IV.E.6. Augmenting the Resonance Parameter Covariance Matrix

The posterior resonance parameter covariance matrix (RPCM) produced by SAMMY is a accurate representation of the uncertainties in the R-matrix evaluation.† Nevertheless, uncertainties for evaluated cross sections reproduced by propagating the RPCM have historically been regarded as "too small." In fact, cross section uncertainties based solely on the RPCM are indeed too small, because it is not possible for the RPCM to convey complete information concerning the evaluated cross section covariance matrix (ECSCM).

There are at least three reasons for this inability: (1) Computation of the RPCM is based on assumptions which are not fully valid. (2) Bayes' equation for the RPCM contains no information about the validity of the fit of theory to data. (3) The experimental data base is not unique. These three reasons are discussed more fully below.

(1) *Assumptions underlying computation of the RPCM*. The RPCM would indeed provide a complete description of the ECSCM, if all underlying assumptions of the evaluation procedure were to have no uncertainty associated with them. However, most underlying assumptions are suspect to some degree.

The most basic assumption is that R-matrix theory provides a correct and complete description of the interactions for which data are being evaluated. All resonances are included, even very small experimentally-invisible resonances and even the (infinite number of) resonances lying outside the energy region under analysis. All spin assignments are correct; there is no unresolved ambiguity. No direct components or other extensions to R-matrix theory exist. Further, everything has been calculated correctly; there are no bugs in the computer code.

Another important assumption is that all experimental conditions are properly understood and included in the analysis. Corrections are accurately made for Doppler and resolution broadening, multiple-scattering, normalization, and backgrounds. No corrections, however minor, have been omitted; each experiment is completely understood and correctly simulated in the code. Everything has been calculated correctly; there are no bugs in the computer code.

Clearly, not one of the assumptions listed in the previous two paragraphs is absolutely valid; each has some non-readily-quantifiable uncertainty associated with it. None of those uncertainties will be reflected in the RPCM.

(2) *Validity of the fit*. The non-iterative form of Bayes' equation for the RPCM can be written as

$$M' = \left(G^t V^{-1} G + M^{-1}\right)^{-1} \quad , \tag{1.1}$$

† This has been confirmed by at least two independent researchers, who compared the SAMMY-produced results with Monte-Carlo simulations. Unfortunately, neither of those studies has been published.

where M is the prior resonance parameter covariance matrix (usually assumed to be large or infinite, so that $M^{-1} \approx 0$), G is the sensitivity matrix (partial derivatives of theory with respect to the parameters), and V is the experimental data covariance matrix. Nowhere in this equation is there any information about the goodness of the fit between theory and measurement. Therefore the RPCM does not contain any information about poor fits, nor can it reflect any discrepancies among the various data sets.

(3) *Non-unique data base*. For every evaluation, the evaluator considers all available relevant measurements, and accepts or rejects each measurement based on his/her determination of the quality of the data. This determination is based on a study of the documentation for the measurement (e.g., whether or not sufficient information is provided to understand the uncertainties associated with the experiment) and on preliminary analyses of the individual data sets. The evaluator may find the need to renormalize the data, subtract a background, or rescale the energies for certain measurements in order to make them consistent with other measurements.

Even though the evaluator can and should attempt to incorporate all known uncertainties into the evaluation (e.g., including normalization uncertainty as a PUP parameter), there is no well-defined methodology for including uncertainties related to the choice of data base. Those uncertainties will therefore not be reflected in the output RPCM.

The logical conclusion is that the resonance parameter covariance matrix alone cannot provide complete information on the uncertainty in the evaluated cross section. Something else is clearly needed.

It is not obvious how one could quantize the effects described above. Nevertheless, the attempt should be made, and some approximate contribution be added to the ECSCM in addition to the contribution from the RPCM.

Historically, what has been done is to increase the RPCM in a rather arbitrary fashion, based on the nuclear data community's judgment of what the ECSCM should look like. For example, for the light element standards for ENDF/B-VI, the ESCSM uncertainties were adjusted upwards so that "… if a modern day experiment were performed today on a given standard using the best techniques, those results should fall within these expanded uncertainties (2/3 of the time)."[†]

For the first release of ENDF/B-VII and for early subsequent evaluations, the usual procedure was for the evaluator to increase either the diagonal elements of the RPCM or (more commonly) increase the uncertainties while maintaining the correlation matrix, while attempting to conform to the evaluator's opinion of what the multigroup cross section covariance matrix should look like. (Various options for accomplishing this task were implemented in SAMMY; these are described in Subsection IV.E.6.a.) This technique, however, is highly subjective and

[†] As quoted by A. D. Carlson at the 2002 Research Coordination Meeting of the IAEA Coordinated Research Project on light element standards.

awkward to use, as the link between the RPCM and the ESCSM (or multigroup covariance matrix) is sufficiently indirect that much trial-and-error is required to achieve the desired result.

More recently, it was recognized by Herve Derrien that normalization and/or background uncertainty components could be added to the RPCM component in order to provide a seemingly realistic description of the expected ECSCM. While these components certainly do not completely reflect all the various types of uncertainties discussed above, they nevertheless may provide a reasonable first approximation for the previously omitted components. The link between normalization and background uncertainty and ESCSM is direct, making this a more satisfying solution than arbitrary increases in the RPCM. An additional positive feature of this option is that it may be implemented directly into ENDF files, without new format requirements, by using ENDF File 33 normalization and background descriptions [NL07c].