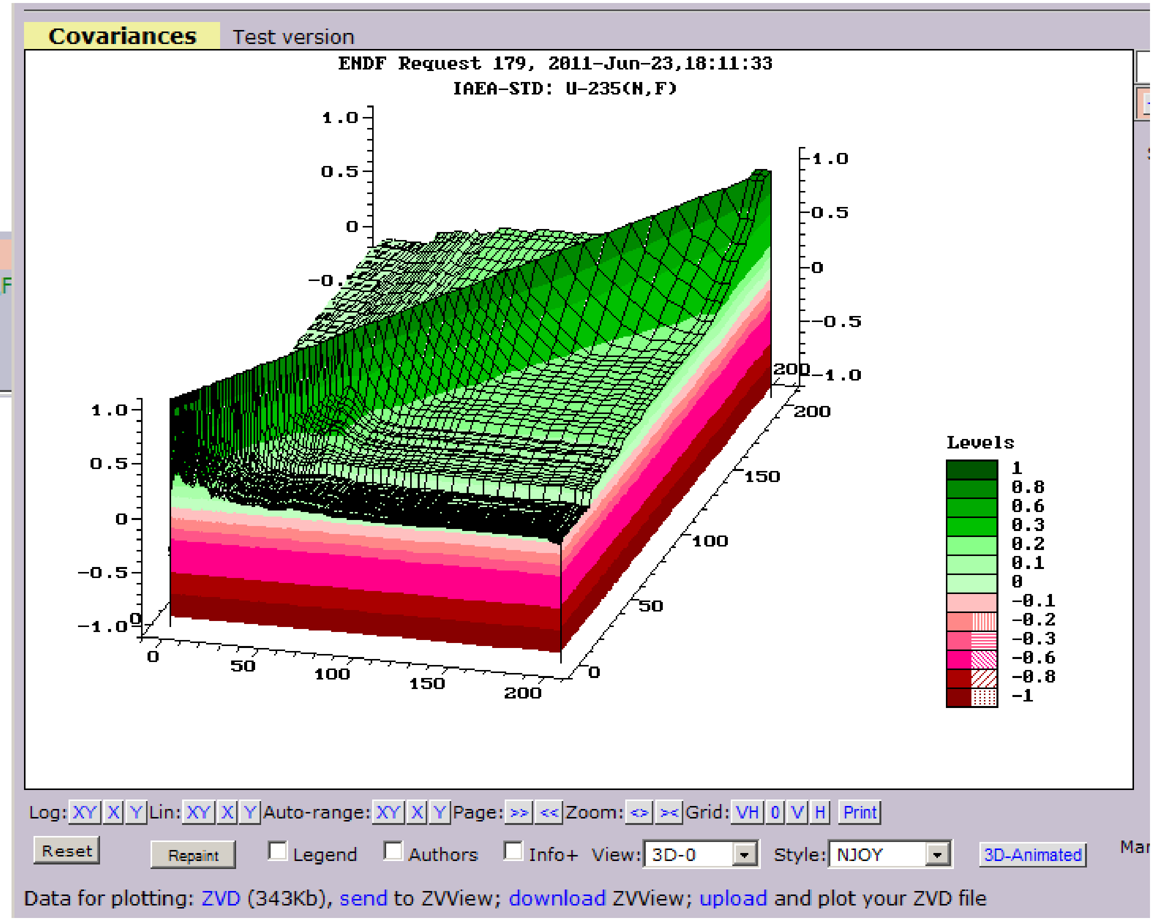


http://www-nds.iaea.org/endf/

Web tool for covariance visualization (cont)







^{235}U(n,f) IAEA Standard

MF33-Plot selected!

http://www-nds.iaea.org/endf/

Web tool for covariance visualization (cont)

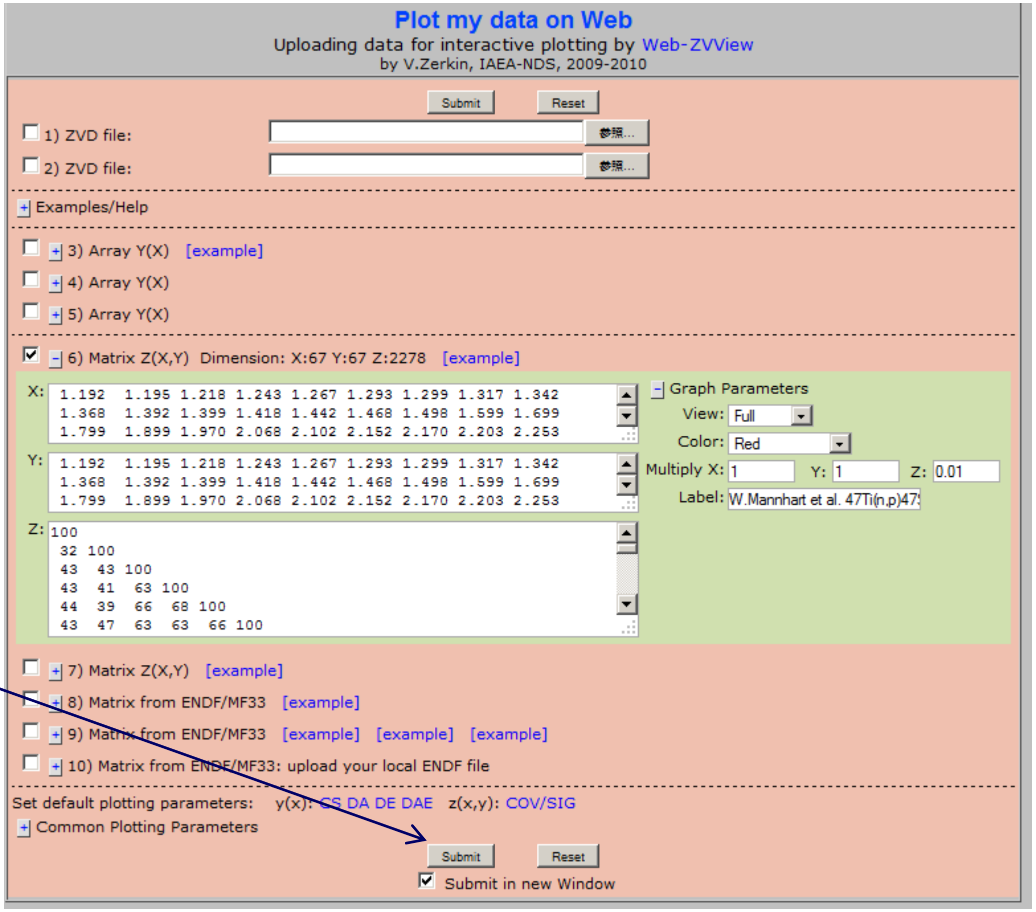
Web-ZVView also helps plotting of your own covariance matrix (or any function Z(x,y)).

x

y

z

Submit!



The ZVView package is based on the universal graphics library DINAMO© *DINAMO - Copyright © - 1998, Viktor Zerkin, registered: Ukraine, ПА N1539

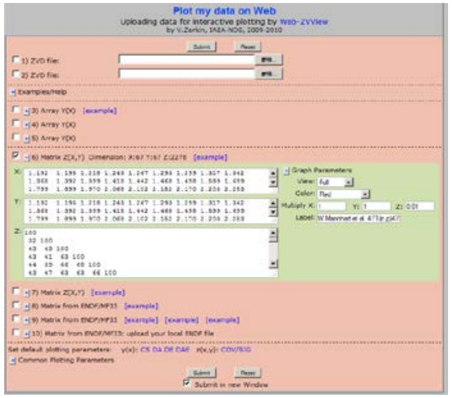
http://www-nds.iaea.org/exfor/myplot.html

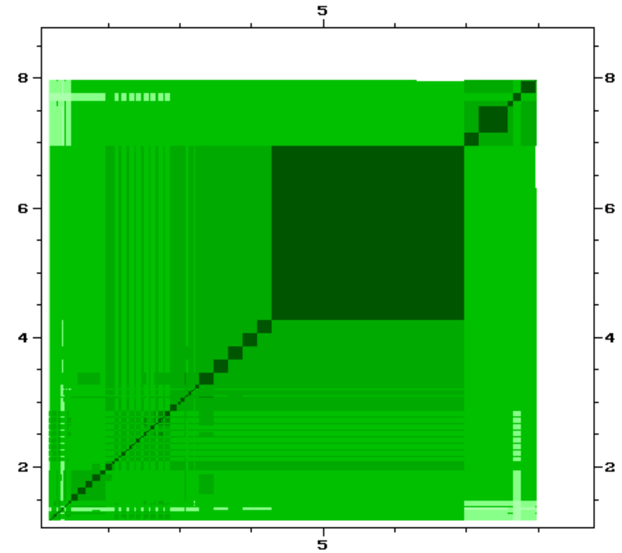
Web tool for covariance visualization (cont)

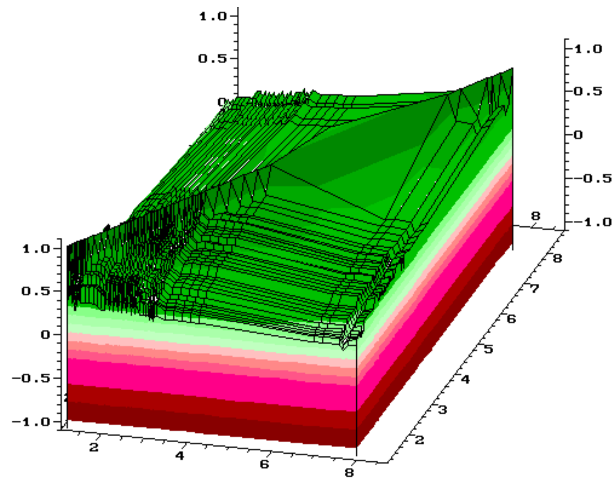
You can also visualize your covariance!

100							
32	100						
43	43	100					
43	41	63	100				
44	39	66	68	100			
43	47	63	63	66	100		
35	57	49	48	48	52	100	
44	39	66	68	73	66	48	100

$^{47}Ti(n,p)^{47}Sc$ covariance by W.Mannhart et al. (1980).







The ZVView package is based on the universal graphics library DINAMO© *DINAMO - Copyright © - 1998, Viktor Zerkin, registered: Ukraine, ПА N1539

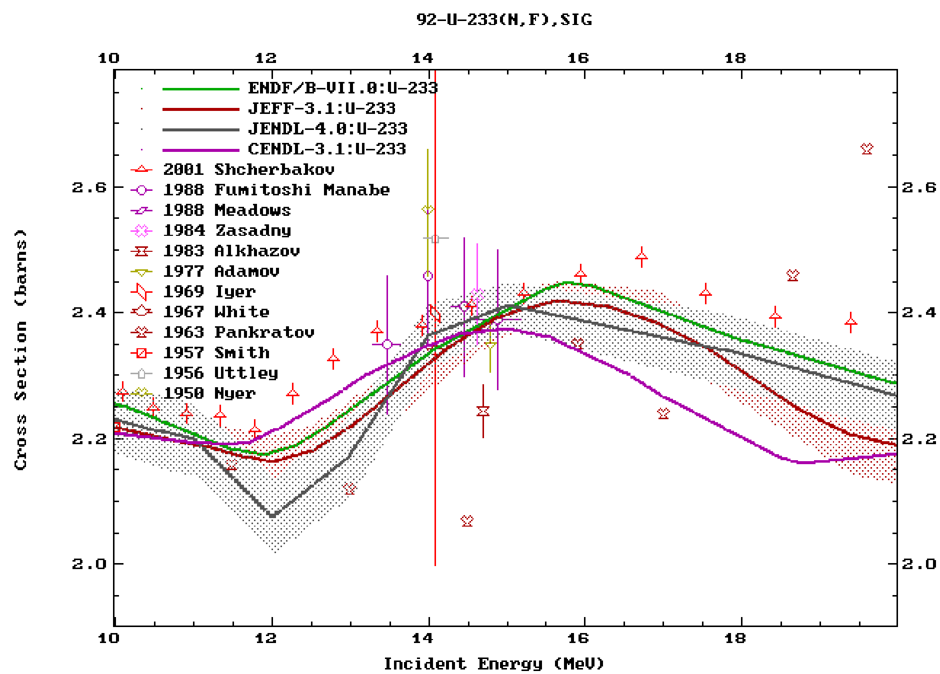
http://www-nds.iaea.org/exfor/myplot.html

Summary

- Experimenters and EXFOR compilers are urged to provide more information about experimental uncertainties and covariances.

- How much detail of uncertainty information is necessary? It is still an open question (for me).

- Development of several data libraries (ENDF, JENDL, CENDL, etc.) with their covariances may keep our knowledge of cross sections in a healthy condition.



$^{233}U(n,f)$, 10 MeV – 20 MeV