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Memo CP-D/680 (Rev.)

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To: Distribution
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Subject: **LEXFOR entry for covariances in the AGS format**
Reference: Memo CP-D/564(Rev.)

IRMM and NDS have recently completed the compilation of neutron transmission data together with and the covariance information. The data resulted from measurements at the GELINA facility (EXFOR 23077) [1]. Two new headings are proposed

Dictionary 24 (Data Headings)

`TOF-MIN`	Lower boundary of time-of-flight
`TOF-MAX`	Upper boundary of time-of-flight.

In order to fulfill the action A51 of the 2010 NRDC meeting, addition to the LEXFOR "**Covariance**" is proposed below. Headings `ERR-1`, `ERR-2` etc. will be interpreted as "AGS vector" when `CHLSK` (Cholesky) is coded under the keyword `COVARIANCE`.

In the example adopted in the LEXFOR input, the uncertainty in normalization factor (0.5%) is not treated as coded information under the `MONIT-ERR`, because the coded total uncertainty (`ERR-T`) does not include this component. If one receives the total uncertainty including the normalization uncertainty, the normalization uncertainty must be coded information under the heading `MONIT-ERR`.

Covariance

Definition

For a measured quantity at two points σ_i and σ_j (e.g., cross section at two incident energies; $i,j=1,2,\ldots,m$), **covariance** between them are defined as

$$\mathrm{cov}(\sigma_i,\sigma_j)=\left\langle\left(\sigma_i-\langle\sigma_i\rangle\right)\left(\sigma_j-\langle\sigma_j\rangle\right)\right\rangle=\langle\sigma_i\sigma_j\rangle-\langle\sigma_i\rangle\langle\sigma_j\rangle \quad (1)$$

If the cross section depends on p parameters (source of uncertainties) $\{x_k\}$ ($k=0,1,2,\ldots,p$),

$$\sigma_i-\langle\sigma_i\rangle=\sum_{k=0}^{p}\frac{\partial\sigma_i}{\partial x_i^k}\left(x_i^k-\langle x_i^k\rangle\right), \quad (2)$$

Eq.(1) can be rewritten as

$$\mathrm{cov}(\sigma_i,\sigma_j)=\sum_{k,l=0}^{p}\frac{\partial\sigma_i}{\partial x_i^k}\mathrm{cov}\left(x_i^k,x_j^l\right)\frac{\partial\sigma_j}{\partial x_j^l}=\Delta_0\sigma_i\cdot\Delta_0\sigma_j\cdot\delta_{ij}+\sum_{k,l=1}^{p}\frac{\partial\sigma_i}{\partial x_i^k}\mathrm{cov}\left(x_i^k,x_j^l\right)\frac{\partial\sigma_j}{\partial x_j^l}. \quad (3)$$

where $k,l=0$ gives the uncorrelated uncertainty $\Delta_0\sigma_i=(\partial\sigma_i/\partial x^0)\Delta x_i^0$.and δ_{ij} is the Kronecker's delta.

…

Cholesky Decomposition of Covariance Matrix

Eq.(3) is expressed as

$$V=MM^t+S_\alpha V_\alpha S_\alpha^t \quad (4)$$

($V=\mathrm{cov}(\sigma_i,\sigma_j)$, $M=\{\Delta_0\sigma_i\}$, $S_\alpha=\{\partial\sigma_i/\partial x_i^k\}$, $V_\alpha=\mathrm{cov}(x_i^k, x_j^l)$)

The $p\times p$ matrix $V_\alpha=\mathrm{cov}(x_i^k, x_j^l)$ is positive definite and symmetric, and therefore there is a matrix L which satisfies $V_\alpha=LL^t$ (**Cholesky decomposition**):

$$V=MM^t+S_\alpha LL^tS_\alpha^t=MM^t+D_\alpha D_\alpha^t, \quad (5)$$

where $D_\alpha=S_\alpha L$ is a $m\times p$ matrix. The ij-th component of the Eq.(5) is

$$\mathrm{cov}(\sigma_i,\sigma_j)=\Delta_0\sigma_i\cdot\Delta_0\sigma_j\cdot\delta_{ij}+\sum_{k=1}^{p}\Delta_k\sigma_i\cdot\Delta_k\sigma_j\,. \quad (6)$$

($D_\alpha=\{\Delta_k\sigma_i\}$, $k=0, 1,2,\ldots,p$ and $i=1,2,\ldots,m$)**.** Therefore the $m\times m$ covariance matrix V can be expressed by p sets of the m-dimension vectors $\{\Delta_k\sigma_i\}$. This vector (AGS vector [2,3]) gives a compact expression of the covariance matrix when m is very huge (e.g., high resolution time-of-flight spectra).

If the covariance matrix $\mathrm{cov}(x_i^k, x_j^l)$ is simplified to $\Delta x_i^k\Delta x_j^l\ \delta_{kl}$ (e.g. $\mathrm{cor}(x_i^k, x_j^l)=\delta_{kl}$ for any i and j), the summation of the last term of Eq.(3) is simplified to the summation of $(\partial\sigma_i/\partial x_i^k)\Delta x_i^k\ (\partial\sigma_j/\partial x_j^l)\ \Delta x_j^l\delta_{kl}$, and $\Delta_k\sigma_i$ in Eq.(6) becomes the k-th partial uncertainty of the quantity σ_i by comparing Eq.(3) and Eq.(6).

Though AGS vector $\{\Delta_k\sigma_i\}$ cannot be interpreted as the partial uncertainty of the quantity σ_i due to the parameter x_k in general, the vectors are coded in the same way, and given under headings `ERR-1`, `ERR-2`,.... with the code `CHLSK` under the keyword `COVARIANCE`.

Example:

```
REACTION    (48-CD-0(N,TOT),,TRN)
MISC-COL    (MISC1) Width of time-of-flight bin
            (MISC2) Uncorrelated uncertainty squared
CORRECTION   Data are corrected for
               - dead time at sample-in detector   (din);
               - background at sample-in detector  (Bin);
               - dead time at sample-out detector  (dout);
               - background at sample-out detector (Bout),
             as follows:
               T=N(din*Cin-Bin)/(dout*Cout-Bout)
             , where
               N: Normalization factor (N=1 +/- 0.5%)
               T:    Transmission;
               Cin:  Count at sample-in detector;
               Cout: Count at sample-out detector.
               Backgrounds were expressed by constant plus sum of
               two exponential: a0+a1*exp(-b1*tof)+a2*exp(-b2*tof)
ERR-ANALYS   ERR-1 to ERR-4 gives "correlation vectors" in the
             AGS format.
            (ERR-T)  Total uncertainty (sigma)
            (ERR-S)  Total uncorrelated uncertainty (sigma)
            (ERR-1)  Correlated component due to dead time
                     correction (sample-in)
            (ERR-2)  Correlated component due to background
                     Correction (sample-in)
            (ERR-3)  Correlated component due to dead time
                     correction (sample-out)
            (ERR-4)  Correlated component due to background
                     Correction (sample-out)
COVARIANCE (CHLSK)  Compiled in ERR-1 to ERR-4 in the AGS format
ENDBIB
NOCOMMON
DATA
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
4.79930E+0    873301.2    873429.2       128.0 1.14780E+0 6.65562E-2
6.65376E-2 4.42725E-3 1.33447E-5-9.12646E-4-1.37145E-5 1.28552E-3
4.79790E+0    873429.2    873557.2       128.0 9.70250E-1 5.63176E-2
5.63021E-2 3.16993E-3 1.09942E-5-8.47529E-4-1.16680E-5 1.00913E-3
…
```

In this example, `ERR-S` gives $\Delta_0\sigma_i$ and `ERR-1` to `ERR-4` give $\Delta_k\sigma_i$ (k=1,2,3,4, i=1,2,…,m) in Eq.(6).

References

[1] S. Kopecky, I. Ivanov, M. Moxon, P. Schillebeeckx, P. Siegler, I. Sirakov, "The total cross section and resonance parameters for the 0.178 eV resonance of ^{113}Cd", Nuclear Instruments and Methods B 267 (2009) 2345 - 2350

[2] C. Bastian, "General procedures and computational methods for generating covariance matrices", Proc. Int. Symposium on Nuclear Data Evaluation Methodology, Brookhaven National Laboratory, USA, October 12-16, 1992, p642.

[3] N. Otuka, A. Borella, S. Kopecky, C. Lampoudis, P. Schillebeeckx, "Database for time-of-flight spectra including covaraince", Proc. Int. Conf. on Nucl. Data for Sci .and Technol., Jeju island, Korea, April 26-30, 2010.

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