

IV.D.2. Propagated Uncertainty Parameters

In the previous section, it was demonstrated that writing the data covariance matrix (DCM) in terms of the theoretical cross sections (rather than in terms of the measured data) leads to equivalent results when fitting to reduced data as are obtained when fitting to raw data. This is particularly important if there are discrepancies in the measured data, a situation for which the usual definition of DCM can lead to strange results. See, for example, Peele's Pertinent Puzzle [RP87] and the many attempts to reconcile this puzzle [ZZ92, SC94, NL04a, NL04b].

To reiterate, the benefits of this definition of DCM are numerous: Consistent and reasonable results are obtained when fitting raw data and when fitting reduced data. (By "results" is meant both parameter values and the corresponding parameter covariance matrix.) All prior uncertainties are reflected in the final results, for varied parameters (as usual) and also for unvaried parameters when the associated uncertainty is properly incorporated in the DCM.

The parameters that are unvaried but whose uncertainties are incorporated into the DCM are hereafter denoted as Propagated Uncertainty Parameters, or PUPs.* In SAMMY, any parameter for which derivatives are available (i.e., any parameter that is capable of being varied) can instead be PUP'd, at the user's discretion. Any of the experiment-related parameters can be treated as PUPs. In addition, although the derivation of Section IV.D.1 discussed only data-reduction parameters, there is nothing to prevent a non-varied theory parameter from being treated as a PUP in an individual run. However, a theory parameter will not currently be treated properly if it is PUP'd in two successive runs because there is then a neglected component of the DCM connecting the two data sets. The SAMMY user should be aware that results will not be correct for that situation.

Specifically, the SAMMY parameter types that can be PUP'd are the shown in Table IV D2.1, along with relevant test cases (see Section XII.B for a discussion of test cases).

Table IV D2.1. Types of parameters that may be PUP'd

| Test case for PUPs | Related test case without PUPs | Type of parameter |
|--------------------|--------------------------------|-------------------------------------|
| tr044 | tr009 | resonance parameters (res) |
| tr059 | tr093 | R-matrix radii (rad) |
| tr040 | tr011 | R-external (ext) |
| tr038 | tr007 | broadening etc (brd) |
| tr041 | tr012 | normalization and background (nbk) |
| tr097 | tr056 | background functions (bgf) |
| tr068 | tr021 | Oak Ridge resolution function (orr) |
| tr096 | tr054 | RPI resolution function (rpi) |
| tr062 | tr029 | nuclide abundance (iso) |
| tr066 | many | miscellaneous parameters (msc) |
| tr055 | tr055 | paramagnetic cross section (pmc) |

* Thanks to Royce Sayer for suggesting this nomenclature.

Extensive testing has been done for each type of parameter, to ensure that the PUP theory and implementation are indeed correct. The tests consisted primarily of running the code with as many different options as possible for treating the parameter uncertainty, and comparing the resulting values and covariance matrices for the varied parameters. The available options are

1. varying the parameter,
2. treating the parameter as a PUP,
3. giving an explicit DCM,
4. providing user-supplied implicit DCM (see Section VI.C.3.b for details), and
5. treating via SAMMY's original IDC parameter method (Section VI.C.3.c), available for normalization and background parameters.

In the tests, options #1 and #2 gave identical results for the first iteration. When available, options #2 and #5 gave exactly identical results for all iterations. Options #3 and #4 gave almost identical results, so long as each element of the explicit DCM was specified with a sufficient number of significant digits. When the data are not discrepant (so that a "fixed" DCM is a good approximation), all methods gave similar results.

To designate that a parameter is a PUP, the SAMMY user must simply set the flag for that parameter equal to "3" rather than "0" (to hold constant) or "1" (to vary). Uncertainties are provided in the same manner as for varied parameters; details are given in Table VI B.2.

In the SAMMY.LPT output file, the ordinal numbers for PUPs are given in angle brackets, for example, <38>, while numbers for varied parameters are given in parentheses, for example (38).

Card sets for most types of parameters may be put into the INPut file (Table VI A.1) rather than the PARAmeter file (Table VI B.2), provided none of that type of parameter is flagged for varying. Varied parameters must always be in the PARAmeter file. PUP'd parameters, on the other hand, may be in either the PARAmeter file or the INPut file. (A card set, however, can occur in at most one of the two files.) A flag = 1 in the INPut file will be ignored; a flag = 3 in either the INPut or the PARAmeter file will signify that the parameter is to be PUP'd. Values (and corresponding uncertainties) for most PUP'd data-related parameters may be different from one run to the next in a series for which the covariance matrix is carried along.

The exception to the above paragraph is any R-matrix parameter, all of which must be in the PARAmeter file. Values and uncertainties for PUP'd R-matrix parameters may NOT be changed from one run to the next in a sequential series. Furthermore, the current implementation neglects the DCM component (caused by PUP'ing the theory parameter) relating one data set to another. Hence, even though the option to PUP the R-matrix parameters is available, its use is not encouraged.

Uncertainties for PUP'd parameters may be input to SAMMY in the same fashion as uncertainties on the varied parameters. The user should be aware, however, that the "EXPLIcit" option (card set "Last B" of the PARAmeter file) is not appropriate for PUPs because it cannot be used when a COVariance file exists (card set "Last A") for the varied parameters. (Therefore,

for example, the final no-Bayes computation would not understand the EXPLIcit uncertainty for PUP'd parameter.) Instead, the uncertainty for the parameter should be input in the card set containing the parameter value itself. For the 2006 revision of the code (sammy-7.0.0), options to include the uncertainties have been added to several of the card sets (e.g., card set 4, the BROADening parameters).

When off-diagonal elements of the PUP covariance matrix exist, input of the covariance matrix for some or all of the PUP'd parameters can be accomplished by means of a separate file. This file can be created by the analyst using available information, or it can be created by preliminary SAMMY runs. Details are given in Section VI.C.3.a.