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

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Outline

- Background Theoretical Notes
- Procedure Used to Generate and Test Multi-Group Low Z MF33 Covariances
- Results of the Testing
  - Easy fixes for some of the ENDF/B VIII data
  - Rejection of some of the ENDF/B VIII data
- Relationship between the χ and the $\sum_{total}$ Covariance Constraints
- A Proposed Covariance Renormalization Procedure for $\sum_{total}$ Covariance Constraints
  - *Should be incorporated into the ENDF-6 Formats Manual Chapter 33*

Some Background Theory to Remember

- Just as $\sum_{totalg}$ = the sum of the partial MF3 cross sections;
  - so must the covariance of $\sum_{totalg}$ = the sum of the covariances of partial MF3 cross sections. I call this the $\sum_{total}$ covariance constraint. It is not explicitly mentioned in the ENDF-6 Formats Manual, but it is implicitly assumed in the formats for MF 33.
- The χ covariance constraint occurs with fission chi multi-group data (which must sum to 1.0) and leads to the zero-sum and zero-column rules for groupwise fission chi covariances. See MF35 and Chapter 35 of the ENDF-6 Format manual.
- What happens when these covariance constraints are not enforced?
  - Replica groupwise χ data does not sum to 1.0
  - Replica groupwise Cross section data does not obey total = the sum of the partials

- An "involutary" matrix is a square matrix which is its own inverse
  - the identity matrix is a simple example
  - Also, the identity matrix with a -1 in the top left position (instead of +1) and +1's in all the other locations

- The identity matrix has an infinite number of square roots
  - We will see that this implies an infinite number of ways to renormalize either the χ or $\sum_{total}$ covariance data.

Procedure

- Process the MF 33 covariance data from all the low Z (thru F19) isotopes in ENDF/B VIII using NJOY (ERRORR module)
  - H3, He3, Be7, **N14**, O17, and O18 do not have any covariance data
- Produce 30g absolute covariance matrices for all the given cross sections including reaction to reaction cross terms
  - NJOY processing does **NOT** cause large negative eigenvalues, though it can add 0.0's.
    - *(Process the original covariance data in the original evaluation energy intervals as groups in NJOY)*
- Assemble a super covariance matrix of 30g x 30g blocks of covariance data. It must be symmetric across the main diagonal.
- Check the super matrix: (*using MATLAB*)
  - Any large negative eigenvalues? *(remember that a valid covariance matrix must be non-negative definite – i.e., all eigenvalues positive or zero)*
  - Verify the cov($\sum_{total}$)= the sum of cov's for all the partial MF3 cross sections.

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ENDF-6 Format Feature which uses MF33 $\sum_{total}$ Covariance Constraint Specification

- 33.2.2.1 NC-type Sub-Subsections with LTY=0
- Here is a sample for C12 (ID=625) in MF 33 covariance data
- Cov(mt4) = Cov(mt1)-Cov(mt2)-Cov(mt28)-Cov(mt102)-Cov(mt103)-Cov(mt104)-Cov(mt107) for the energy range 4.812 to 20 MeV

```
 6012.00000 11.8936500          0          0          0          1 62533  4
 0.000000+0 0.000000+0          0          4          1          1 62533  4
 0.000000+0 0.000000+0          0          0          0          0 62533  4
 4.812000+6 2.000000+7          0          0         14          7 62533  4
 1.000000+0 1.000000+0-1.000000+0 2.000000+0-1.000000+0 2.800000+1 62533  4
-1.000000+0 1.020000+2-1.000000+0 1.030000+2-1.000000+0 1.040000+2 62533  4
-1.000000+0 1.070000+2                                             62533  4
 0.000000+0 0.000000+0          1          5          6          3 62533  4
 1.000000-5 4.812000+6 1.500000+8 0.000000+0 0.000000+0 0.000000+0 62533  4
```

However, There is a "Gotcha" in this Otherwise Very Convenient Format Feature for MF 33 Data

- Some MT reactions have threshold energies and a cross section of 0.0 below that energy.
- The 0.0 is understood to have no uncertainty, i.e., it is a hard 0.0.

- Therefore, reactions with thresholds (e.g., inelastic, n2n, …) **SHOULD NOT** be used as the covariance defined in terms of other covariances in the energy ranges where the cross section is 0.0. Reactions without thresholds (e.g., total, elastic, ...) should be used instead.

  – This is the main problem with H2, B10, C12, and O16 covariance data in ENDF/B VIII

Summary Table of Covariance Testing Results

isotope	MF 33 covariance mt's	meets the Sigma-total constraint	any large negative eigenvalues	notes
H1	1,2,102	yes	no	uses mt 1 sum
H2	1,2,16,102	**no**	no	**shouldn't use mt 16 for constraint**
He4	1,2	yes	no	uses mt 1 sum
Li6	2,105	**no**	no	**could use mt 1 = sum**
Li7	1,2,4,25,102,104,851	yes	no	uses mt 2 sum + more
Be9	1,2,16,102,103,104,105,107	yes	no	uses mt 2 sum
B10	1,2,4,102,102,104,113,800,801	**no**	no	**shouldn't use mt 4 for constraint**
B11	1,2,4,16,22,28,102,103,105,107	yes	no	uses mt 2 sum
C12	1,2,4,51,102,103,104,107	**no**	no	**shouldn't use mt 4 for constraint**
C13	2,51	**no**	no	**could use mt 1 = sum**
N15	1,2,4,16,22,28,102,103,104,105,107	yes	no	uses mt 2 sum
O16	1,2,4,16,22,23,28,102,103,104,105,107,108	**no**	no	**shouldn't use mt 4 for constraint**
JO16	1,2,4,16,22,28,102,103,104,107	yes	no	uses mt 2 sum
F19	1,2,4,16,22,28,102,103,104,105,107	yes	yes	uses mt 2 sum

Details of the problems with H2, B10, C12, and O16

- For H2, B10, and C12
  - Cov(MT1) is full
  - Cross terms for Cov(MT1) to Cov(MT4) or Cov(MT16) are only defined at energies > threshold
    - No other covariance matrix data for covariance cross terms involving MT1
    - Cov(MT1) to Cov(MT2) could be very useful
  - Therefore: $\sum_{total}$ Covariance Constraint is satisfied only at energies > threshold
  - is **NOT** satisfied at energies < threshold

- For O16
  - Cov(MT1) is full
  - Cross Terms involving Cov(MT1) are only available for Cov(MT4)
    - No other covariance matrix data available for cross terms involving MT1
    - Cov(MT1) to Cov(MT2) could be very useful
  - Cov(MT4) is full (**oops**, there should be an energy threshold!)
  - What is the actual uncertainty of a hard 0.0 cross section? (zero!)
  - Therefore: the $\sum_{total}$ Covariance Constraint is **NOT** satisfied < threshold

The χ Covariance Renormalization Formula is already in the ENDF-6 Format Manual …

- See MF 35 or Chapter 35 (eqtn 35.2) in the ENDF-6 Format Manual
- Uses Absolute Covariance Matrices
- The "zero-sum" and "zero-column" rule are a multi-group manifestation of this χ Covariance Constraint
- At least 1 eigenvalue should be 0.

- Compare with the Perko paper – this ENDF-6 procedure is identical with FN or "Full Normalization" (see eqtn 38), and it forces machine precision compliance with the "zero-sum" and "zero-column" rules and also a hard 0 eigenvalue. This procedure does not fix bad data; it only normalizes pretty good data to satisfy the covariance constraints exactly.
- Other normalization procedures are also available; "partial", "control parameter", etc.
- Normalization is "idempotent" – only do it once, further iterations do not change anything

- *Perko et al, "Ambiguities in the Sensitivity and Uncertainty Analysis of Reactor Physics Problems involving Constrained Quantities",* ***NSE****, 180:3, 345-377, 2015.*

ENDF-6 Manual (MF 35)

If the above constraint has not been applied in the evaluation process, corrected values $\widehat{F}_{k,k'}$ may be obtained from the following relation:

$$\widehat{F}_{k,k'} = F_{k,k'} - S_k Y_{k'} - S_{k'} Y_k + Y_k Y_{k'} \sum_j S_j . \qquad (35.2)$$

The correction is applicable not only to the covariance matrix in the ENDF file, but also to derived covariance matrices (for example, after processing and condensation on the user's energy grid).

Perko paper

The usual fission spectrum covariance normalization procedure is a special case of Eq. (37). To see this, one needs to consider a linear constraint of $C_f(\underline{\alpha}) = \underline{W}^T \underline{\alpha} = C^0$ and full normalization [i.e., Eq. (17)]. In this case the correction formula, i.e., the (i,j)'th element of the normalized covariance matrix, is

$$\left[\underline{\underline{C}}^{FN}_{\vec{\alpha}}\right]_{i,j} = \left[\underline{\underline{C}}_{\vec{\alpha}}\right]_{i,j} - \frac{\alpha_i^0}{C^0} \sum_{k=1}^{N} \left[\underline{\underline{C}}_{\vec{\alpha}}\right]_{k,j} W_k - \frac{\alpha_j^0}{C^0} \sum_{k=1}^{N} \left[\underline{\underline{C}}_{\vec{\alpha}}\right]_{i,k} W_k + \frac{\alpha_i^0 \alpha_j^0}{(C^0)^2} \sum_{k=1}^{N} \sum_{l=1}^{N} \left[\underline{\underline{C}}_{\vec{\alpha}}\right]_{k,l} W_k W_l . \qquad (38)$$

Substituting $W_i = 1, \ \alpha_i^0 = \chi_i \ \ \forall \ \ i = 1, \ldots, N$, and $C^0 = 1$ into Eq. (38) yields a formula that is identical to the ENDF/B-6 Manual suggestion for the fission spectrum covariance matrix normalization [Eq. (35.2) of Ref. 28].

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New Result for Renormalizing an Abs. Cov. Matrix with the $\sum_{Total}$ Constraint (MF 33)

- Assume that the **sigma total block** is in the leftmost column and the topmost row
- Define a transformation (permutation?) matrix from the identity matrix (assume total and 3 partial cross sections, and each 4x4 matrix entry below represents a groups x groups block matrix.)
- **This "mult" transformation converts a $\sum_{total}$ constraint form into a χ constraint form (and vice versa, like a toggle switch)**

$$\text{mult} = \begin{matrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{matrix}$$

[mult] * [mult] = the identity matrix
[mult] is a square root of the identity matrix
[mult] is an involutory matrix

Simple Visualization of the "mult" Process

- Original Super Block Matrix – even number of mult iterations
  - (with total (1), elastic (2), inelastic (4), and n2n (16))
  - (should obey left value = the rest of the row, and top value = the rest of the column)

Cov11	Cov21	Cov41	Cov161
Cov12	Cov22	Cov42	Cov162
Cov14	Cov24	Cov44	Cov164
Cov116	Cov216	Cov416	Cov1616

- Intermediate Super Block Matrix – odd number of mult iterations
  - (should obey "zero-sum" and "zero-column" rules)

Cov11	-Cov21	-Cov41	-Cov161
-Cov12	Cov22	Cov42	Cov162
-Cov14	Cov24	Cov44	Cov164
-Cov116	Cov216	Cov416	Cov1616

- The Whole Renormalization Process was Verified Numerically in MATLAB

New Result for Renormalizing an Abs. Cov. Matrix with the $\sum_{Total}$ Constraint (MF 33) – Continued

- Perform the full multiplication:
  - [mult] * [an abs cov matrix which needs a sigma total constraint] * [mult]
- Apply the already existing χ renormalization procedure (i.e., FN or Full Normalization) – because this intermediate matrix needs to comply with the zero-sum and zero-column rule. (The FN procedure is not unique.)
  - Eqtn 35.2 from the ENDF-6 manual –or– Eqtn 38 from the Perko paper
- Perform a second full multiplication on the result of the renormalization procedure
  - [mult] * [an abs cov matrix which has an exact χ constraint] * [mult]
  - which gives **[an abs cov matrix with an exact $\sum_{total}$ constraint]**

- *This procedure should probably be added to the ENDF-6 formats manual in the MF 33 section*
- **Like the MF 35 procedure, this does not fix large negative eigenvalues or bad data, it only enforces the $\sum_{total}$ covariance constraint of pretty good data to machine precision and forces a hard zero eigenvalue. The normalization is also idempotent. (i.e., a second normalization does not change anything)**

Summary

- Good News
  - Low-Z Covariance data in ENDF/B VIII MF33 does NOT have large negative eigenvalue problems (except F19)
  - Some of the Low-Z Covariance data is just fine
  - Li6 and C13 can be easily fixed by defining MT 1 as the sum of the partial covariances

- Bad News
  - Some of the data is not (yet) available, e.g., N14
  - D2, B10, C12, and O16 MF 33 covariance data must be rejected
    - They do not comply with the $\sum_{total}$ Covariance Constraint

- CSEWG ENDF-6 Format Follow-up
  - Include the proposed MF33 Covariance Renormalization Procedure
    - Analogous to the MF35 Procedure already in place