

### VI.C.3.a. Input for propagated uncertainty parameters

The Propagated Uncertainty Parameter (PUP) option is described in detail in Sections IV.D.1 and IV.D.2. Essentially, the PUP method takes any of the SAMMY parameters (either R-matrix parameters or parameters from the experiment-related corrections to the cross sections) and incorporates the uncertainty on that parameter into the data covariance matrix (DCM). The value of the parameter is held fixed.

As indicated in Table VI B.2, SAMMY input parameters generally have both a flag and an uncertainty associated with them. If that flag is zero, the parameter is treated as a constant and the uncertainty is ignored. When the flag is 1, the value of that parameter is refined (“fitted” or “searched on”) during the analysis process; the uncertainty is taken as the “prior” uncertainty on that parameter (unless, of course, a prior COVariance file is used). If the flag is 3, the parameter value remains fixed, but the uncertainty becomes a component of the DCM.

Nearly all the data-related card sets of the PARAmeter file (Table VI B.2) can now be inserted into the INPut file (see the end of Table VI A.1). When the card set is in the INPut file, flags = 1 will be ignored but flags = 3 will be honored.

Sometimes it is desirable to provide an off-diagonal covariance matrix for the PUP'd parameters. For example, the set of resolution-function parameters may be determined altogether, by fitting a functional form to measured data; those parameters are then correlated. To input such information to SAMMY, create an ASCII file containing the following information:

1. A title on the first line.
2. A line containing “Number of parameters = #”, where # is replaced by the integer number of PUP parameters for which covariances will be provided. [In fact, only the equal sign and the number are absolutely necessary on this line.]
3. One or more lines containing the exact values of the PUPs, in free-format. These values must be within 0.1 % of the actual value of the parameters as given in the PARAmeter or INPut file. (Caution: if there are two PUPs whose values are nearly identical, and it is the second one that you are intending to use here, SAMMY might misinterpret the information. To avoid this problem, include the first PUP, and all in between, in the PUP covariance matrix.)
4. One or more lines containing the lower triangular covariance matrix elements for those parameters (reading across the matrix from the left-hand side to the diagonal in the usual SAMMY fashion), in free format.

It is NOT necessary to include every PUP in this file, but those that are included must be consecutively located in the SAMMY.LPT listing; that is, the PUP numbers inside the pointed brackets must be consecutive, as in <6> and <7>. For example, one might have a covariance matrix for the resolution-function parameters but wish to PUP the Doppler width plus the normalization and background parameters as well. See test case tr168 for examples.

To use the PUP covariance file in a SAMMY run, include the phrase “PUP COVARIANCE IS IN an ascii file” in the command section of the INPut file.

It is possible to use SAMMY to generate PUP covariance information and write it into a file to be used as input for subsequent runs. For example, to predetermine resolution-function parameters, a SAMMY run (or series of runs) might be made on “clean” data with well-defined resonance parameters. Only the resolution parameters would be flagged. The command “CREATE PUP FILE FROM varied parameters used in this run” would be included in the INPut file for this run (or for the final run of the series). The output file SAMPUP.COV is in the appropriate format for use as the input PUP covariance file for future runs. Again, see test case tr168 for an example of this.

Caveat: The implementation of the PUP covariance input option is new and has not been extensively tested. Because there are so many possibilities for parameters to be PUP’d, it has not been possible for the author to test each and every potential combination. The user is therefore strongly advised to carefully examine the SAMMY.LPT output file to be sure that the PUP covariance matrix information has been properly interpreted by the code. In particular, look at the array printed following the phrase “Correlation matrix for PUPped parameters” and check that the uncertainties and correlations correspond to the appropriate PUPs.

For sequential runs in which the varied-parameter COVariance file from one run is used as input to the next run, values and uncertainties for varied parameters cannot be modified. (The exception is via the use of program SAMAMR; see Section X.C.) However, values and uncertainties for PUPs can be modified, since they are associated with the data set rather than with the parameters whose values are being determined. (The exception is that the treatment of R-matrix parameters may not be changed during a sequence of runs.) If the user wishes to be certain that values for PUPs do not change, s/he can insert the command “DO NOT ALLOW VALUES for data-related parameters to change” into the INPut file.

R-matrix parameters should not be PUP’d during sequential runs: One of the assumptions underlying the use of sequential analysis is that the data sets being analyzed are completely independent of each other, that is, they are not united via a common DCM. Therefore, if a parameter (e.g., a channel radius) is PUP’d for two data sets, the associated components of the DCM uniting the two data sets will be ignored. This would violate the assumption of independent data sets. The same is also true for simultaneous runs of two or more data sets, as described in Section IV.E.1, because the scheme described there also assumes that the data sets are independent.

It is expected that future development work will provide a means of properly including the effect of a PUP’d variable that connects two otherwise-independent data sets.