Converting EXFOR data to C5M - computational format with correlation matrices.

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Since June 2007 full EXFOR database is regularly converted to extended computational format XC4 and distributed through the IAEA-NDS Web site for the members SG30 group. Resulting XC4 file (~1Gb) is used by software packages (Empire, TALYS, GANDR) as source of experimental data. Since 2010, new software (x4toc5.java) converting EXFOR to C5 format was developed. (C5 is the same format as XC4 but extended by two additional columns with statistical and total systematic uncertainties). After that Web Tool for constructing a covariance matrix from EXFOR uncertainties was developed [1]. The Tool offers to user a lot of "manual" options and parameters, but also two "default algorithms" to produce covariance matrix:

- Default-1 using only statistical and systematic uncertainties given in C5;
- Default-2 with very general assumptions: using statistical uncertainties as given in C5, and splitting systematic uncertainties 50/50 to fully correlated and MERC (medium energy range) correlated uncertainties with parameters depending on the method of measurements (see [2]).

After two years of experience dealing with the Web tools, computational output format C5 was extended to include correlation matrix. The correlation matrix is calculated using Default-2 algorithm (but in the future it can contain data coded in EXFOR file instead). It is simple (see Appendix 1 and 2 with examples), uses grouping if dimension of matrix is larger than 50*50. Now it is generated only for energy dependent cross sections and ratios (format does not foresees more complex correlations like correlations between different reactions or datasets).

C5M format is on the testing phase. Output to C5M format is available in NDS EXFOR Web retrieval system via interactive and non-interactive requests, and via standalone program (being tested at NNDC). This year full EXFOR was converted to C5M format for testing in GANDR package (total size of C5M file: ~1.4Gb, contains 20,851 correlation matrices among total 71,753 EXFOR datasets having cross sections and ratios).

C5M can be offered to developers of evaluation software packages not only as further extension of C4 format (allowing experimental covariance data, but not really having them). C5M file offers covariance data generated by tested (and trusted, see [3]) methods already now, i.e. before covariance data massively reported by experimentalists and appear in EXFOR database. This could help to develop new methodologies of data evaluation.

References:

1. V.Zerkin, Web Tool for Constructing a Covariance Matrix from EXFOR Uncertainties, EPJ Web of Conferences 27, 00009 (2012), DOI: 10.1051/epjconf/20122700009
2. V.Zerkin, Development of Web Tool for constructing a covariance matrix from EXFOR uncertainties, NRDC-2012, WP2012-42/Rev.1 http://www-nds.iaea.org/nrdc/nrdc_2012/working/wp2012-42rev.pdf
3. S.A. Badikov, Chen Zhenpeng, A.D. Carlson, E.V. Gai, G.M. Hale, F.-J. Hambsch, H.M. Hofmann, T. Kawano, N.M. Larson, V.G. Pronyaev, D.L. Smith, Soo-Youl Oh, S. Tagesen and H. Vonach, International Evaluation of Neutron Cross-Section Standards, STI/PUB/1291, http://www-nds.iaea.org/publications/tecdocs/sti-pub-1291.pdf

Appendix-1

```
#ENTRY      30998
#AUTHOR1    Xia Yijun+
#YEAR       1994
#INSTITUTE  (3CPRSIU)
#TITLE      Measurements of neutron capture cross sections of
#+          wolfram and thulium
#AUTHOR(S)  Xia Yijun,  Wang Chunhao,  Yang Jingfu,
#+           Yang Zhihua, Luo Xiaobing,  Liu Jianfeng
#REF-CODE   (C,91BEIJIN,,147,1991)
#REFERENCE  Conf. Symp.on Fast Neutron Physics, Beijing, 9-13 Sep 1991
#+          p.147, 1991
#DATASETS   2
. . . . . .
#DATASET    309980032
#DATE       19930902
#REACTION   69-TM-169(N,G)69-TM-170,,SIG
#PROJ       1
#TARG       69169
#MF         3
#MT         102
#PRODUCT    69-TM-170
#C4BEGIN    [    1 69169   3 102   ]
#DATA       19
```

# Prj	Targ	M	MF	MT	PXC	Energy	dEnergy	Data	dData	Cos/LO	dCos/LO	ELV/HL	dELV/HL	I78	Refer (YY)	EntrySubP	dSys	dStat
1	69169	3	102			11200.	360.	2.509	0.393913		69170				Xia Yijun,ET.AL.	(88)30998	32	0.180648	0.35126
1	69169	3	102			12900.	450.	2.132	0.27716		69170				Xia Yijun,ET.AL.	(88)30998	32	0.1066	0.25584
1	69169	3	102			14000.	500.	1.713	0.226116		69170				Xia Yijun,ET.AL.	(88)30998	32	0.095928	0.20556
1	69169	3	102			15100.	560.	1.749	0.19239		69170				Xia Yijun,ET.AL.	(88)30998	32	0.08745	0.1749
1	69169	3	102			16400.	640.	1.593	0.157707		69170				Xia Yijun,ET.AL.	(88)30998	32	0.086022	0.132219
1	69169	3	102			17900.	730.	1.328	0.111552		69170				Xia Yijun,ET.AL.	(88)30998	32	0.070384	0.08632
1	69169	3	102			19600.	840.	1.244	0.098276		69170				Xia Yijun,ET.AL.	(88)30998	32	0.065932	0.069664
1	69169	3	102			21600.	960.	1.291	0.089079		69170				Xia Yijun,ET.AL.	(88)30998	32	0.056804	0.068423
1	69169	3	102			23900.	1100.	1.236	0.075396		69170				Xia Yijun,ET.AL.	(88)30998	32	0.053148	0.053148
1	69169	3	102			26500.	1300.	1.062	0.060534		69170				Xia Yijun,ET.AL.	(88)30998	32	0.045666	0.040356
1	69169	3	102			29600.	1600.	1.01	0.05555		69170				Xia Yijun,ET.AL.	(88)30998	32	0.04343	0.03434
1	69169	3	102			33300.	1900.	0.979	0.050908		69170				Xia Yijun,ET.AL.	(88)30998	32	0.041118	0.02937
1	69169	3	102			37800.	2200.	0.925	0.049025		69170				Xia Yijun,ET.AL.	(88)30998	32	0.0407	0.026825
1	69169	3	102			43200.	2700.	0.83	0.04565		69170				Xia Yijun,ET.AL.	(88)30998	32	0.04067	0.02158
1	69169	3	102			49800.	3400.	0.802	0.0401		69170				Xia Yijun,ET.AL.	(88)30998	32	0.034486	0.02005
1	69169	3	102			58100.	4300.	0.732	0.035136		69170				Xia Yijun,ET.AL.	(88)30998	32	0.031476	0.016104
1	69169	3	102			68800.	5600.	0.632	0.030336		69170				Xia Yijun,ET.AL.	(88)30998	32	0.026544	0.01264
1	69169	3	102			82300.	7200.	0.609	0.034104		69170				Xia Yijun,ET.AL.	(88)30998	32	0.031059	0.013398
1	69169	3	102			100000.	9800.	0.552	0.064584		69170				Xia Yijun,ET.AL.	(88)30998	32	0.062376	0.017664

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#/DATA      19
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#COVARIANCE     2              Generated
#COMMENT        Default2. EXFOR software ver.2012/05/17, by V.Zerkin@iaea.org (IAEA-NDS)
#+              1) If only total uncertainties are given, assume uncertainties: statistical/systematic=50/50.
#+              2) Statistical uncertainties ara added to full covariance matrix as uncorrelated components
#+              3) Total systematic uncertainties are split to (50/50) and added as fully correlated and MERC-correlated components
#ALGORITHM      2          1          100.        50.         50.         1          1.0E-5      2.0E7       0.05
#+              Type       Groupping  Stat.SERC   Syst.LERC   Syst.MERC   Log/Lin    En-Min      En-Max      Length
#COVARDATA      1          19         19
#EnMin(eV)  EnMax(eV)   Data(b)     Std.dev.(%) Correlations(%)
#---------><---------><---------><---------><---Values: separated by space; line length: unlimited....
11200.      11200.      2.509       15.7        100
12900.      12900.      2.132       13.0        17 100
14000.      14000.      1.713       13.2        18 16 100
15100.      15100.      1.749       11.2        18 16 18 100
16400.      16400.      1.593       9.9         22 19 22 24 100
17900.      17900.      1.328       8.4         24 21 24 27 33 100
19600.      19600.      1.244       7.7         25 23 26 28 35 42 100
21600.      21600.      1.291       6.9         22 20 23 25 31 38 42 100
23900.      23900.      1.236       6.1         24 21 24 26 33 40 45 44 100
26500.      26500.      1.062       5.7         24 21 25 27 34 41 46 44 51 100
29600.      29600.      1.01        5.5         24 21 24 27 34 41 46 45 51 56 100
33300.      33300.      0.979       5.2         23 21 24 26 33 40 45 44 51 56 61 100
37800.      37800.      0.925       5.3         22 20 23 25 32 39 44 43 49 55 60 65 100
43200.      43200.      0.83        5.5         21 19 22 25 32 38 44 43 49 55 60 65 70 100
49800.      49800.      0.802       5.0         20 17 20 22 29 35 40 39 45 50 55 60 65 73 100
58100.      58100.      0.732       4.8         20 17 19 21 27 33 38 37 43 48 53 58 63 70 73 100
68800.      68800.      0.632       4.7         21 17 19 20 25 30 35 34 40 45 50 55 59 67 69 76 100
82300.      82300.      0.609       5.6         21 18 19 21 25 29 32 31 37 41 46 51 56 63 65 72 78 100
100000.     100000.     0.552       11.7        22 19 20 22 26 30 33 31 34 38 43 48 53 60 63 69 75 82 100
#/COVARDATA
#/COVARIANCE
#/DATASET
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#DATASET    40890002
#DATE       20100704
#REACTION   92-U-236(N,G)92-U-237,,SIG,,AV
#PROJ       1
#TARG       92236
#MF         3
#MT         102
#PRODUCT    92-U-237
#C4BEGIN    [    1 92236   3 102   ]
#DATA       57
# Prj Targ M MF MT PXC  Energy  dEnergy  Data      dData   Cos/LO   dCos/LO   ELV/HL  dELV/HL I78 Refer (YY)              EntrySubP  dSys     dStat
#---><---->o<-><-->ooo<-------><-------><-------><-------><-------><-------><-------><-><----------------------><---><->o<-------><------->
    1 92236   3 102       3500.     500.    2.275    0.303             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102       4500.     500.    1.929     0.22             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102       5500.     500.    1.647    0.165             92237                     L.E.Kazakov,ET.AL.   (85)40890  2           0.070821
    1 92236   3 102       6500.     500.    1.376    0.117             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102       7500.     500.    1.166    0.086             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102       8500.     500.    1.101     0.07             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102       9500.     500.    1.086    0.063             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
    1 92236   3 102      11000.    1000.    0.919    0.051             92237                     L.E.Kazakov,ET.AL.   (85)40890  2           0.017461
    1 92236   3 102      13000.    1000.    0.876    0.046             92237                     L.E.Kazakov,ET.AL.   (85)40890  2
. . . . . .
    1 92236   3 102     410000.   10000.    0.185    0.009             92237                     L.E.Kazakov,ET.AL.   (85)40890  2           0.002035
#/DATA      57
#COVARIANCE     2              Generated
#COMMENT        Default2. EXFOR software ver.2012/05/17, by V.Zerkin@iaea.org (IAEA-NDS)
#+              1) If only total uncertainties are given, assume uncertainties: statistical/systematic=50/50.
#+              2) Statistical uncertainties ara added to full covariance matrix as uncorrelated components
#+              3) Total systematic uncertainties are split to (50/50) and added as fully correlated and MERC-correlated components
#ALGORITHM      2           2           100.        50.         50.         1           1.0E-5      2.0E7       0.05
#+              Type        Groupping   Stat.SERC   Syst.LERC   Syst.MERC   Log/Lin     En-Min      En-Max      Length
#COVARDATA      1           29          29
#EnMin(eV)  EnMax(eV)   Data(b)     Std.dev.(%) Correlations(%)
#----------><----------><---------><----------><---Values: separated by space; line length: unlimited....
3500.       5500.       2.102       10.7        100
5500.       7500.       1.5115      8.5         62 100
7500.       9500.       1.1335      6.0         49 66 100
9500.       13000.      1.0025      5.2         48 66 67 100
13000.      17000.      0.8745      4.5         36 51 54 65 100
17000.      21000.      0.7505      4.2         33 44 47 58 60 100
21000.      25000.      0.6995      4.1         33 39 42 53 55 62 100
25000.      29000.      0.6475      4.1         33 37 38 48 51 58 63 100
29000.      37500.      0.6025      4.3         37 41 39 50 53 60 66 71 100
37500.      47500.      0.538       4.1         33 37 33 38 42 48 53 57 68 100
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47500.      57500.      0.4615      4.1          33 37 33 37 36 42 47 52 62 61 100
57500.      67500.      0.403       4.2          33 37 33 37 33 38 43 47 56 57 62 100
67500.      77500.      0.355       4.2          33 37 33 37 33 34 39 43 52 53 58 63 100
77500.      87500.      0.3225      4.0          33 37 33 37 33 33 36 40 49 50 55 60 63 100
87500.      97500.      0.289       3.9          33 37 33 37 33 33 33 37 45 47 52 57 61 64 100
97500.      115000.     0.2745      4.2          37 41 37 41 37 37 37 39 48 49 56 61 65 68 72 100
115000.     135000.     0.25        4.0          33 37 33 37 33 33 33 33 38 40 46 50 54 57 60 70 100
135000.     155000.     0.2305      3.9          33 37 33 37 33 33 33 33 37 37 42 47 50 54 56 66 63 100
155000.     175000.     0.2115      4.1          33 37 33 37 33 33 33 33 37 33 39 43 47 50 53 62 60 63 100
175000.     195000.     0.215       4.0          33 37 33 37 33 33 33 33 37 33 36 40 44 47 50 59 57 61 64 100
195000.     215000.     0.2085      4.4          37 40 37 40 37 37 37 37 41 37 37 42 46 49 53 62 60 64 67 71 100
215000.     235000.     0.208       4.2          33 37 33 37 33 33 33 33 37 33 33 36 39 43 46 54 52 56 59 62 71 100
235000.     255000.     0.204       4.0          33 37 33 37 33 33 33 33 37 33 33 34 37 41 43 51 50 54 57 60 69 65 100
255000.     275000.     0.199       3.9          33 37 33 37 33 33 33 33 37 33 33 33 35 39 41 49 48 52 55 58 66 63 65 100
275000.     295000.     0.1945      4.0          33 37 33 37 33 33 33 33 37 33 33 33 34 37 40 47 46 50 53 56 64 61 63 65 100
295000.     330000.     0.202       4.4          37 41 37 41 37 37 37 37 42 37 37 37 37 39 42 51 50 54 57 61 70 66 68 71 73 100
330000.     370000.     0.1935      4.0          33 37 33 37 33 33 33 33 37 33 33 33 33 33 35 42 42 46 49 52 60 57 59 61 62 71 100
370000.     410000.     0.186       4.2          33 37 33 37 33 33 33 33 37 33 33 33 33 33 33 39 39 43 46 49 57 54 56 58 60 68 64 100
410000.     410000.     0.185       4.9          40 44 40 44 40 40 40 40 44 40 40 40 40 40 40 44 44 48 52 56 65 61 64 66 68 78 73 77 100
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#/COVARIANCE
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