OAK RIDGE National Laboratory

ENDF/B-VIII.1 Validation: Covariance

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Work flow

- Use ExSite to generate templates to make inputs (1-D data and puff)
- By default PUFF corrects for $|\text{correlation}| > 1$, but this can be switched off
- Use cadillac to combine all ENDF covariances into a library
- Use cognac to correct
- Use covcomp to compare with existing covariance library
- Also can use covcomp to assess effect of corrections.

Inconsistencies in the ENDF files

- 54Cr LRF=3 in File 2 and LRF=7 in File 32 (corrected after Beta 1)
- Cross material covariance data:
- **Au197**:
  - Has cross covariances U235, U238 and Pu239
    But only U233 has the requisite covariance
- **U233**
  - Has cross covariance with U235, U238, Pu239, Pu240, Pu241
    But none of these materials have the requisite cross covariances
- **U235**
  - Has cross covariances with Au197, Li6, U238, Pu239
    But none of these materials have the requisite cross covariances

Derived matrices

- Matrices can be denoted as derived (LTY=0), for example:
  Total = sum over all other cross sections : $\sigma_x = \sum_i c_i \sigma_i$
- The covariance the is given as: $\langle \sigma_t^m, \sigma_t^n \rangle = \sum_{i,j} c_i c_j \langle \sigma_i^m, \sigma_j^n \rangle$ which also applies cross correlation between this redundant cross section and all between all constituents.
- The ENDF format allow to define a cross section as redundant in some energy range only and be part of another redundant cross section in another range.
- There are several cases in Beta 1, where there are two layers of redundance:
  - For example, O16:
    MT=4 = 1 - 16 - 22 - 23 - 28 - 32 - 41 - 44 - 45 - 102 - 103 - 104 - 105 - 106 - 107 - 108 - 112 (whole range
    MT=103 = 600 + 601 + 602 + 603 (whole range)
    MT=104 = 650 + 651 + ... + 659 (whole range)
    MT=104 = 700 + 701 + ...+ 749 (whole range)
- If it is given over the same range, a processing code can just simply internally change the sum for, MT=4 = 1 - 16 - 22 - 23 - 28 - 32 - 41 - 44 - 45 - 102 – (600 + 601 + 602 + 603) – (650 + 651 + ... + 659) -…
- If the ranges don't overlap, this definition is not consistent, it. Would be better for the evaluator to give the explicit summation
- PUFF has been changed to do the above substitution and throw and error if the ranges are incompatible.

Lumped Reactions

Process ENDF data file with PUFF

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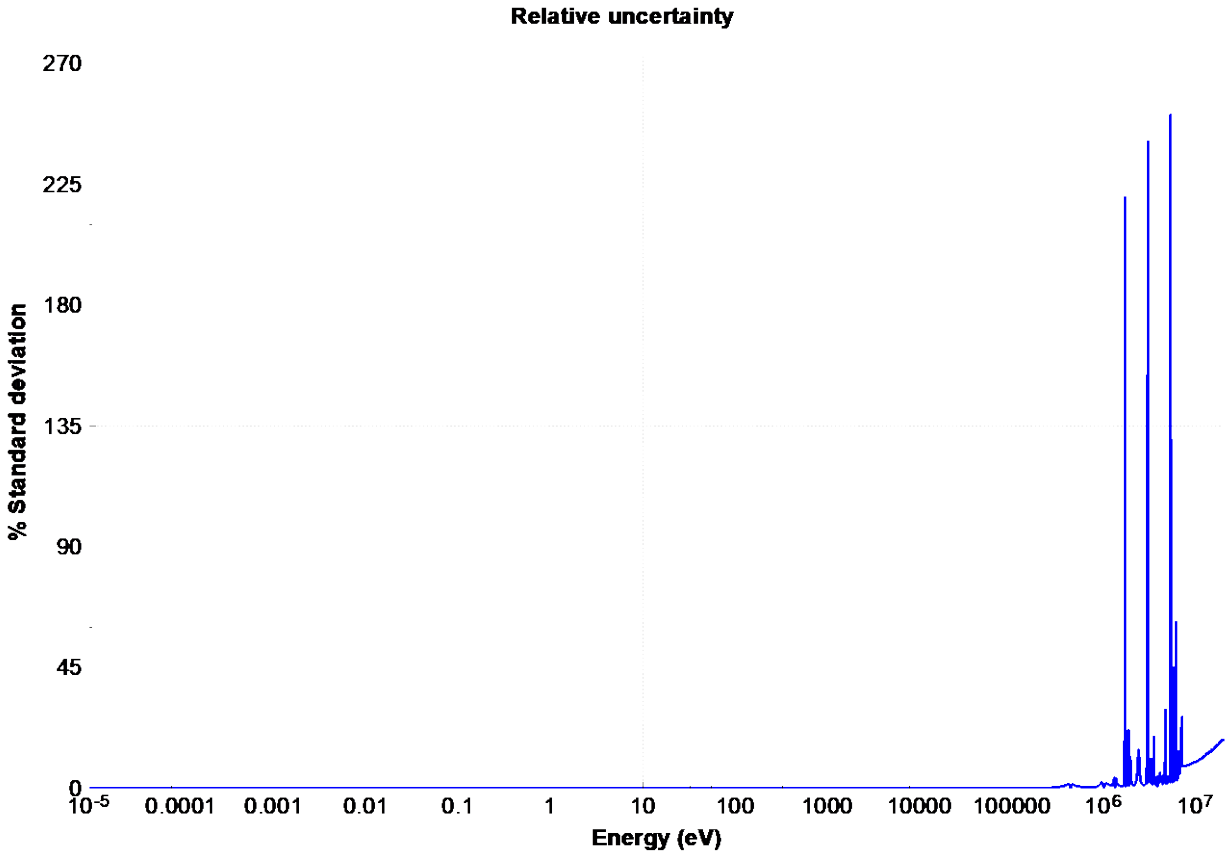
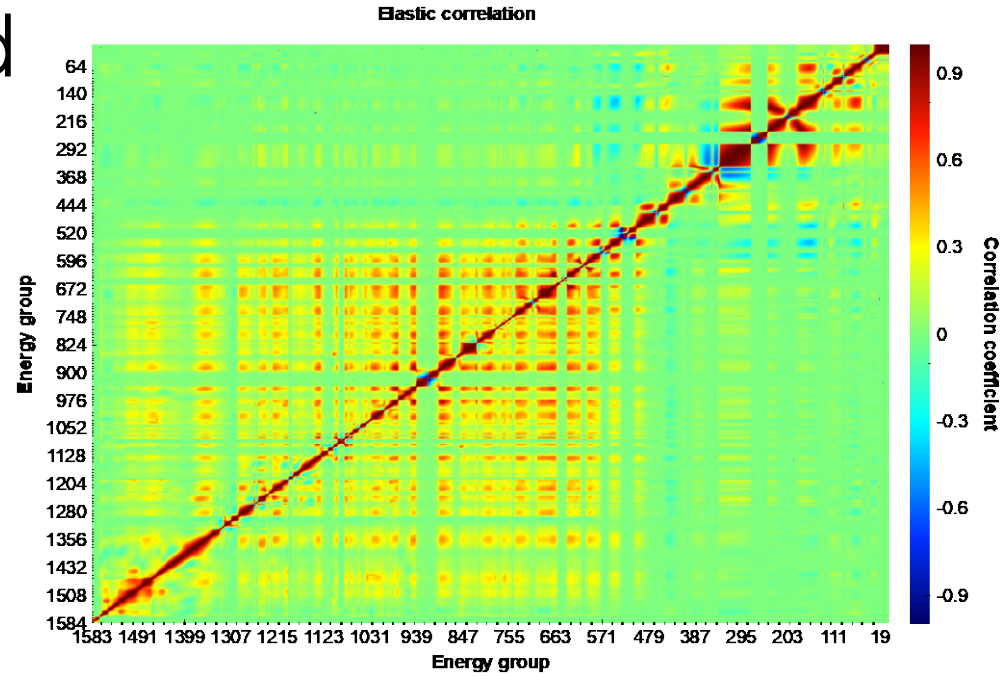
- Expand all File 31 and File 33 covariance to super-grid (all evaluator energy grids plus user group structure)
- Convert to absolute covariance as needed. This will allow to add the matrices. At this point there can still be two or more covariance for each pair of material and reaction, for example one covariance in the fast and one in the resolved.
- Add them to
- Check that there are not correlation greater than 1 or smaller than -1. Reset as needed

Affected:

- ^{19}F <4,22>, <16,22>, <22,28>. All smaller than |1.13|
- ^{7}Li <4,851> (851 = lumped reaction = 16 + 24. Correlation is 1.5 for one matrix element.
- ^{16}O <2,2> Correlation and uncertainties for some groups are huge, see plots
- ^{239}Pu <456. 456> All smaller than |2.04|

^{16}O elastic on the evaluator grid





<51,1621> = 23509.5
<51,1622> = 286378
<52,978> = 23289.1
<52,979> = 362877
<53,978> = 23289.1
<53,979> = 362877
<54,978> = 23289.1
<54,979> = 362877
<62,749> = 24.0086
<63,1264> = 84645.8
<63,1265> = 2.24205e+06
<239,1189> = 54853.7

Process ENDF data file with PUFF cont.

- Add all matrices together
- Calculate all sum and ratio matrices
- Check that there are not correlation greater than 1 or smaller than -1. Reset as needed

Affected:

- MT=5 (defined as 1 – 2) in ^{12}C
- MT=2 (defined as 1 – 5 – 851) in 7Li (851 = 16 + 24)

Note: PUFF also has an option to delete covariance matrices with correlation > 1 or < -1. The assumption is that correcting the correlation can make the matrix highly non-positive definite.

Note: Puff reports that it has corrected data after each of these steps, but it only lists the matrices for which the correction happened.

However, correction can be switched off and results with and without correction on the super grid can be compared with covcomp.

Correct data with cognac

We correct for relative uncertainty >1, which can happen for threshold reactions at threshold due to numerics (small cross sections, relative uncertainty).

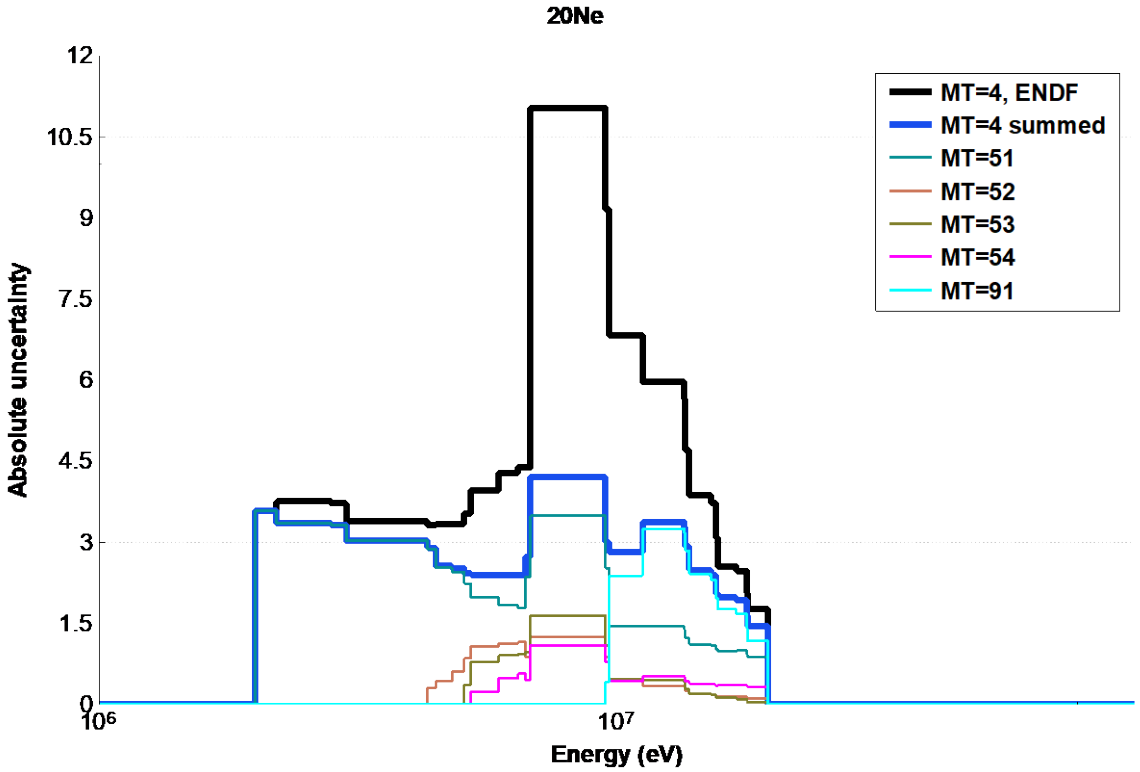
In ENDF/B-VIII.1 there are also many corrections for non-threshold reactions. Cognac lists the reactions for which the uncertainties have been updated

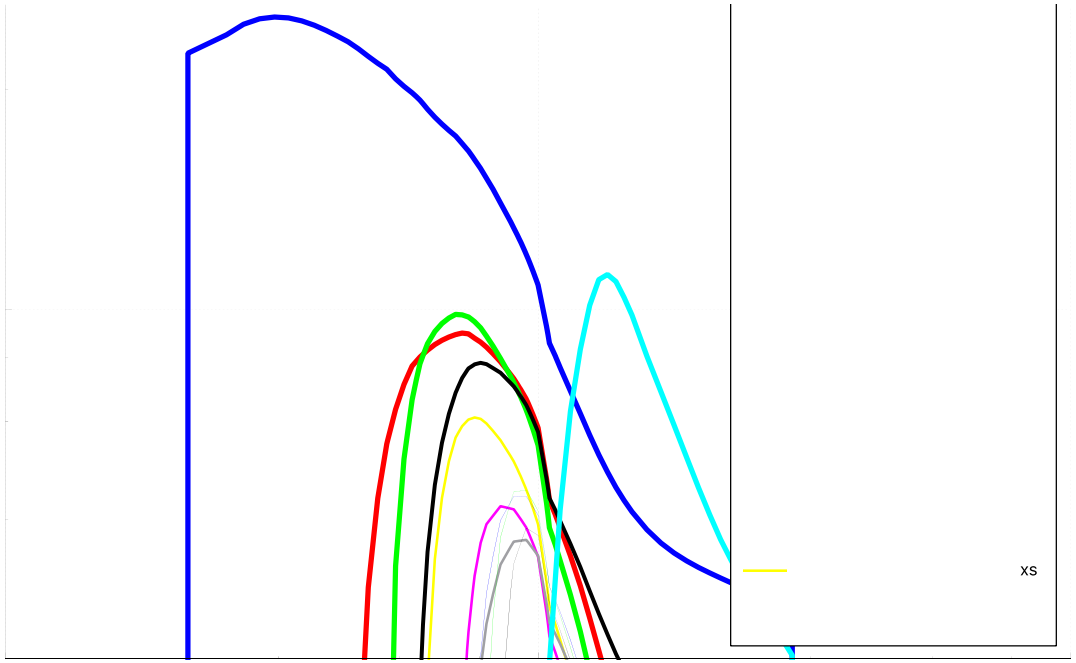
If uncertainty exist for higher energies, but not for lower energies, for which cross section exist, we extend the diagonal on the covariance done to lower energies.
Affected:

- mat=26054 mt=1, 2, 102
- mat=40094 mt=1
- mat=79197 mt=1
- mat=90232 mt=18
- mat=93237 mt=456, 452, 1, 2, 18, 102,
- mat=94238 mt=1, 18

Note: More detailed differences can be retrieved using covcomp to compare covariance library before and after correction by cognac.

Redundant covariance are not consistent cont.





- MT=4 is given in File 33, as are MT=51,52,53,54, 91. But covariances for the other discrete inelastic data are not given.
- MT=4 recalculated is out of sync with the one in ENDF (missing covariances). Could be solved by giving a covariance for a lumped reaction of 55 +.. + 72.
- Why it matters: Using data in codes like SAMPLER will not correctly perturb all discrete inelastic

Redundant covariance are not consistent cont.

Isotopes where MT=4 is inconsistent for this above reason:

- 20Ne, 21Ne, 22Ne, 37Ar, 41Ar, 45Ca, 47Ca, 51Cr, 54Mn, 56Mn, 75Se, 81Kr, 93Mo, 98Tc, 97Ru, 109Cd 143Pm, 144Pm, 145Pm, 145Sm, 191Os, 192Os, 190Pt, 191Pt, 192Pt, 193Pt, 194Pt, 195Pt, 196Pt, 197Pt, 198Pt, 203Hg, 204Tl. 205Pb, 208Po, 210Po

Total covariance on ENDF file is not directly used in SCALE, but internally resumed from partial covariance data.

However, there are some inconsistencies in the ENDF files regarding covariance data for total cross sections.

- Zr94: Covariance for MT=1 only has data for E >= $9 * 10^4$, MT=2 and 102 have data starting at $1*10^{-5}$.