IV.E.4. Covariances for Calculated Cross Sections

Let T_i represent the theoretical cross section (or transmission), at energy point E_i, as calculated from the "final" set of resonance parameters and parameter covariance matrix. The covariance matrix element connecting theory point T_i with point T_j is found from

$$\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_j}{\partial u_n} \quad , \tag{IV E4.1}$$

where M_{kn} is the covariance matrix element connecting parameter u_k with parameter u_n . The theoretical uncertainty on theory T_i is the square root of the diagonal element; that is,

$$\Delta T_i = \sqrt{\Delta^2 T_i} = \sqrt{\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_i}{\partial u_n}} \quad . \tag{IV E4.2}$$

When the phrase

```
INCLUDE THEORETICAL uncertainties in plot file
```

is given in the command section of the INPut file, values of ΔT_i will be reported in the plot file. See Section VII.C for specific details about where to find which uncertainties.

To create an ASCII listing of cross section (or transmission), uncertainty, and correlation matrix, include the phrase

```
CROSS SECTION COVARIance matrix is wanted
```

in the command section of the INPut file. The desired listing will be given in the SAMMY.LPT file. This is a no-Bayes run (i.e., no fitting can be accomplished in the same SAMMY run).

Using this command will also give the cross-section covariance matrix formatted into a "publishable" file named SAMCOV.PUB. This file is formatted with values separated by tabs so that it can be easily ported to a spreadsheet or other program, for example, to be plotted in three dimensions. This SAMCOV.PUB file contains the following information:

Row 1: three tabs, followed by the T_i separated by tabs
Row 2: three tabs, followed by the ΔT_i separated by tabs
Row 3: three tabs, followed by the E_i separated by tabs
Row 4: T_1, ΔT_1, E_1, followed by the first row of the covariance matrix separated by tabs
Row 5: T_2, ΔT_2, E_2, followed by the second row of the covariance matrix separated by tabs
. . .
Row N+3: T_N, ΔT_N, E_N, followed by the N^{th} row of the covariance matrix separated by tabs

In this format, it is easily possible to manipulate the results in a spreadsheet program. For example, the correlation matrix is found by dividing the covariance matrix element by the uncertainty in the same column in Row 2 and by the uncertainty in the same row in Column 2. See test case tr010, run e, for an example of this. (Caution: The user should exercise caution in porting this file to a spreadsheet, as the number of data points can easily become too large to fit into a normal spreadsheet.)

The SAMMY user should note that the covariance matrix constructed in this fashion is not a complete representation of the evaluated cross section covariance matrix. Detail arguments concerning this assertion are presented in Section IV.E.6.