

## A Systematic Description of the Generation of Covariance Matrices

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Although the importance of covariances has been recognized by the nuclear community, there appears to be limited understanding of the nature of covariances and the manner in which they contribute to the solution of physical problems. This paper is an attempt to provide a systematic description of the various sources of uncertainty, their contributions to covariance matrices (CMs), and the effect they may have on the calculated values and uncertainties of integral quantities such as  $k_{eff}$ .

Our intent is to elucidate some important, but often overlooked, properties of CMs. First, one must recognize that the set of quantities (data, parameters, etc.) associated with the CM must be specified in order for the term “covariance matrix” to be meaningful. For example, the CM associated with the energy-differential experimental cross section provides a measure of the uncertainty on each individual data point (cross section at a particular energy) and of the relationship (correlation) between those data points. In this paper, we discuss the various techniques used to determine realistic and appropriate CMs associated with quantities of interest at the many different stages of nuclear data processing, starting from measurement of energy-differential neutron cross sections through the final calculations of integral quantities. Emphasis is placed on the propagation of uncertainties through each step of the process.

Step 1: the data reduction process. We begin with the “raw data,” i.e., with the experiment which is intended to measure the differential cross section as a function of energy. For example, in neutron time-of-flight measurements, what the experiment actually measures is “number of counts” vs. “time of flight.” Various operations are used to convert from counts to cross section; for example, a background  $b$  is subtracted and the counts are normalized by a value  $a$  related to the duration of the experiment [1,2]. Values for  $b$  and  $a$  are measured by separate experiments; each has an associated uncertainty which the experimentalist can estimate. The uncertainties in  $b$  and  $a$  are propagated to the cross sections; that is, the uncertainty on the cross section has a component due to the uncertainty in  $b$  and another due to the uncertainty in  $a$ , as well as a component due to the measurement uncertainty. In addition, the cross-section uncertainty at one energy is related to the cross-section uncertainty at another energy via the uncertainties on  $b$  and  $a$ ; this relationship is described mathematically by the experimental-data CM.

Step 2: the data evaluation process. Neither the raw data nor the differential cross section is the appropriate quantity for use in nuclear reactor or transport calculations. Rather, what is needed is the *evaluated* cross section, which reflects the “best” measured cross section value and also the best theoretical knowledge both of the shape of the “true” cross section (e.g., R-matrix theory) and of the real-world modifications to the true cross section (e.g., resolution or Doppler broadening, finite-size effects, etc.). Sophisticated computer codes such as SAMMY [3] are used to determine a best-fit set of resonance parameters and the associated CM. This CM reflects all the experimental uncertainties from Step 1 and also includes uncertainties related to the corrections for real-world effects.

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The uncertainty in the model itself (i.e., R-matrix theory plus corrections) should also be incorporated at this stage, but to date very little effort has been made in this regard.

Step 3: conversion to pointwise cross sections plus covariance matrix. Processor codes such as AMPX [4] or NJOY [5] then calculate pointwise cross sections (i.e., cross sections as a function of energy) directly from the R-matrix parameters, on an energy grid which is sufficiently dense to define the structure in the cross section. The associated CM can also be generated, using the partial derivatives of the cross sections with respect to the resonance parameters to propagate uncertainty information stored in the resonance-parameter CM. The resulting pointwise cross section CM will, in general, bear little resemblance to the experimental data CM from Step 1, but it nevertheless incorporates the same information (plus much more, from Step 2).

Step 4: averaging to give multigroup cross section plus covariance matrix. The pointwise cross sections and associated CM are averaged using appropriate flux weighting to give multigroup cross sections and the associated CM. Two codes used for this purpose are PUFF [6] and ERRORJ [7]; SAMMY can also produce multigroup results.

Step 5: calculating integral quantities. The multigroup cross sections and associated CM found in Step 4 are then used to calculate  $k_{eff}$  (or other integral quantities). The mathematics is well understood for propagating the multigroup cross section CM, yielding a reasonable estimate for the nuclear data component of the uncertainty on  $k_{eff}$ . The statistical uncertainty associated with the Monte Carlo computation of  $k_{eff}$  is also well represented. Two additional components of the uncertainty are, however, generally omitted or ignored: (1) the uncertainty associated with the model used to calculate  $k_{eff}$ , and (2) the uncertainty associated with the use of multigroup cross sections rather than pointwise cross sections.

In the full paper, a simple example will be used to illustrate all steps of this process. Dangers inherent in ignoring the CM will be demonstrated. The effects of using rigorous vs. approximate CMs will also be examined.

## References

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