Coding of Partial Uncertainties and Correlation Matrices

Memo CP-D/704 (N. Otsuka, 2011-04-20)

Though compilation of detailed uncertainty information has been often stressed in the NRDC Meeting [1], the EXFOR Format is still not satisfactory to include all available information from experimentalists. For example, we have only one heading `ERR-S` for uncorrelated (statistical) uncertainty.

In this memo, I will present some examples of error analysis information available from experimentalists, and propose the format to keep experimental information for evaluators and programmers in a computer readable manner. I limit the scope of this paper to the energy dependent cross sections (excitation function) of a reaction, i.e., only energy-energy correlation of a given reaction is discussed. In addition to this correlation, there has been other experimental information of correlations (e.g., reaction-reaction correlation in fission spectrum averaged cross sections provided from KURRI etc., correlation between Legendre coefficients from PTB etc.). But I will not treat these correlations in this memo to simplify discussion and avoid drastic changes in the EXFOR Formats. Hereafter "correlation" always means correlation in a quantity between two incident neutron energies (cross energy correlation).

An example of a recent experiment - C. Sage et al. (2009, 2010) at Geel [2,3]

Below is an example of ^{241}Am(n,2n)^{240}Am energy dependent activation cross section derivation with the ^{27}Al(n,α)^{24}Na monitor cross section (*i*: index of incident neutron energy point, *k*: type of correction).

$$\sigma_{\mathrm{Am}}(i) = \sigma_{\mathrm{Al}}(i) \frac{S_{\mathrm{Am}}(i)}{S_{\mathrm{Al}}(i)} \frac{[I\,\varepsilon\, f_{\Sigma}(i) f_r(i)\, n(i)\, \Phi_0(i)]_{\mathrm{Al}}}{[I\,\varepsilon\, f_{\Sigma}(i) f_r(i)\, n(i)\, \Phi_0(i)]_{\mathrm{Am}}} \prod_k \frac{C_{k,\mathrm{Am}}(i)}{C_{k,\mathrm{Al}}(i)}$$

Definitions of parameters:

$\sigma_{\mathrm{Am}}(i)$: ^{241}Am(n,2n)^{240}Am cross section
$\sigma_{\mathrm{Al}}(i)$: ^{27}Al(n,α)^{24}Na cross section
$S(i)$: number of counts
I: gamma-ray emission probability (constant)
ε: peak efficiency for emitted gamma (constant)
$f_r(i)$: 1-exp($-\lambda t_r(i)$) where $t_r(i)$ is irradiation time
$f_\Sigma(i)$: $(1/\lambda)\ \Sigma\ \exp(-\lambda t_d(i))[1-\exp(-\lambda t_m(i)]$ where $t_d\,(i)$ and $t_m\,(i)$ are starting and measuring time
$n(i)$: number of target nuclei in the sample
$\Phi_0(i)$: neutron flux
$C_{\mathrm{flux}}(i)$: correction due to flux fluctuation
$C_{\mathrm{low}}(i)$: correction due to low-energy secondary neutron

Creating the full covariance matrix of the results of measurements we may present the component of the uncertainties in accordance with their correlation properties. It is usually classified to (1) uncorrelated (short energy range correlation; SERC), (2) fully correlated (long energy range correlation; LERC), and (3) partly correlated (medium energy range correlation; MERC) [4]. These are also introduced at the beginning of the ENDF-6 Formats Manual Chapter 33.

The numbers of count $\boldsymbol{S}$ are uncorrelated for both isotopes. The decay gamma intensity $\boldsymbol{I}$ and detector efficiency $\boldsymbol{\varepsilon}$ are fully correlated for both isotopes because one gamma line was used for one reaction. The monitor cross section $\boldsymbol{\sigma_{Al}}$ was adopted from a standard library with its correlation matrix, which takes a value between -1 and 1 for each element.

Special care has to be directed to the numbers of nuclei $\boldsymbol{n}$ for the samples used in the experiment. The authors used different Al samples at each neutron energy i, and therefore it should be treated as uncorrelated assuming that there is no systematic bias in the results of the sample thickness measurement. On the other hand, the authors used 4 Am samples at neutron energy i=(1,6,9), (2,3,4), (5,7) and 8. Within each group, they are strongly correlated while it can be assumed as uncorrelated between neutron energies belonging to two different groups. (This example shows us that details of samples are important for correlation property analysis.)

Correlation properties considered by authors are tabulated below. The uncertainties of parameters not listed in this table were neglected by authors.

Source	σ_{Al}	S_{Am}	S_{Al}	I_{Am}	n_{Al}	n_{Am}	$\varepsilon_{Al}/\varepsilon_{Am}$	$[f_\Sigma f_f]_{Am}$	$C_{low,Am}/C_{low,Al}$
Property	P	U	U	F	U	P	F	F	U

U: Uncorrelated (SERC), F: Fully correlated (LERC), P: Partly correlated (MERC)

These are defined under `ERR-ANALYS` in EXFOR 23114 as follows:

```
ERR-ANALYS (ERR-T) Total uncertainty.
           (MONIT-ERR) Uncertainty of monitor cross section.
           (ERR-S) Counting statistics uncertainty for Am .
           (ERR-1) Counting statistics uncertainty for Al.
           (ERR-2) Uncertainty of gamma-rays intensities .
           (ERR-3) Uncertainty of Al target nuclei number
           (ERR-4) Uncertainty of Am target nuclei number
           (ERR-5) Uncertainty of ratio of detection efficiency
                   for Al to Am one.
           (ERR-6) Uncertainty of time factors for Am.
           (ERR-7) Uncertainty due to correction for presence of
                   low-energy breakup neutrons.
```

In comparison with above the table, we realize inconsistency between the heading and its correlation property:

1) The heading `ERR-1` (defined as the 1st *systematic* uncertainty in the EXFOR dictionary) is applied to an uncorrelated (statistical) uncertainty ΔS_{Al} because only one heading `ERR-S` is available for uncorrelated (statistical) uncertainties in the current EXFOR Formats.
2) The headings `ERR-3` (defined as 3rd *systematic* uncertainty in the dictionary) and `ERR-7` (defined as 7th *systematic* uncertainty in the dictionary) are applied to uncorrelated uncertainties Δn_{Al} and $\Delta(C_{low,Am}/C_{low,Al})$.

Also correlation properties (LERC or MERC) are not indicated by the compiler.

“Correlation Factors” in the EXFOR Formats

The EXFOR Formats Manual defines a data field for “correlation factors”. What is “correlation factors”? Its definition has not been clear from the EXFOR Formats manual. This field has been used by only two entries (EXFOR 10921 [5] and 12869 [6]), which report neutron cross sections measured by the ANL Dynamitron. Partial uncertainties and (macro) correlation matrix are tabulated in [5]. Partial uncertainties are defined under `ERR-ANALYS` of EXFOR 10921.001 as follows:

```
ERR-ANALYS (ERR-T) total error
           Partial errors and their sources:
           (ERR-S) statistical error
           (ERR-1,,,1.0) Gamma-ray detection efficiency.
           (ERR-2,,,0.0) Irradiation geometry.
           (ERR-3,,,1.0) Uranium deposit,mass,and isotope content.
           (ERR-4,,,1.0) Extrapolation correction for fissions and
                         correction for finite thickness of deposit.
           (ERR-5,,,1.0) Correction for neutron absorption in Cu
                         sample.
           (ERR-6,,,1.0) Error in correction for neutron
                         scattering by the sample and fission chamber
                         components.
           (ERR-7,,,0.5) Neutron source characteristics.
           (ERR-8,,,0.0) Correction of fissions for neutron
                         background and neutron scattering due to
                         tantalum cup.
```

Three values 1.0, 0.5 and 0.0 are coded as “correlation factors” in EXFOR 10921, and they are corresponding to “c(100): 100% correlated”, “c(50): 50% correlated” and “uc: uncorrelated” uncertainties in Table III of the article. Thanks to the guidance of Dr. D.L. Smith, I could reproduce the (macro) correlation matrix tabulated in Table IV of the article from the coded partial uncertainties by the following formula

$$V_{ij} = \sum_{q=1}^{12} K_{ijq} e_{iq} e_{jq}$$
$$C_{ij} = V_{ij} / \sqrt{V_{ii} V_{ij}} ,$$

where 12 partial uncertainties are considered. The coefficient K_{ijq} =1.0 for i=j, 0.0, 0.5 or 1.0 for $i \neq j$, while e_{iq} and e_{jq} are partial per-cent uncertainties for the i-th and j-th neutron energy bin, respectively. Similar equations are seen in p.130 of [7].

In general, we can compile correlation properties within the current format when the authors assume a constant “correlation factor” for off-diagonal element K_{ijq} (=1.0 for i=j, =constant for $i \neq j$) for each source q. Use of 3 values (1.0, 0.5 and 0.0) seems to me a good solution to avoid unnecessary complication (named as *Occam’s Lazor assumption* by Dr. Smith).

However, the current EXFOR format is not sufficient when authors provided various values between -1 to 1 as K_{ijq} . (Micro) correlation matrices considered by Sage *et al.* [3,4] show such examples. See Appendix B of [4]. We should be able to compile detailed correlation properties when authors provide them by an appropriate methodology.

Proposal

In order to improve this situation, I propose to apply ERR-1, ERR-2 etc. for any partial uncertainties regardless of their correlation property (unless there is a more specific heading, e.g., MONIT-ERR), and indicate correlation properties in the 4th field by

U: Uncorrelated (random, statistical)
F: Fully correlated
P: Partially correlated
C: Correlated (when information is insufficient to determine F or P).
(blank): Correlation property unknown

Example 1: EXFOR 23114

```
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/Al)
```

Example 2: EXFOR 10921

```
ERR-ANALYS (ERR-T,,,P) Total uncertainty
           (ERR-1,,,U) Counting statistics and reproducibility
           (ERR-2,,,F) Gamma-ray detection efficiency.
           (ERR-3,,,U) Irradiation geometry.
           (ERR-4,,,F) Uranium deposit,mass, and isotope content.
           (ERR-5,,,F) Extrapolation correction for fissions and
                       correction for finite thickness of deposit.
           (ERR-6,,,F) Correction for neutron absorption in Cu
                       sample.
           (ERR-7,,,F) Uncertainty in correction for neutron
                       scattering by the sample and fission chamber
                       components.
           (ERR-8,,,P) Neutron source characteristics.
           (ERR-9,,,U) Correction of fissions for neutron
                       background and neutron scattering due to
                       tantalum cup.
```

If authors give (micro) correlation matrices for partial uncertainties defined with the flag P, it can be given under the keyword COVARIANCE. Such coding samples are appended to this Memo.

The heading ERR-1, ERR-2... will be defined as 1st, 2nd ... partial uncertainties in the dictionary. The heading ERR-S can be kept where only one uncorrelated (statistical) uncertainty is considered.

I thank M. Herman, and P. Obložinský, A. Plompen, V. Pronyaev, P. Schillebeeckx and D.L. Smith for their instruction and discussion.

References

[1] For example, M. Lammer, O. Schwerer (ed.), INDC(NDS)-0141, p23, 1982.
[2] C. Sage, V. Semkova, *et al.*, Phys. Rev. C**81**(2010)064604.
[3] C. Sage, Thèse de Doctorat, Universitè de Strasbourg (2009).
[4] For example, W. Mannhart, INDC(NDS)-0558, D.2.1, 2011 (in print).
[5] G. Winkler *et al.*, Nucl. Sci. Eng.**76**(1980)30.
[6] P. Guenther *et al.*, Nucl. Phys. **A448**(1986)280.
[7] D.L. Smith, "Probability, statistics, and data uncertainties in nuclear science and technology", American Nuclear Society, Inc., Illinois, USA (1991).

Appendix: Coding samples (where `COVARIANCE` gives free text information)

EXFOR 23114.002 (in preparation) [2-3]

Because partial correlation matrix for monitor cross section is given, evaluators can revise the total correlation matrix when they renormalize cross sections by a new standard cross section!!

```
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/Al)
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) Total correlation
            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) Partial correlation due to standard
            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-5,PER-CENT) Partial correlation due to sample mass
            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
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
ENDSUBENT
```

EXFOR 10921.002-003 [5]

```
SUBENT
BIB
REACTION    ((29-CU-63(N,A)27-CO-60,,SIG)/(92-U-238(N,F),,SIG))
...
ERR-ANALYS (ERR-T,,,P)  Total uncertainty
           (ERR-1,,,U)  Counting statistics and reproducibility
           (ERR-2,,,U)  Irradiation geometry
           (ERR-3,,,F)  Gamma-ray detector efficiency
           (ERR-3,,,F)  Uranium deposit, mass, isotope content
           (ERR-4,,,F)  Extrapolation correction for fissions and
                        correction for finite thickness of deposit
           (ERR-5,,,P)  Neutron source characteristics 7Li(p,n)
           (ERR-6,,,P)  Neutron source characteristics D(d,n)
           (ERR-7,,,P)  Correction for activity induced in the
                        sample by neutron background
           (ERR-8,,,U)  Correction of fission for neutron background and
                        neutron scattering due to Ta cup,
                        7Li(p,n) source
           (ERR-9,,,U)  Correction of fission for neutron background and
                        neutron scattering due to gas-cell components,
                        D(d,n) source
           (ERR-10,,,F) Correction for neutron absorption in the copper
                        sample
           (ERR-11,,,F) Correction for neutron scattering by the sampl
                        and fission chamber components
COVARIANCE (EN,MEV)
            3.560 3.800 4.065 4.361 4.656 4.954 5.120 5.185
            ...
           (COR,ERR-T,PER-CENT) Total correlation
            100
              2   100
              4    17   100
              5    19    37   100
            ...
           (COR,ERR-5,PER-CENT)
            100
             50   100
             50    50   100
             50    50    50   100
            ...
           (COR,ERR-6,PER-CENT)
            100
             50   100
             50    50   100
             50    50    50   100
            ...
           (COR,ERR-7,PER-CENT)
            100
             50   100
             50    50   100
             50    50    50   100
            ...
ENDBIB
NOCOMMON
DATA
EN         EN-RSL-HW  DATA       ERR-T      ERR-1      ERR-2
ERR-3      ERR-4      ERR-5      ERR-6      ERR-7      ERR-8
ERR-9      ERR-10     ERR-11     ERR-12
MEV        MEV        NO-DIM     PER-CENT   PER-CENT   PER-CENT
PER-CENT   PER-CENT   PER-CENT   PER-CENT   PER-CENT   PER-CENT
PER-CENT   PER-CENT   PER-CENT   PER-CENT
 3.560      0.044        7.27E-05 50.        50.        3.0
 1.5        1.0        0.5        1.5
                       1.8        2.2
 3.800      0.08        2.204E-04 11.5       10.5       3.0
 1.5        1.0        0.2        1.5
                       1.8        2.2
 ...
ENDDATA
ENDSUBENT
```