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Memo CP-D/680

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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.

Covariance

Definition

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

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

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

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

Eq.(1) can be rewritten as

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

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.

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Cholesky Decomposition of Covariance Matrix

Eq.(3) is expressed as

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

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

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

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

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

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

($D_\alpha = \{\Delta_k \sigma_i\}$, $k=0, 1, 2, \dots, p$ and $i=1, 2, \dots, m$). 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 $\text{cov}(x_i^k, x_j^l)$ is simplified to $\Delta x_i^k \Delta x_j^l \delta_{kl}$ (e.g. $\text{cor}(x_i^k, x_j^l) = \delta_{kl}$ 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:

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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*Count-Bout)
               , where
               N: Normalization factor (N=1 +/- 0.5%)
               T: Transmission;
               Cin: Count at sample-in detector;
               Count: 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-ANALYSIS  ERR-1 to ERR-4 gives "correlation vectors" in the
               AGS format.
               (ERR-T) Total uncertainty (sigma)
               (ERR-S) Uncorrelated uncertainty (sigma)
               (ERR-1) Correlation dead time correction (sample)
               (ERR-2) Correlation background correction (sample)
               (ERR-3) Correlation dead time correction (open beam)
               (ERR-4) Correlation background correction (open beam)
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
...
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In this example, ERR-S gives $\Delta_0\sigma_i$ and ERR-1 to ERR-4 give $\Delta_k\sigma_i$ ($k=1,2,3,4$, $i=1,2,\dots,m$) 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 covarainces", Proc. Int. Conf. on Nucl. Data for Sci. and Technol., Jeju island, Korea, April 26-30, 2010.

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