Web Tool for constructing a covariance matrix from EXFOR uncertainties

V.Zerkin, IAEA-NDS, 21/05/2011

Last few years there is growing interest and usage of covariances in nuclear data community. Covariance data in evaluated data files are used already very long time, have well defined formats (ENDF-6) and developed software of different types. Although EXFOR does not even have established formats for storage of covariance data, most of experimentalists could not provide these data – they published partial uncertainties which finally have appeared in EXFOR, and for some old experiments this information is absent at all. But even in the cases when information about uncertainties is very poor or absent, nowadays evaluators would like to be able to have some covariance matrix using some assumptions. Presented Web tool was developed for such evaluators, and also for experimentalists and EXFOR compilers who are interested in this subject. The tool was created in October-2010 and until now has status “under development”. The general ideas of algorithms are based on the relevant part of the methodology used in the work under IAEA Coordinated Research Project "Neutron Cross-section Standards" [1].

How it works.

1. The tool starts from converting EXFOR file to computational format C5 (C4 + systematic and statistical uncertainties) and presenting to user report with full relevant information:
   - C5 data points (energy, central values of cross sections)
   - C5 uncertainties (total, systematic, statistical)
   - all uncertainties given in EXFOR file
   - text from EXFOR given in ERR-ANALYS and METHOD sections
2. Then user can setup new values of uncertainties (or confirm existing uncertainties), introduce new (artificial) uncertainties splitting systematic uncertainties to parts, etc. This group will be used on the next step as input variables.
3. After that user defines how to use existing and newly introduced uncertainties for constructing covariance matrix: correlation type (uncorrelated, fully correlated and partially correlated). For partially correlated uncertainties (named medium energy range (MERC) correlation components in [1]) user defines additional parameters: correlation length and scale.
4. Finally user submits calculation and receives intermediate and final results in the following forms: raw data, data in ENDF-6 format (MF33) and link to Web-ZVView plotting package, where user can generate output in EXFOR format (draft) and text input for Fortran users including Fortran code.

The tool is available in the IAEA-NDS EXFOR Web retrieval system: http://www-nds.iaea.org/exfor; link [cov] will be offered to user for every dataset having Web-Quantity=’CS’. EXFOR compilers can also use it when using EXFOR uploading system: http://www-nds.iaea.org/exfor/x4up1.htm .

Concluding remarks

Hopefully this tool can be practically useful for some users and may help in the development of the methods using experimental data with covariances for various applications. It will probably need further improvements and development. Suggestions and feed back are very welcome. It may also help in development of EXFOR formats for storage of the partial uncertainties.

Acknowledgment

I thank to V.Pronyaev for useful discussions.

References

1. V.G. Pronyaev, S.A. Badikov, A.D. Carlson, Chen Zhenpeng, E.V. Gai, G.M. Hale, F.-J. Hambsch, H.M. Hofmann, T. Kawano, N.M. Larson, D.L. Smith, Soo-Youl Oh, S. Tagesen, H. Vonach, chapter “Evaluation Methodology and Codes”, pp.10-12, “International Evaluation of Neutron Cross-Section Standards”, IAEA-2006, http://www-pub.iaea.org/MTCD/publications/PDF/Pub1291_web.pdf

Attachment-1.

On-line help

X4/Servlet: Help Title - Mozilla Firefox

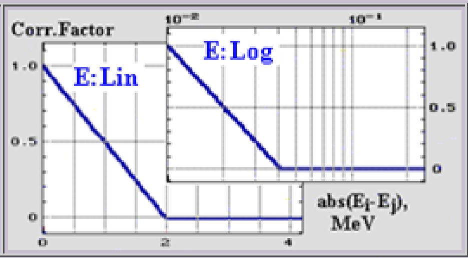
http://161.5.149.112/exfor1/x4js/x4covar_hlp.htm

Constructing covariance matrix from EXFOR uncertainties

programmer: V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)
International Atomic Energy Agency, October 2010
(Status: under development)

MERC (Medium Energy Range Correlations).
Applicable for partially-correlated uncertainties.
The correlation length of partially correlated uncertainties (Medium Energy Range Correlation) is determined as energy range of which correlations between uncertainties in two energy points disappear*. Log scale for energy correlations is probably more common for the time of flight measurements and linear scale - for discrete energy source measurements.
Typical examples of usage:

1) Scale:Lin; Energy: from 0 to 20MeV; Length: 0.1 (to 0.25)
*(means: points farer than 2 MeV (20MeV*0.1) are not correlated; between 0 and 2MeV, correlation factor = 1-abs(E_i-E_j)/2MeV)*
2) Scale:Log; Energy: from 10^{-5}eV to 20MeV; Length: 0.05
(means: points farer than 1/20 of the energy range are not correlated, otherwise correlation factor decreases from 1 to 0 proportionally to differences of energies in the logarithmic scale)
3) User can choose Energy range corresponding to Min-Max of selected dataset, set up type of Energy scale to Lin/Log, and define correlation Length on the basis of own consedirations



Note. This Web-tools presents an independent implementation of the algorithms of construction of covariance matrix for experimental data used under IAEA Coordinated Research Project "Neutron Cross-section Standards", 2004-2006 (see [page]).

SERC (Short Energy Range Correlations).
Applicable for uncorrelated uncertainties.
Example: statistical uncertainties.

LERC (Long Energy Range Correlations).
Applicable for fully-correlated uncertainties
Example: uncertainties in the determination of mass of the sample.

Uncorrelated
SERC (Short Energy Range)

1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1

Fully-correlated
LERC (Long Energy Range)

1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1

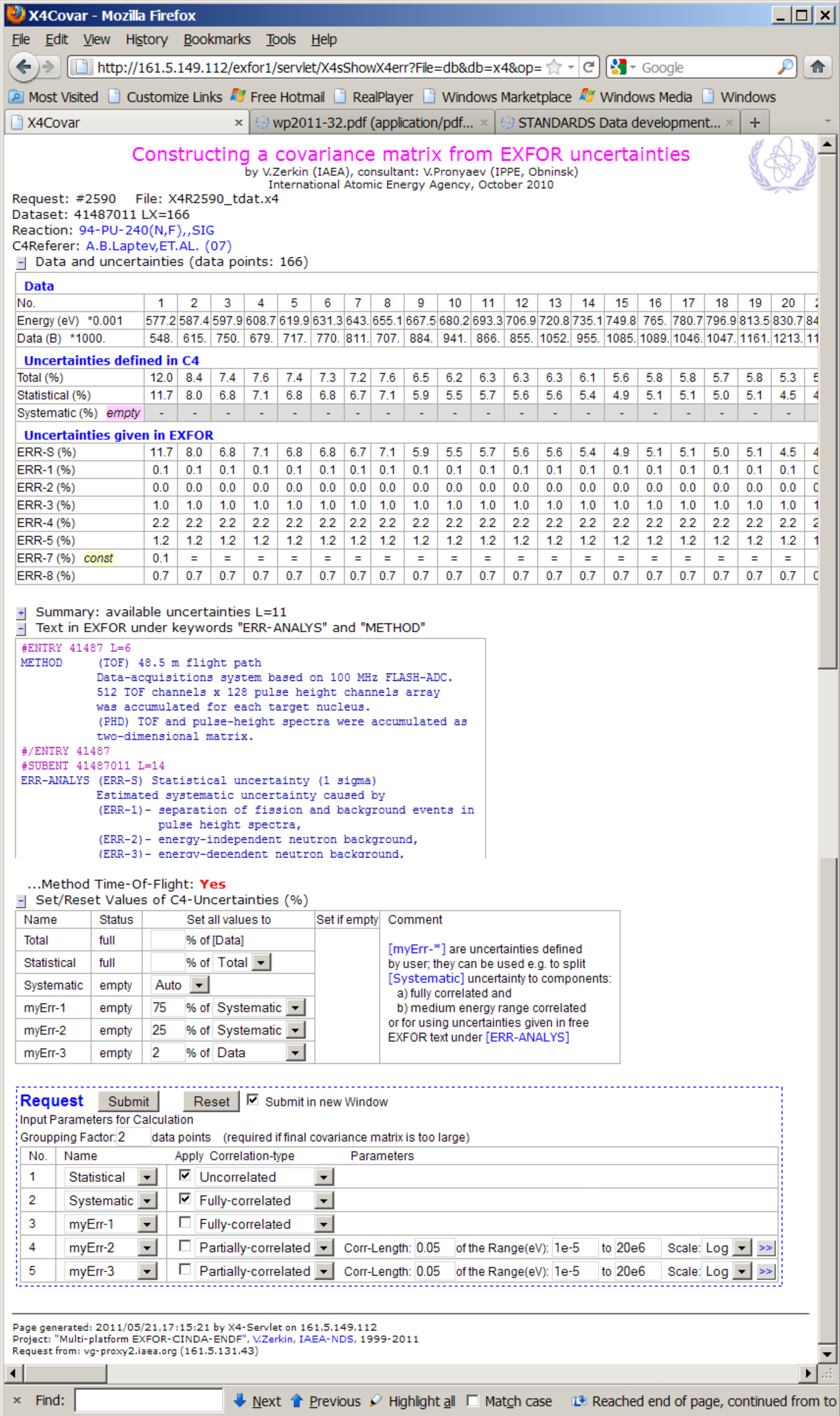
Partially-correlated
MERC (Medium Energy Range)

1	.7	.4	.1	0	0	0	0
.7	1	.7	.4	.1	0	0	0
.4	.7	1	.7	.4	.1	0	0
.1	.4	.7	1	.7	.4	.1	0
0	.1	.4	.7	1	.7	.4	.1
0	0	.1	.4	.7	1	.7	.4
0	0	0	.1	.4	.7	1	.7
0	0	0	0	.1	.4	.7	1

Last modified: 11/04/2010 18:39:13
Project: EXFOR-Relational V.Zerkin, IAEA, 1999-2010

Working Screenshot-1

Attachment-2.



X4Covar - Mozilla Firefox

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http://161.5.149.112/exfor1/servlet/X4sShowX4err?File=db&db=x4&op=

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X4Covar | wp2011-32.pdf (application/pdf... | STANDARDS Data development...

Constructing a covariance matrix from EXFOR uncertainties

by V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)
International Atomic Energy Agency, October 2010

Request: #2590 File: X4R2590_tdat.x4
Dataset: 41487011 LX=166
Reaction: 94-PU-240(N,F),,SIG
C4Referer: A.B.Laptev,ET.AL. (07)

Data and uncertainties (data points: 166)

Data

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Energy (eV) *0.001	577.2	587.4	597.9	608.7	619.9	631.3	643.	655.1	667.5	680.2	693.3	706.9	720.8	735.1	749.8	765.	780.7	796.9	813.5	830.7
Data (B) *1000.	548.	615.	750.	679.	717.	770.	811.	707.	884.	941.	866.	855.	1052.	955.	1085.	1089.	1046.	1047.	1161.	1213.
Uncertainties defined in C4																				
Total (%)	12.0	8.4	7.4	7.6	7.4	7.3	7.2	7.6	6.5	6.2	6.3	6.3	6.3	6.1	5.6	5.8	5.8	5.7	5.8	5.3
Statistical (%)	11.7	8.0	6.8	7.1	6.8	6.8	6.7	7.1	5.9	5.5	5.7	5.6	5.6	5.4	4.9	5.1	5.1	5.0	5.1	4.5
Systematic (%) *empty*	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Uncertainties given in EXFOR																				
ERR-S (%)	11.7	8.0	6.8	7.1	6.8	6.8	6.7	7.1	5.9	5.5	5.7	5.6	5.6	5.4	4.9	5.1	5.1	5.0	5.1	4.5
ERR-1 (%)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
ERR-2 (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ERR-3 (%)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
ERR-4 (%)	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2
ERR-5 (%)	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
ERR-7 (%) *const*	0.1	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
ERR-8 (%)	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7

Summary: available uncertainties L=11
Text in EXFOR under keywords "ERR-ANALYS" and "METHOD"

```
#ENTRY 41487 L=6
METHOD      (TOF) 48.5 m flight path
            Data-acquisitions system based on 100 MHz FLASH-ADC.
            512 TOF channels x 128 pulse height channels array
            was accumulated for each target nucleus.
            (PHD) TOF and pulse-height spectra were accumulated as
            two-dimensional matrix.
#/ENTRY 41487
#SUBENT 41487011 L=14
ERR-ANALYS (ERR-S) Statistical uncertainty (1 sigma)
            Estimated systematic uncertainty caused by
            (ERR-1)- separation of fission and background events in
                     pulse height spectra,
            (ERR-2)- energy-independent neutron background,
            (ERR-3)- energy-dependent neutron background,
```

...Method Time-Of-Flight: **Yes**

Set/Reset Values of C4-Uncertainties (%)

Name	Status	Set all values to	Set if empty	Comment
Total	full	% of [Data]		[myErr-*] are uncertainties defined by user; they can be used e.g. to split [Systematic] uncertainty to components: a) fully correlated and b) medium energy range correlated or for using uncertainties given in free EXFOR text under [ERR-ANALYS]
Statistical	full	% of Total		
Systematic	empty	Auto		
myErr-1	empty	75 % of Systematic		
myErr-2	empty	25 % of Systematic		
myErr-3	empty	2 % of Data		

Request Submit Reset ☑ Submit in new Window

Input Parameters for Calculation
Groupping Factor: 2 data points (required if final covariance matrix is too large)

No.	Name	Apply	Correlation-type	Parameters
1	Statistical	☑	Uncorrelated	
2	Systematic	☑	Fully-correlated	
3	myErr-1	☐	Fully-correlated	
4	myErr-2	☐	Partially-correlated	Corr-Length: 0.05 of the Range(eV): 1e-5 to 20e6 Scale: Log >>
5	myErr-3	☐	Partially-correlated	Corr-Length: 0.05 of the Range(eV): 1e-5 to 20e6 Scale: Log >>

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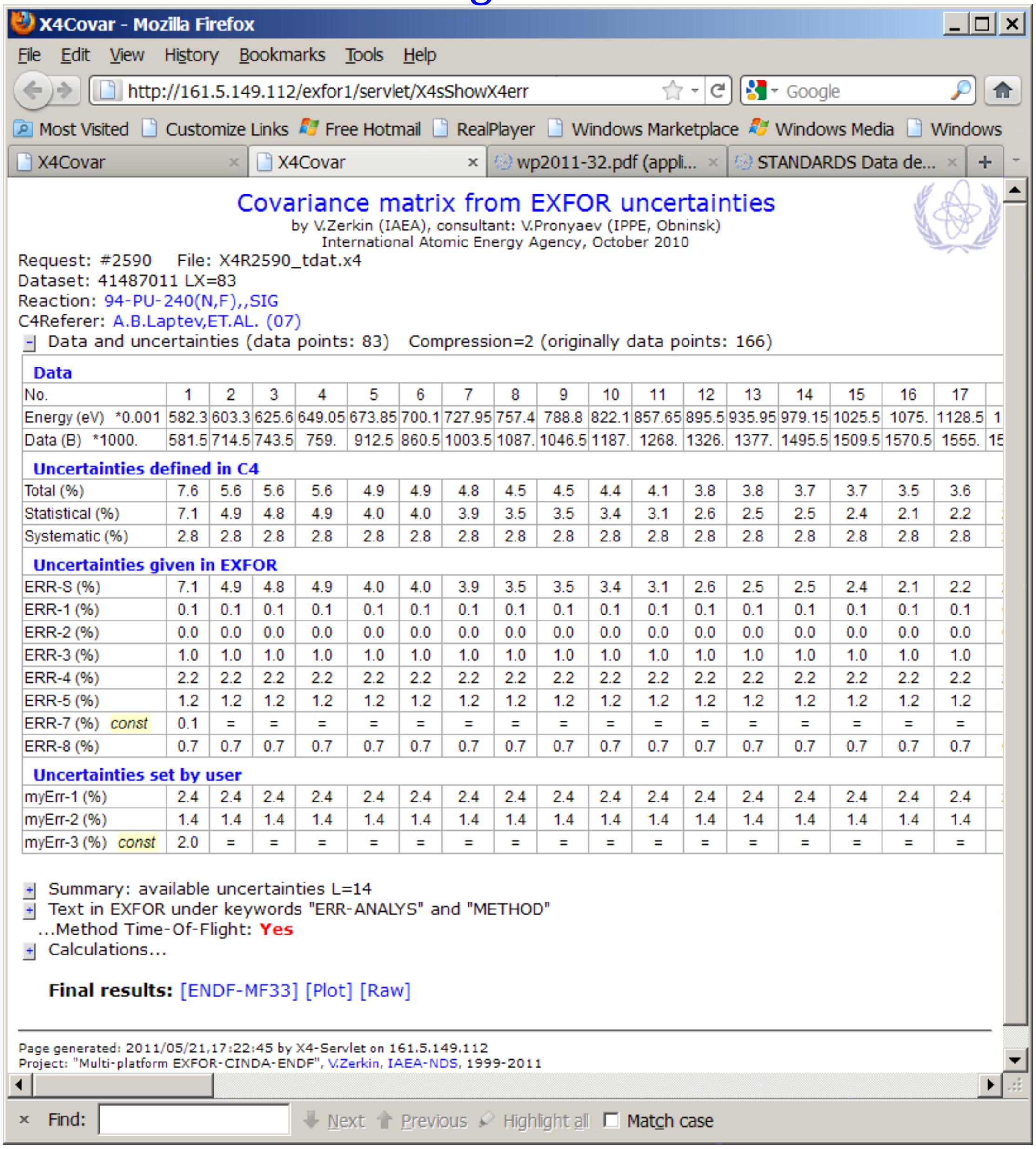
Attachment-3.

Working Screenshot-2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X4Covar | X4Covar | wp2011-32.pdf (appli... | STANDARDS Data de...

Covariance matrix from EXFOR uncertainties

by V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)
International Atomic Energy Agency, October 2010

Request: #2590 File: X4R2590_tdat.x4
Dataset: 41487011 LX=83
Reaction: 94-PU-240(N,F),,SIG
C4Referer: A.B.Laptev,ET.AL. (07)
Data and uncertainties (data points: 83) Compression=2 (originally data points: 166)

Data

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
Energy (eV) *0.001	582.3	603.3	625.6	649.05	673.85	700.1	727.95	757.4	788.8	822.1	857.65	895.5	935.95	979.15	1025.5	1075.	1128.5	1
Data (B) *1000.	581.5	714.5	743.5	759.	912.5	860.5	1003.5	1087.	1046.5	1187.	1268.	1326.	1377.	1495.5	1509.5	1570.5	1555.	15
Uncertainties defined in C4																		
Total (%)	7.6	5.6	5.6	5.6	4.9	4.9	4.8	4.5	4.5	4.4	4.1	3.8	3.8	3.7	3.7	3.5	3.6	
Statistical (%)	7.1	4.9	4.8	4.9	4.0	4.0	3.9	3.5	3.5	3.4	3.1	2.6	2.5	2.5	2.4	2.1	2.2	
Systematic (%)	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	
Uncertainties given in EXFOR																		
ERR-S (%)	7.1	4.9	4.8	4.9	4.0	4.0	3.9	3.5	3.5	3.4	3.1	2.6	2.5	2.5	2.4	2.1	2.2	
ERR-1 (%)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	
ERR-2 (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
ERR-3 (%)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
ERR-4 (%)	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	
ERR-5 (%)	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	
ERR-7 (%) const	0.1	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	
ERR-8 (%)	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	
Uncertainties set by user																		
myErr-1 (%)	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	
myErr-2 (%)	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	
myErr-3 (%) const	2.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	

+ Summary: available uncertainties L=14
+ Text in EXFOR under keywords "ERR-ANALYS" and "METHOD"
...Method Time-Of-Flight: **Yes**
+ Calculations...

Final results: [ENDF-MF33] [Plot] [Raw]

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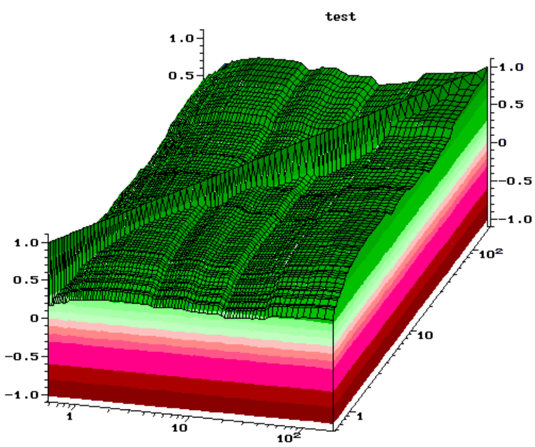
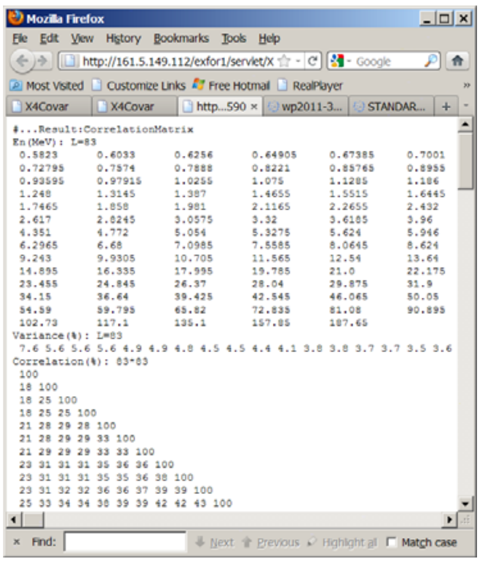
Plot and output data

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http://161.5.149.112/exfor1/servlet/X

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X4Covar | X4Covar | http...590 | wp2011-3... | STANDAR...

```
#...Result:CorrelationMatrix
En(MeV): L=83
 0.5823     0.6033     0.6256     0.64905    0.67385    0.7001
 0.72795    0.7574     0.7888     0.8221     0.85765    0.8955
 0.93595    0.97915    1.0255     1.075      1.1285     1.186
 1.248      1.3145     1.387      1.4655     1.5515     1.6445
 1.7465     1.858      1.981      2.1165     2.2655     2.432
 2.617      2.8245     3.0575     3.32       3.6185     3.96
 4.351      4.772      5.054      5.3275     5.624      5.946
 6.2965     6.68       7.0985     7.5585     8.0645     8.624
 9.243      9.9305     10.705     11.565     12.54      13.64
 14.895     16.335     17.995     19.785     21.0       22.175
 23.455     24.845     26.37      28.04      29.875     31.9
 34.15      36.64      39.425     42.545     46.065     50.05
 54.59      59.795     65.82      72.835     81.08      90.895
 102.73     117.1      135.1      157.85     187.65
Variance(%): L=83
 7.6 5.6 5.6 5.6 4.9 4.9 4.8 4.5 4.5 4.4 4.1 3.8 3.8 3.7 3.7 3.5 3.6
Correlation(%): 83*83
 100
 18 100
 18 25 100
 18 25 25 100
 21 28 29 28 100
 21 28 29 29 33 100
 21 29 29 29 33 33 100
 23 31 31 31 35 36 36 100
 23 31 31 31 35 35 36 38 100
 23 31 32 32 36 36 37 39 39 100
 25 33 34 34 38 39 39 42 42 43 100
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Find: Next Previous Highlight all Match case