Appendix A.7 MODIFICATIONS AND ADDITIONS IN REVISION 7

(This section is modified slightly from Section I.A in Revision 7 of this manual, with ~~strikeouts~~ and {inserts} to clarify topics that might otherwise cause confusion.)

Modifications, additions, and improvements to SAMMY subsequent to the publication of Revision 6 of this manual are summarized here.

New or expanded options in the resolved resonance region (RRR)

1. The ability to quickly and efficiently generate and use the data covariance matrix (DCM) has been greatly enhanced with the development of two features:
   a. The Propagated Uncertainty Parameter (PUP) option allows the uncertainty associated with any parameter to be incorporated into the data covariance matrix, while holding the value for that parameter constant. Sections IV.D.1 and IV.D.2 give details; input is described in Section VI.C.3.a.
   b. The User-Supplied Implicit Data Covariance (IDC) option allows the components of the DCM to be generated external to SAMMY. See Sections IV.D.3 and VI.C.3.b.
2. Covariances associated with point-wise cross sections can now be calculated and printed; see Section IV.E.4 for details.
3. Techniques have been improved for simultaneous fitting using the M+W scheme for solution of Bayes' Equations. For example, either explicit or implicit data covariance matrices may be used for the individual data sets. Details regarding simultaneous fitting are in Section IV.E.1.
4. Options have been introduced to perform true least-squares fitting (as opposed to Bayes techniques, which require estimation of finite prior parameter uncertainties). Least-squares fitting implicitly assumes infinite prior parameter uncertainties. See Section IV.E.3.
5. The "retroactive covariance method" has received considerable attention to ensure that it is working properly. Also, it is now possible to make a SAMMY run using the original parameter values together with the retroactive covariance matrix to test whether the combination is reasonable. See Section IV.E.2 for details.
6. Ad hoc methods have been created for modifying the output uncertainties in the parameter covariance matrix, in order to report more realistic uncertainties in ENDF files or other publications. These methods are discussed in Section ~~IV.E.6~~ {IV.E.6.a}.
7. The RPI resolution function has been extended in order to provide capabilities to simulate the GELINA and nTOF resolution functions. Extensions include a continuously varying time-channel width. Thanks to Frank Gunsing for providing appropriate forms and parameter values for those. Details are given in Section III.C.3.
8. An option has been created to efficiently calculate unweighted energy-averaged cross sections (Section V.C.3).
9. As an alternative to the energy dependence of the flux used in the Watt spectrum average [Section V.B, Eq. (V B.7)], the user may specify the flux numerically on an energy grid. Details are given in Section V.B.1.
10. An optional correction for neutron sensitivity has been added to the multiple-scattering correction for capture yields. See Section III.D for details.

11. An externally generated direct capture component may be added to the R-matrix cross section, with a variable normalization on this component. See Section II.B.4.

12. The ENDF connection has been strengthened:
    a. A new ENDF format for File 2 resonance parameters (LRU = 1, LRF = 7, titled "R-Matrix Limited") was developed by the SAMMY author and approved by the Cross Section Evaluation Working Group in November of 2004. This format provides capability for reporting virtually any SAMMY R-matrix parameterization (for incident neutrons) into the evaluated nuclear data files. SAMMY can both read and write this format. Sections VI.F.2, VI.F.3, and IX discuss this and other ENDF formats.
    b. To facilitate use of the new R-matrix format, the auxiliary code SAMRML was developed as an aid to processor-code developers. This code calculates cross sections and derivatives from the R-matrix parameters, much as SAMMY itself does, but does not contain any of the measurement-related capabilities (e.g., Doppler or resolution broadening, multiple-scattering corrections) found in SAMMY. See Section X.Q for details.
    c. A second new ENDF format, for File 32 (covariances for resonance parameters), was developed by the SAMMY author and approved by CSEWG in 2004. This format (denoted the Compact Covariance Format, and defined by parameter LCOMP = 2 allows the parameter uncertainties and an abbreviated correlation matrix to be stored in the ENDF file. Again, SAMMY can both read and write this format; see Sections VI.F.2, VI.F.3, and IX.
    d. SAMMY can also read and write other ENDF File 32 covariance formats (LCOMP = 0 for Breit Wigner; LCOMP = 1 for any of the Breit Wigner, Reich Moore, and R-matrix limited formats), though not in all possible permutations. See Section IX for details.
    e. For comparison purposes, it is now possible to read and write ENDF File 2 (resonance parameters) in either of the Breit-Wigner formats (LRF = 1 or 2). SAMMY users are reminded, however, that these crude approximations should *not* be used for new evaluations.

Input and output improvements in RRR

1. Most of the data-related parameters (e.g., abundances, Doppler temperature, resolution-broadening parameters) can now be specified in the INPut file rather than the PARameter file. See the end of Table VI A.1 for a list of parameter types (card sets) that can be moved to the INPut file.

2. A flag to include the uncertainty on a parameter while holding the parameter fixed (i.e., to treat the parameter as a PUP, as described in Section IV.D.2) will be acknowledged in either the INPut file or the PARameter file. A flag to vary a parameter will be ignored in the INPut file. The option to PUP a parameter in the INPut file makes it far easier for the user to organize a sequence of SAMMY runs involving several different data sets.

3. To specify reactions such as inelastic or (n,p), the input has been somewhat cumbersome. With this release, a more intuitive key-word-based input is available. See Section II.B.1.c and card sets 4 and 8 of Table VIA.1 for details.

4. The PUBLISH command was updated to include spins J and L. See Section VII.F for details.

5. Simpler options have been created for the input of prior uncertainties for various classes of resonance parameters. See card set "Last D" in Table VI B.2.

6. Simpler options have been created for input of prior uncertainties for broadening parameters (card set 4 of the PARameter file) and for channel radii (card set 7a).

Streamlining and modernization changes

1. A new distribution system was created for SAMMY by Dorothea Wiarda. For details, see Section XIII.F.
2. The use of temporary data files has been substantially lessened but not yet completely eliminated. The functions previously performed by "reads to" and "writes from" the temporary files are now performed within the code.
3. Array sizes have been reduced where possible.
4. Modifications were introduced to make it easy to use extremely large arrays, for those rare situations in which those modifications are necessary. Thanks to Goran Arbanas for his work on this feature. For details, see Section XIII.A.
5. Sections II, III, and IV of this manual have been reorganized into a more sensible and legible ordering with greatly expanded descriptions.
6. Section XI of this manual, "Helpful Hints for Running SAMMY," has been completely rewritten. Both novice and experienced users are encouraged to read this section.

Bugs eliminated in the RRR

1. The conversion of the covariance matrix from *u*-parameters to *p*-parameters had previously ignored the dependence of the neutron (or other) widths on the resonance energy. This deficiency has now been corrected; details are in Section II.D.1.e.
2. The RPI resolution function (Section III.C.3) has been corrected to work properly at low energy.
3. Bondarenko averaging (Section V.C.2) now works with "make no corrections," that is, when the unaveraged cross sections were not Doppler- or resolution-broadened prior to averaging.
4. For average cross sections:
   a. The energy- or time-weighted average (Section V.C.1) had been working correctly but also had great potential for abuse: The implementation of this feature assumed that the "unaveraged" cross sections had been averaged over the time-channel width –that is, the implementation assumed that these are measured values, not theoretical cross sections. Therefore this method should not be used when accurate averages of theoretical cross sections are wanted.
   b. To obtain accurate averages of theoretical cross sections, one can use the Bondarenko averaging technique (Section V.C.2). However, for more efficient calculations of unweighted (weighted with a constant) averages, the new unweighted energy average described in Section V.C.3 is the method of choice.
5. The Watt spectrum average (Section V.B) was previously calculated incorrectly; this has been fixed.

6. Kinematics equations for angular distributions with non-zero Q value have been derived and implemented in the code. (See Section II.C.2.b.) It therefore is now possible to properly calculate angular distribution reaction cross sections. (Previously, these cross sections had been calculated incorrectly.)
7. In some cases, especially those involving high orbital angular momentum, elastic scattering angular distributions for incident charged particles (Section II.C.4.a) had been calculated incorrectly. This is now corrected.
8. A bug affecting very-low-energy cross sections has been eliminated from the Leal-Hwang Doppler-broadening method (Section III.B.2). This method now produces virtually the same results as does the free-gas model of Section III.B.1.
9. A bug has been corrected in the "`RECONSTRUCT CROSS SEctions from resonance parameters`" option, so that fission cross sections are also correctly generated.

Auxiliary programs

1. The SAMQUA program has been enhanced to additional information, useful in determining whether a particular spin group and/or channel must be included. See Section X.J.
2. Input for and output from the SAMMY run which prepares input for the Monte Carlo simulation code SAMSMC has been changed, to eliminate redundancies and reduce mistakes; see Section X.M for details.
3. The SUGGEL program is now portable to LINUX systems. See Section X.P.
4. A code SAMRML was developed to calculate cross sections and partial derivatives at any specified energy, starting from ENDF File 2. See Section X.Q.

Improvements in the unresolved resonance region (URR)

1. Elastic data may be fitted. Previously, only total, inelastic, fission, or capture were allowed.
2. The ability to perform a "no-Bayes" run (calculation of cross section with no fitting to data) was added.
3. Calculation of the Dresner integration was upgraded.
4. The Moldauer prescription for width fluctuations was implemented. Previously, it had been inadvertently disabled in the coding.
5. Options were added to include direct capture and/or direct inelastic.
6. Options for interfacing with ENDF were enhanced.
7. The interior of the code was redesigned (modernized) a bit.
8. Bugs related to sequential runs were found and eliminated.
9. Previously, the value of $\left\langle \Gamma_f \right\rangle$ would occasionally become negative during an analysis; when this happens, the value is now set to the absolute value of $\left\langle \Gamma_f \right\rangle$.

10. The PARameter file has been modified for increased human legibility. Spin and orbital angular momentum may be added to the listing of $\left\langle \Gamma_f \right\rangle$ to reduce possibilities for confusion.
11. Usage of the parameter covariance matrix has been generalized to include features previously available only in the RRR.

Prognostication

Though it is never possible to precisely predict the path forward, it is possible to itemize options under consideration for future implementation into the code. Below are listed some of these options for the resolved resonance region. (For a similar list in the unresolved resonance region, see Section VIII.) Comments on these options, suggestions for prioritization, and proposals for additional items are always welcome.

1. Put each nuclide's R-matrix information into a separate file. Analysis of measurements with multiple nuclides in the sample would then use multiple PARameter files rather than one combined file.
2. Provide measurement-related information (e.g., thickness, temperature, resolution function, background) in a separate file for each data set. Information concerning the measurement would then be thoroughly isolated from information concerning the R-matrix.
3. Implement a technique for analyzing inverse reaction data without rewriting the resonance parameters or the experimental data. This would allow, for example, n+^{16}O data to be analyzed simultaneously with α + ^{13}C data.
4. Implement convergence criteria when iterating for non linearity (Section IV.A.3).
5. Simplify the simultaneous fitting of more than one data set (Section IV.E.1) and the use of least-squares (Section IV.E.3).
6. Invent methodologies for incorporating uncertainty in the *theory* into the analysis. For example, what is the effect of our limited knowledge of spin assignments for the very small resonances?
7. When two mostly independent measurements are marginally related (e.g., by having used the same physical sample), provide options for incorporating uncertainties from that relationship into the analysis.
8. Currently, the auxiliary grid (Section III.A) is generated only once during the fitting procedure. When resonance energies are varied, and the values change significantly in early iterations, the original auxiliary grid may not be adequate. Implement an option to regenerate this grid for each iteration.
9. Currently, corrections for experimental effects in angular-distribution data are rather unsophisticated. Is there a need for improvement here?
10. Create a graphical user interface.
11. Introduce a modern configuration control and archival system for the code.
12. Introduce modern matrix-manipulation techniques, especially for very large runs. Preliminary studies have indicated that this will significantly reduce the time requirements for extremely large runs.