Annex to Memo CP-D/627

Automatic test of EXFOR with TALYS: Attempt 1

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The objective of WPEC Subgroup 30 *Quality improvement of the EXFOR database* is to make EXFOR an easy accessible database of experimental nuclear reaction data, and to systematically check and correct EXFOR entries for errors. In 2007-2008, significant progress has been made to make EXFOR available as a complete computational database. One obvious advantage of a computational database is that automatic comparisons with nuclear model codes can be made, to test the quality of either the data or the model code. This is exactly the topic of this document.

The objective is to compare two large databases:

- The entire EXFOR database in so called XC4 format, made available by the IAEA (Zerkin).
- A complete nuclear reaction database, SALTY, created by default (”blind”) TALYS calculations.

The term ”complete” in the second item above means that we have stored all the output that Talys gives us, if we specify maximum output with the Talys keywords. In this first stage, we use only part of the SALTY library. For the current comparison with EXFOR we consider:

- Projectiles: gamma’s, neutrons, protons, deuterons, tritons, helions and alpha’s
- Targets: all stable isotopes in the Z=9-83 range
- Incident energies from thermal energies up to 200 MeV
- Cross sections: total, elastic, non-elastic, exclusive (i.e. per MT number) and residual production cross sections.

This exercise is an EXFOR test and a Talys test at the same time. This global comparison obviously does not replace a ”true” evaluation for one particular isotope, which involves careful studying all experimental work, precise nuclear model fitting, etc. However, it has already been shown in many occasions that Talys provides very reasonable ”blind” estimates for many reaction processes, with the thermal range and fission as notable exceptions (Talys can be used for that also, but only a ”true” isotopic evaluation brings the results somewhere near the experimental data for those processes). Hence, with the exception of certain reactions, Talys should be able to give a reasonably good prediction of many reaction data, and obviously we will constantly try to extend such a prediction to as many reactions as possible. At first sight, the problem is simple: If we know that Talys is usually within e.g. 30% of the experimental

data for a certain reaction channel, alarm bells should start ringing if the deviation for such a channel is suddenly much larger. We note that large deviations may also come from bad Talys performance, even if the visual agreement on linear scale is good. For example, for threshold reactions the difference between Talys and experiment may easily be a factor of 10, close to threshold, and there may be experimental and theoretical reasons for that. In general the rule holds that the smaller the cross section, the larger the relative error. It is therefore important to watch not only the calculation/experiment (C/E) values, but also the absolute deviation. In several cases, it turns out that there are problems in EXFOR, and many of them can not so easily be detected with ways other than with a model code (which is why these problems are still in EXFOR in the first place). The problems which are easiest to detect are C/E values around 0.001 or 1000, suggesting the well known error of mixing barns and millibarns. Unfortunately, the majority of cases is more difficult to judge. This is an attempt to categorize possible problems of EXFOR (or Talys). The current comparison may also help to solve one of the largest problems of EXFOR: reaction identifiers which are assigned in wrong, inconsistent or even multiple ways. If Talys is expected to give a reasonably good prediction for a reaction and we obtain a large deviation, it may be that we are not comparing the Talys result with the correct quantity.

To discover and classify problems, we use 4 goodness-of-fit estimators. If they are all very large (or in the case of R very small), something is wrong somewhere. They are the F-factor

$$F = 10^{\sqrt{\frac{1}{N}\sum_i^N \left(\log \frac{\sigma_T^i}{\sigma_E^i}\right)^2}}, \tag{1}$$

the C/E value, also called R,

$$R = \frac{1}{N}\sum_i^N \frac{\sigma_T^i}{\sigma_E^i}, \tag{2}$$

the χ^2,

$$\chi^2 = \frac{1}{N}\sum_i^N \left(\frac{\sigma_T^i - \sigma_E^i}{\Delta\sigma_E^i}\right)^2, \tag{3}$$

and the absolute deviation

$$\Delta = \frac{1}{N}\sum_i^N |\sigma_T^i - \sigma_{exp}^i|, \tag{4}$$

where the subscript T stands for theory or Talys and E for experimental. In all cases, we average over the number of energy points, N, in each set. Hence, each EXFOR subentry (data set) that contains a cross section excitation function (or only 1 point) is described by four numbers: F, R, χ^2 and Δ, while we also keep track of all individual components F_i, R_i, χ_i^2 and Δ_i for e.g. C/E plots.

The F-factor is a kind of twisted R value. In fact, each individual component of the sum inside F is equal to R if it is larger than 1, and 1/R if it is smaller than 1. This is a helpful quantity, since averaging R values over many points may not be very meaningful if the values cross 1 at some point. A value of F=1.2 means that for the entire data set we are roughly 20% off on average. We use F as the leading indicator in our statistical study, i.e. we sort our results in order of increasing F to identify the worst cases.

In our data evaluation system, the most versatile use of experimental data is made if nuclear reactions are stored directory-wise per reaction type. For example, all experimental data sets for (n,2n) reactions on

^{54}Fe are stored in a subdirectory n/fe/054/016, inside which there are various files, one per experiment, e.g.

```
......
Bahal1984.tot
Bormann1976.tot
Cross1963.tot
Csikai1965.tot
......
```

where e.g. the Bormann1976.tot file looks as follows

```
# Target  : Z= 26 A= 54       Isomer=   Projectile=n
# Reaction: MT= 16 (n,2n   )  Isomer=
# Quantity: Cross section          Frame: L
# X4 ID: 20614002  C4: MF   3 MT  16 X4 Code: 26-FE-54(N,2N)26-FE-53,,SIG
# Author  : M.Bormann+                Year: 1976
#    E(MeV)       xs(mb)      dxs(mb)      dE(MeV)       TALYS         F       R(C/E)       Chi-2      Delta(mb)
  1.40500E+01  1.01000E+01  1.00000E-01  9.00000E-02  3.41057E+00   2.961      0.3377       4475.       6.689
  1.45500E+01  1.75000E+01  1.20000E-01  1.00000E-01  1.10903E+01   1.578      0.6337       2853.       6.410
  1.48100E+01  2.25000E+01  1.50000E-01  1.00000E-01  1.65837E+01   1.357      0.7371       1556.       5.916
  1.50800E+01  2.36000E+01  1.50000E-01  1.00000E-01  2.23218E+01   1.057      0.9458       72.61       1.278
  1.53500E+01  2.90000E+01  1.70000E-01  1.00000E-01  2.81392E+01   1.031      0.9703       25.64      0.8608
  1.56100E+01  2.95000E+01  2.00000E-01  1.10000E-01  3.37412E+01   1.144       1.144       449.7       4.241
  1.59200E+01  3.70000E+01  2.10000E-01  1.10000E-01  4.04205E+01   1.092       1.092       265.3       3.421
  1.64300E+01  4.55000E+01  2.40000E-01  1.10000E-01  4.92008E+01   1.081       1.081       237.8       3.701
  1.69400E+01  5.60000E+01  3.00000E-01  1.10000E-01  5.75702E+01   1.028       1.028       27.39       1.570
  1.75600E+01  5.62000E+01  3.10000E-01  1.10000E-01  6.44940E+01   1.148       1.148       715.8       8.294
  1.82300E+01  5.81000E+01  3.00000E-01  1.20000E-01  7.06126E+01   1.215       1.215       1740.       12.51
#M.Bormann,  H-K.Feddersen,  H.-H.Holscher,
# W.Scobel, H.Wagner
#Jour. Zeitschrift fuer Physik, Section A
#Vol.277, p.203, 1976
#-(N,2N) EXCITATION FUNCTIONS FOR FE-54, GE-70, SE-74,
#RB-85, SR-86,88, Y-89, MO-92, AND HG-204 IN THE
#NEUTRON ENERGY REGION 13-18 MEV-. (GERMAN)
```

For this particular study, we simply print the blind, default, unadjusted (i.e. be gentle, please) Talys result, and the statistical factors for each point in the table, while we keep the average values for this set in another summary table. While we make the translation from the XC4 computational database to our own directory-structured database, we do our Talys comparison, checks and statistical analyses on the fly. After about 10 minutes, the conversion is done and all checking and statistical results are available.

We show a few examples here. Fig. 1 shows the distribution of the F-values for all (n,2n) reactions that we managed to get out of the XC4 database. We logged the number of cases per F-bin, whereby we distributed the range F=1-1000 over 100 logaritmically equidistant bins. Hence, the first bin means that Talys is inside 7% of the experimental data, the second bin between 7-15%, the third bin 15-23%, and so on. All cases with F$>$1000 are put in the last bin. The high peak at the lowest bins probably means good news for Talys. The cases with very high F-values probably mean trouble for EXFOR (or XC4). The cases in between mean trouble for either Talys or Exfor, or both. For SG-30, the interesting cases are in the tail of the distribution and it is probably best to start checking and working on the highest values. Note that there is always the possibility of an erroneous XC4 interpretation from my side, leading to false alarm, and hopefully this improves over time. These distributions are available for all MT numbers, and also for residual production cross sections. Fig. 1 also shows the result for all neutron-induced reactions.

The most interesting are of course the specific cases with large deviation. The conversion process produces a file called *x4.sort* which has all EXFOR entries sorted by F-value. The bottom of that list looks

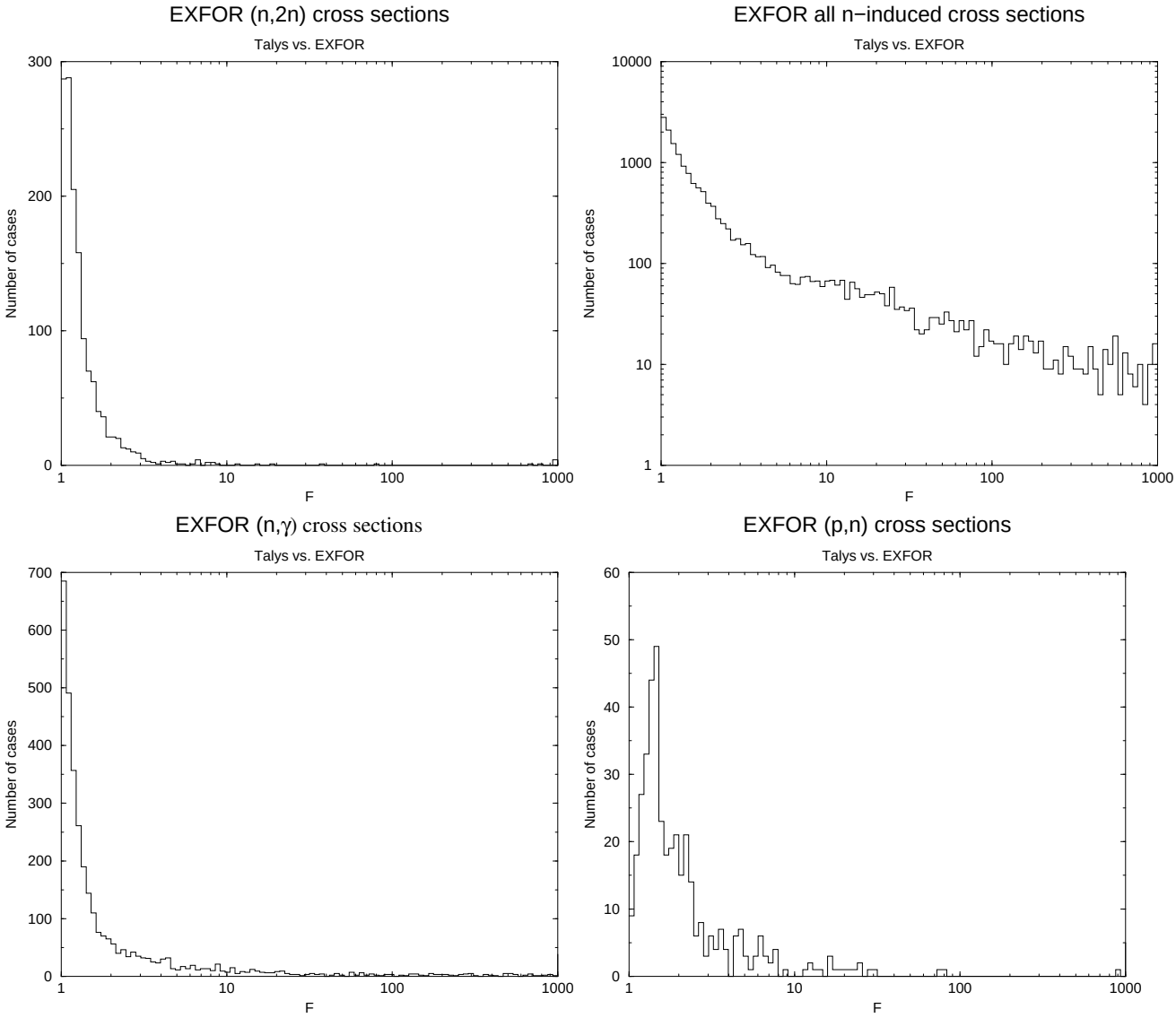

Figure 1: Frequency table for the F-values for (n,2n) reactions, all neutron-induced reactions, (n,γ), and (p,n) reactions.

as follows

```
  EXFOR    C4 New  #C4  #New     Reaction                                F          R        chi-2     Delta
.......
 11491007   1  1     1     1 25-MN-55(N,HE3)23-V-53,,SIG              1.080E+15  9.262E-16   0.00      0.420
 11590082   1  1     1     1 81-TL-205(N,HE3)79-AU-203,,SIG           1.448E+15  6.908E-16   0.00      7.000E-02
 30106012   1  1     1     1 57-LA-139(N,2P)55-CS-138,,SIG            1.523E+15  6.568E-16   2.25      3.000E-02
 11491015   1  1     1     1 40-ZR-94(N,HE3)38-SR-92,,SIG             4.892E+15  2.044E-16   0.00      0.400
 30152014   1  1     1     1 52-TE-130(N,HE3)50-SN-128,,SIG           5.786E+15  1.728E-16   3.52      1.500E-02
```

i.e. we find F-values above 10^{15}, and they even are probably not EXFOR errors! (Talys is known to miss the (n,He3) threshold by at least 1 MeV, resulting in a huge deviation near threshold. Note the small deviation in millibarns in the last column). More interesting is perhaps to filter out one kind of reaction. If under Linux, we do *grep 'N,2N' x4.sort* the bottom of that list looks as follows.

```
  EXFOR    C4 New  #C4  #New     Reaction                                F          R        chi-2     Delta
.......
 303220122  1  1     1     1 49-IN-115(N,2N)49-IN-114-M1,,SIG          107.       107.      3.368E+05  1.161E+03
 22662014   1  1     6     6 58-CE-140(N,2N)58-CE-139-M,,SIG           140.       141.      1.175E+07   793.
 23018004   1  1     6     6 80-HG-196(N,2N)80-HG-195-G,,SIG           638.       642.      2.852E+07   582.
 23018002   1  1     6     6 80-HG-196(N,2N)80-HG-195,,SIG             702.       703.      7.502E+07  1.578E+03
 23018003   1  1     6     6 80-HG-196(N,2N)80-HG-195-M,,SIG           748.       754.      6.158E+07   996.
 11684003   1  1     1     1 25-MN-55(N,2N)25-MN-54,,SIG               786.       786.       0.00       785.
 23018007   1  1     6     6 80-HG-198(N,2N)80-HG-197-G,,SIG           880.       881.      8.661E+07  1.007E+03
 31454005   1  1     1     1 72-HF-179(N,2N)72-HF-178-M2,,SIG          908.       908.      1.039E+07   290.
 20033003   1  1     1     1 37-RB-85(N,2N)37-RB-84,,SIG               960.      1.042E-03   399.      1.010E+06
 22969007   1  1     4     4 72-HF-176(N,2N)72-HF-175,,SIG             961.       975.      1.119E+08  1.194E+03
 23018014   1  1     6     6 80-HG-204(N,2N)80-HG-203,,SIG             993.       994.      4.301E+08  2.135E+03
 23018005   1  1     6     6 80-HG-198(N,2N)80-HG-197,,SIG             994.       995.      2.696E+08  2.075E+03
 23018006   1  1     6     6 80-HG-198(N,2N)80-HG-197-M,,SIG          1.139E+03  1.140E+03  2.872E+08  1.069E+03
 22347006   1  1     3     3 53-I-129(N,2N)53-I-128,,SIG              1.450E+03  1.454E+03  1.164E+08  1.640E+03
```

Here we see the F-values around 1000 suggesting the b-mb problem. Indeed, the (n,2n) cross sections of the various Hg isotopes were a factor of 1000 too small and this has recently been corrected. Note that the R-factor indicates that 37-RB-85(N,2N) concerns kilobarns instead of barns (hence the deviation of 1.010E+06 mb). Unfortunately, not all problems are that simple. There may be an inconsistency between Talys and Exfor on the definition of an isomer, leading to large discrepancies and the list above may also suggest that isomeric, ground state and total cross sections may have been mixed.

After *grep 'N,TOT' x4.sort* we find near the bottom

```
  EXFOR    C4 New  #C4  #New     Reaction                                F          R        chi-2     Delta
.......
 21676005   1  1     1     1 23-V-51(N,TOT),,SIG,,AV                   914.       914.      1.442E+10  4.924E+06
 11026015   1  1     1     1 23-V-0(N,TOT),,SIG                        920.       920.      4.948E+09  4.924E+06
 22007002   1  1   121   121 14-SI-0(N,TOT),,SIG                       937.       983.       0.00      5.151E+05
 31468004   1  1     7     7 24-CR-0(N,TOT),,SIG                       972.       973.      9.116E+08  3.790E+03
 20602009   1  1     1     1 23-V-51(N,TOT),,SIG                       974.       974.      5.870E+10  4.846E+06
 31468006   1  1     6     6 28-NI-0(N,TOT),,SIG                      1.010E+03  1.010E+03  7.236E+08  3.603E+03
 31468005   1  1     6     6 26-FE-0(N,TOT),,SIG                      1.013E+03  1.014E+03  8.609E+08  3.642E+03
 31468007   1  1     2     2 29-CU-0(N,TOT),,SIG                      1.031E+03  1.031E+03  6.671E+08  3.442E+03
 31468003   1  1     7     7 23-V-0(N,TOT),,SIG                       1.039E+03  1.040E+03  9.202E+08  3.987E+03
 11204004   1  1    12    12 4-BE-9(N,TOT),,SIG                       1.045E+03  1.058E+03   0.00      1.528E+06
.......
```

of which some (maybe all?) are indeed mb-b problems. Note however that at very low energies Talys may be a factor 1000 off (while above a few MeV Talys should be within 1-3 %).

In the future, this procedure should also be applied to secondary distributions such as angular distributions and (double-)differential spectra. Before this can be done, the secondary energies and angles in the XC4 database first need to be sorted (with the sortC4 code).

As stated above, the first obvious use of all this information is to identify problems and to correct them. However, with all these results available, it is now also possible to set-up some ”zeroth-order” quality flagging. Although we can never be 100% sure, it is very probable that the subentries with small F-values (where ”small” depends on the reaction channel) represent indeed the type of quantities that are reported in EXFOR. In other words, the reaction identifier assigned by the compiler for these subentries is correct.

Note that here I am not yet talking about renormalization of wrongly interpreted experimental conditions (there has been some recent discussion about this and that may be very valuable too). The quality flagging mentioned above would simply ensure that e.g. a cross section reported as being (n,2n) in EXFOR is indeed just that, and not e.g. a compound (n,n') + (n,2n) cross section (which would place it further down the tail of our F-distribution since Talys is being compared with the wrong quantity). In this way we would obtain a large ”verified” set of EXFOR data, while ”validation” of the data would involve a more precise study of the detailed experiment and possible renormalization. To start with, such a quality list could exist of only the EXFOR subentry number and e.g. a 1 for a verified set and a 0 for a non-verified set. This requires some further study and discussion.

Finally, all experimental uncertainties of EXFOR were also sorted per reaction or MT number and stored in files, e.g. *mterr.102*. The largest errors for capture are obtained with *sort -g -k 3,3 mterr.016*:

```
.............
 10340007  52-TE-130(N,G)52-TE-131,,SIG              354.     %
 11507090  74-W-180(N,G)74-W-181,,SIG,,MXW           400.     %
 13742004  38-SR-88(N,G)38-SR-89,,SIG,,RAW           619.     %
 400070051 34-SE-80(N,G)34-SE-81,,SIG                749.     %
 40975014  68-ER-170(N,G)68-ER-171,,SIG            1.538E+03 %
```

which may or may not be wrong, closer inspection is required. The largest errors in the entire list are

```
.............
 20668004  74-W-180(N,P)73-TA-180-M,,SIG             960.     %
 21264010  42-MO-92(N,N+P)41-NB-91,,SIG            1.344E+03 %
 22640003  8-O-18(N,P)7-N-18,,SIG                  1.478E+03 %
 40975014  68-ER-170(N,G)68-ER-171,,SIG            1.538E+03 %
 21288007  20-CA-48(N,2N)20-CA-47,,SIG             5.565E+03 %
 20909003  6-C-12(N,TOT),,SIG                     1.629E+04 %
 21288005  20-CA-44(N,A)18-AR-41,,SIG              1.714E+04 %
 41163008  52-TE-126(N,P)51-SB-126-G,,SIG          2.000E+04 %
 C0774002  39-Y-89(P,N)40-ZR-89,,SIG               7.334E+04 %
 12940004  40-ZR-0(N,TOT),,SIG                    9.071E+04 %
```

Only results for incident neutrons were given here, but the same is done for other projectiles. More refined test are possible and I hope to find the time to perform them in the near future. All results described in this document, i.e. all resulting numerical files, have been sent to the IAEA for further inspection.