A Study of the Covariance Data in ENDF/B VIII.0 for Low Z Isotopes

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Abstract. Thirty group covariance data have been produced from ENDF/B VIII.0 MF 33 for H1, H2, He4, Li6, Li7, Be9, B10, B11, C12, C13, N15, O16, the JENDL O16 and F19. Multi-group cross section covariance data was produced by NJOY routine ERRORR. Negative eigenvalues were found only for F19, but the covariance constraints required for the condition of the sum of partial cross sections being equal to the resultant total cross section were found to be incorrect for H2, Li6, B10, C12, C13, and O16. An easy correction is suggested for Li6 and C13. An expansion of the ENDF-6 formats manual is suggested for the MF 33 chapter and a new proposed covariance normalization scheme is proposed.

1 Introduction

Thirty group covariance data have been produced for analysis and checking for H1, H2, He4, Li6, Li7, Be9, B10, B11, C12, C13, N15, O16, JENDL O16 and F19 (H3, He3, Be7, N14, O17, and O18 do not have any covariance data.) In processing these ENDF/B VIII.0 evaluations, cross section covariance data was produced from the data given in the MF 33 section. NJOY [1] routine ERRORR produces the multi-group covariances.

The standard Los Alamos “td” weighting function was used in the group collapse to 30 groups. Experience has shown that NJOY does not add any large negative eigenvalues while processing, though it can add some extra 0.0 eigenvalues. The 0.0 eigenvalues may assume small negative values due to numerical round-off.

A big combined covariance matrix was also assembled for each isotope. All the processing calculations used “absolute” covariance matrices, not relative covariances (i.e., relative to the means of the cross sections). Nor were correlation matrices (i.e. using covariances and the standard deviations of the cross sections) used. The big combined covariance matrix is important, since it would be used to generate replica cross section data and libraries for all of the reactions (at the same time) with covariance data.

2 Testing the Low Z Multi-group Covariance Data

Two methods were used to test the covariance matrices. An eigenvalue decomposition was performed on the big combined covariance matrix for each isotope. For example, the big covariance matrix for Be9 is 240x240 with the following reactions included – total (nt 1), elastic (mt 2), n2n (mt 16), ng (mt 102), np (mt 103), nd (mt 104), nt (mt 105), and nalpha (mt 107). Each sub-block of the big matrix is 30x30. Quite a few of the sub-blocks are 0.0.

All of the isotopes listed above except for F19 were free from any “large” negative eigenvalues. The negative eigenvalues were all close to 0.0 and several orders of magnitude smaller than the dominant large positive eigenvalues.

The largest negative eigenvalue in the 30g big combined F19 covariance data is worrisome because it is -0.003744... against a backdrop of the 3 largest eigenvalues being 0.264990..., 0.408761..., and 0.647917... This gives a ratio of only ~173, or only 2 orders of magnitude. Comparable ratios from all the other tested isotopes were all larger than 2.2e6, or 6 orders of magnitude. The 6 orders of magnitude is roughly equivalent to the limits of the single precision covariance data in the evaluation files.

The second test was a check of the covariance restraint imposed by having a total cross section and a bunch of partial cross sections which sum to the total cross section. This covariance constraint requires that the covariance block of the total cross section be equal to the sum of all the other cross sections’ covariance block matrices.

In gxg (i.e., groups by groups) sub-block matrix terms (assuming 4 reactions), the covariance constraints can be expressed as:

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The zeros on the RHS of the equations 1-4 are understood to be gxx matrices will all elements equal to or very nearly equal to 0.0. These covariance checks are quite easy to implement on a spreadsheet.

These sigma total covariance constraints are satisfied for all 30 groups for H1, He4, Li7, Be9, B11, N15, and the JENDL O16. They are satisfied ONLY in the higher energy groups (and NOT in the lower energy groups) for H2, B10, and C12. The common factor in the B10, C12, and O16 evaluations is that the covariance for inelastic (mt 4) is defined as a combination of all the other covariances. This feature is a very convenient evaluator option in the ENDF-6 format [2] for defining covariance data.

The problem is that inelastic (mt 4) cross sections exist only above some threshold energy (for C12, it is 4.812 MeV) – and are 0.0 at lower energies. Therefore, the covariances for inelastic (mt 4) cross sections must also be 0.0 at lower energies. This means that ERRORR in NJOY can NOT impose the covariance constraint on any cross sections in the lower energies with an inelastic (mt 4) covariance definition. Similarly, H2 hits a similar threshold limitation since its covariance constraints are defined with n2n (mt 16) cross sections.

The covariance data for H2, B10, and C12 is, in truth, more complicated than this simple explanation. There are layers of covariance definition built upon layers. Nevertheless, the essential problem is that cross sections of 0.0 (below some threshold) and with no uncertainty, are called upon to balance out the covariances from other reactions. It simply cannot be done.

Li6 and C13 have a different covariance constraint problem. They do not specify any cross terms between reactions. In fact, Li6 only specifies (within reaction) covariance data for elastic (mt 2) and nt (mt 105). C13 only specifies elastic (mt 2) and inelastic (mt 51). Therefore, any user would have to make some sort of assumption about the across reaction correlations to use these data to sample cross sections (otherwise, the sampled cross sections will not balance between total and the sum of the partials).

For example, the user could allow changes in elastic (mt 2) and then impose exactly the same changes (in magnitude) into the total (mt 1) cross sections. Such a common-sense approach preserves cross section balance. A more general approach would be to change the evaluation file to define covariance data for the total (mt 1) cross section in terms of the other cross sections.

### 3 The Relationship Between Different Covariance Constraints

The most well-known constraint occurs in fission chi data found in MF 5 and MF 35. Since multi-group chi values must sum to 1.0, any increase in a fission chi value for one group must be accompanied by a fission chi decrease in 1 or more other groups.

In a similar way, the multi-group covariance data for fission chi’s is also constrained. Specifically, if the covariances are in absolute form, then the sum of any row or column of fission chi covariances must be 0.0. This rule is mentioned in the ENDF-6 formats manual [2]. Without this constraint, replica values of the multi-group fission chi vectors generated from the covariances will not sum to 1.0.

Also, there is a renormalization formula given for fission chi covariances which is designed to eliminate small round-off type errors by normalization. The formula does not magically create normalized good data from bad data; such an attempt would only produce normalized bad data.

The covariance constraint discussed in this paper is a constraint related to the total cross section being equal to the sum of all its partial cross sections in sections MF 3 and MF 33.

These two covariance constraints (fission chi and sigma total) are related through a transformation matrix in the general form of an identity matrix. Assume that the total covariance blocks are in the leftmost and topmost blocks of the big combined covariance matrix. Then the transformation matrix is an identity matrix which has -1’s along the diagonal of the first (gxx) block of the big combined matrix and +1’s along the diagonal of the other main diagonal blocks.

For a 4-reaction system, with sigma total in the top row and left column, the transformation looks like this:

\[
\begin{bmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

Where the [] entries are assumed to be gxx, and the -1 or +1 are diagonal only entries.

This transformation matrix is a square root of the identity matrix. So, it can be pre- and post-multiplied into any matrix without changing the eigenvalues.
However, several of the signs of the eigenvector elements are changed.

By pre- and post-multiplying this transformation matrix into a big combined covariance matrix with the sigma total constraint, the matrix is transformed into a form of covariance matrix like the fission chi constraint. That is, the covariance constraints are changed from the form of equations 1-4 to a form in which the well-known zero sum and/or zero column rules apply.

For a four reaction system (total, elastic, inelastic, and n2n), the transformation changes the matrix from:

\[
\begin{bmatrix}
\text{Cov1,1} & \text{Cov2,1} & \text{Cov4,1} & \text{Cov16,1} \\
\text{Cov1,2} & \text{Cov2,2} & \text{Cov4,2} & \text{Cov16,2} \\
\text{Cov1,4} & \text{Cov2,4} & \text{Cov4,4} & \text{Cov16,4} \\
\text{Cov1,16} & \text{Cov2,16} & \text{Cov4,16} & \text{Cov16,16}
\end{bmatrix}
\]

\[\text{(6)}\]

where Covnm is a g\times g covariance matrix,

to the following: (note the sign changes)

\[
\begin{bmatrix}
\text{Cov1,1} & -\text{Cov2,1} & -\text{Cov4,1} & -\text{Cov16,1} \\
-\text{Cov1,2} & \text{Cov2,2} & \text{Cov4,2} & \text{Cov16,2} \\
-\text{Cov1,4} & \text{Cov2,4} & \text{Cov4,4} & \text{Cov16,4} \\
-\text{Cov1,16} & \text{Cov2,16} & \text{Cov4,16} & \text{Cov16,16}
\end{bmatrix}
\]

\[\text{(7)}\]

Since the total cross section covariances are in the leftmost row and topmost column, a visual inspection of the form of equation 7 verifies that the sum of the elements of any row or column must be 0.0.

A further pre- and post-multiplication operation will change this big combined matrix in the form of equation 7 back to its original form of equation 6.

Therefore, the ENDF-6 normalization procedure for fission chi covariance data can be applied to sigma total covariance data – after the sigma total covariance data has been transformed into the fission chi form (equation 7). When the normalization has been completed, then pre- and post-multiply the normalized matrix by the transformation again to produce the final normalized sigma total covariance matrix in the form of equation 6.

A numerical sample problem verifying this procedure, as well as other aspects of correlated random sampling, is available as a tutorial document [3].

Like the fission chi normalization procedure, this sigma total covariance matrix procedure is not designed to produce good data from bad data – it is only designed to normalize good data with some small errors into normalized covariance data. Any attempt to use this normalization procedure on bad data will only produce normalized bad data.

Both normalization procedures will also produce at least one 0.0 eigenvalue because one of the elements of any row or column is redundant due to the covariance constraints.

It should also be noted that the fission chi normalization formula given in the ENDF-6 formats manual is a form of “full normalization” (FN) discussed elsewhere [4]. In fact, the ENDF-6 formula is explicitly called out as a simplified form of FN normalization. Compare Equation. 35.2 from reference [2] with Equation 38 of reference [4].

It is proposed that the ENDF-6 manual [2] should be extended in Chapter 33 to include this broader understanding of sigma total covariance constraints and covariance normalization.

4 Summary

An extensive verification test of evaluated low Z reaction rate covariances in ENDF/B VIII.0 has been carried out at Los Alamos. The good news was that there was only 1 significant negative eigenvalue (in F19) in the covariance data sets. The bad news was that some of the low Z data sets do not preserve the covariance constraint condition that the total (nt 1) covariance matrix must be equal to the sum of all the partial cross section covariances.

The MF 33 covariance data for H2, B10, C12, and O16 should be revisited and corrected. Likewise, the covariance data for Li6 and C13 should be revisited, and some simple fixes have been proposed.

An expanded discussion of covariance constraints and covariance renormalizations has also been presented which should be included into the next revision of chapter 33 of the ENDF-6 formats manual.

References