IV.E.2. Retroactive Parameter Covariance Matrix Method

Occasionally it is necessary to produce an approximate covariance matrix associated with a pre-existing set of resonance parameters.

For example, most current evaluated nuclear data files (ENDF) contain resonance parameters, but not uncertainties / covariances for those parameters. The ideal cure for this situation would be to re-analyze the experimental data, including all appropriate uncertainties (both measurement and theory related), thus producing a new set of resonance parameters and the corresponding covariance matrix. However, it is not possible to immediately produce complete new evaluations for all nuclides in the ENDF. Therefore, a method is needed to generate an approximate covariance matrix appropriate for the current ENDF resonance parameters.

This may be accomplished using a scheme called the "retroactive parameter covariance matrix method": First, create representative data sets covering the energy range of the R-matrix evaluation. This may be done by running SAMMY in the no-Bayes mode with suitable energy grids, and using the calculated cross sections as the "experimental data" in later runs. Make reasonable choices for the covariance matrix for this set of data. Do a simultaneous fit to all those data sets, taking the ENDF File 2 parameter set for initial values and varying all resonance parameters. Check whether the output parameter values are not very different from the input values. If that is the case (as it should be, with the artificial experimental data in use here), then the output parameter covariance matrix (PCM) may safely be assumed to be a reasonable approximation for the covariance matrix associated with the input parameter values.

Test case tr149 gives an example of the procedure for retroactively producing an approximate covariance matrix.

After the retroactive covariance matrix has been produced, it is possible to use that covariance matrix with the original parameter values in another SAMMY run. To do this, include one of the following (equivalent) commands

```
RETROACTIVE OLD PARAmeter file new covariance or
RETROACTIVE or
U COVARIANCE MATRIX is correct, p is not
```

in the INPut file. In addition, make a new file, identical to the original PARameter file but containing the phrase "COVARiance matrix exists" at the end of the file (after the final blank line signifying the end of the previous card set, or immediately after card set 2 if there are no other card sets). This new file, and the now-renamed SAMMY.COV file from the run that created the retroactive parameter covariance file, are used as the input *.par and *.cov file for this run. See test case tr083, step r, for which the PARameter file t083r.par is identical to the original file ../tr082/tr082a.par except for the final line.

Variations on this procedure are possible. Instead of assuming that the *u*- PCM is correct, one could assume that the *p*-PCM is correct. (For a discussion of *u*- vs. *p*-parameters, see the end of Section IV.C.) Ideally, there should be virtually no differences in results obtained from the two

assumptions, since only insignificant changes should occur to the value of the parameters in the retroactive process. In practice there will be small differences. To use the *p*-PCM instead of the *u*-PCM from the *.cov file, include the command

```
P COVARIANCE MATRIX is correct, u is not
```

The user may wish to modify (increase) the uncertainties on some of the parameters. To give explicit values for the uncertainties, while maintaining the correlation matrix currently in the *.cov file, include both of these commands in the INPut file:

```
P COVARIANCE MATRIX is correct, u is not     and
MODIFY P COVARIANCE matrix before using
```

In addition, create a file (the "new uncertainty" file) containing, in free format, the values you want for the uncertainties for all of the varied parameters (*p*-parameters), in the numerical order as indicated in the LPT file. An uncertainty equal to zero in this file indicates that SAMMY should use the uncertainty from the *.cov file. The name of this file is given at the end of the input stream. See also Table VI E.2 for a complete listing of the ordering of input files.

It is possible to use the MODIFY P COVARIANCE option with U COVARIANCE MATRIX rather than P COVARIANCE MATRIX. In this case, the *u*-PCM is taken from the *.cov file and transformation is made to give the associated *p*-PCM; this matrix is then modified using the uncertainties from the new uncertainty file. The reverse transformation then gives the *u*-PCM to be used in the SAMMY calculations.

For additional details on modifying the SAMMY-produced PCMs, see Section IV.E.6.