

Generating covariance libraries with AMPX

D. Wiarda

M. L. Williams

B. J. Marshall



Outline

- Quick guide to making a covariance library
- What ENDF provides
- SCALE covariance library
- AMPX process cross section covariance matrices
- Resonance range covariance matrices

For the impatient

- Generate an XML listing from the desired ENDF files using ExSite
- Generate a template file containing input for:
 - **point1d**: broadens point-wise cross section data to desired temperature
 - **puff**: generates covariance matrices from ENDF on the user-defined grid
 - **combine_cov**: combines the files for each nuclide generated in the last step into a library (including cross reaction and cross material covariance matrices)
- Expand the templates using ExSite
- Run the input files (in order) generated in the last step
- Run **cognac** to correct the library and/or remove certain reactions

For the impatient (continued)

- The SCALE recommended covariance library has covariance information (low-fi) for more nuclides than are usually given in ENDF
- If the new library is generated on the same energy grid as the SCALE covariance library (56 or 252 neutron groups), cadillac can be used to add SCALE covariance information for any nuclide and reaction not included from ENDF
- Fulcrum can be used to view the COVERX formatted covariance library
- cognac has an option to print a text version of the COVERX library (not to be confused with the COVERX library in ASCII format)

Covariance data for thermal moderators

- In SCALE, thermal moderators like H in H₂O have a special ID. The fast region repeats the cross section data from H
- Therefore, covariance information for the fast evaluations must be repeated for the thermal moderators
- If generating the XML listing:
Include ENDF files for thermal moderators and update the configuration file for the listing

Corrections applied to SCALE covariance libraries

The following corrections are applied by cognac:

- All redundant covariance matrices are removed: for example, if $\langle 1,2 \rangle$ and $\langle 2,1 \rangle$ are present, only $\langle 1,2 \rangle$ is retained
- Cross section data without covariance information are removed
- Relative uncertainties larger than 1 are set to 1
- Correlation values with absolute values larger than 1 are set to +1 or -1
- If a higher energy group has uncertainty data and the lower energy groups do not (but they do have non-zero cross section data), then diagonal elements of the covariance matrix are extended

cognac prints a summary of the corrections that were applied

Comparing data in your new library with SCALE

- Use covcomp to compare two covariance libraries
- Before comparing, ensure that
 - All uncertainties will be converted to relative uncertainties
 - All covariance matrices will be converted to correlation matrices

```

The following cross section data are missing on the right coverx file
-----
      4007      2
      4007      1
      4007     103
      ...
     1092235     16
The following matrices are missing on the right coverx file
-----
      4007      2      4007      2
      4007      1      4007      1
      ...
     1092235      4     1092235      2
     1092235     16     1092235      2

Differences in relative uncertainty for cross section 8016 mt =2
  1 5.70708e-02 1.71275e-02 6.99890e-01
  2 1.14614e-02 1.44984e-02 2.64978e-01
  ..
 19 2.27706e-01 4.56564e-01 1.00506e+00

Differences in correlation *1000 for Matrix 8016 2 8016 2
  Row      Column      left      right difference
  1         2           73         29         44
  1         3           62          0         62
  1         4            9          0          9
  1         6           -3          0          3
  1         7            9          0          9
  1         8          -10          0         10
  1         9          -19          0         19
  1        10          -11          0         11
    
```

```

1 =shell
2 cp /Users/dw8/scale_data/data/scale.rev08.252groupcov7.1 scalelibrary
3 cp ${RTNDIR}/newLibrary library
4 end
5 =covcomp
6 left=scalelibrary right=newlibrary out=compar eps=1.0E-5 corr=0.002
7 end
    
```

Configure covcomp

Use: left

Name of the first file to be compared

Use: right

Name of the second file to be compared

Use: out

Name of the output file if desired

Use: eps

Precision to which to compare cross section data and uncertainties

Use: corr

Precision to which to correlation matrix elements are compared

OK Cancel

What ENDF provides

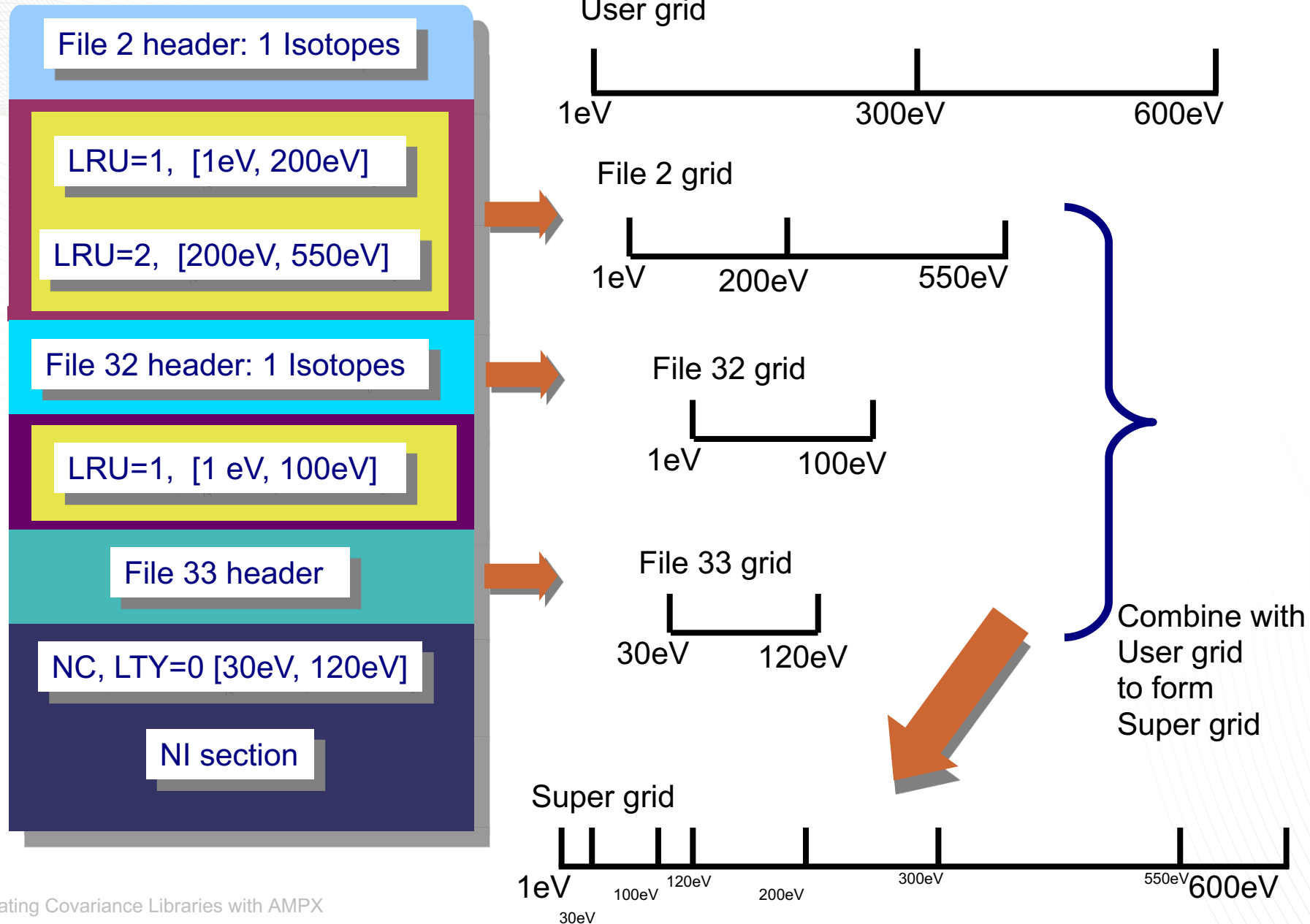
- Point-wise cross section covariance matrices in File 31 and File 33
 - The grid is fairly coarse, and on the grid, the data are given as a histogram
 - Data are stored in ENDF ASCII format: that is, with 11 digits per floating point number. **This often means the covariance matrix is no longer positive definite due to insufficient precision**
- Covariance matrix for resonance parameters in the resolved and unresolved range
 - Since there can be many resonance parameters, this matrix can be very large
- Covariance matrices for exit energy distribution for fission reaction (Chi)
 - This is given for a few incident energies and is to be treated as a histogram between incident energies
 - No correlation between incident energies is allowed
- In a few cases, covariance matrices are used for angular distributions, but they are not currently processed by PUFF
- For most of the covariance matrices, there is more than one format to allow for compression, which makes processing more difficult

SCALE-6.2 Covariance Library

- The SCALE-6.2 covariance library includes:
 - ENDF/B-VII.1 for 187 isotopes, SCALE-6.1 data (mainly Lo-Fi) retained for ~215 missing nuclides
 - Chi uncertainties (file 35) processed from ENDF/B-VII.1
 - Chi uncertainties from JENDL4.0 for ^{241}Am , ^{242}Am , ^{243}Am , ^{244}Am , ^{237}Np , ^{231}Pa , ^{233}Pa , ^{241}Pu , ^{232}Th , ^{233}U , ^{234}U , ^{236}U , ^{237}U
 - Updated thermal capture values for ^{255}Eu , ^{147}Pm , ^{103}Rh , ^{149}Sm , ^{151}Sm (to be equal to Atlas values)

SCALE sensitivity tools currently only use the following reactions: 1, 2, 4, 16, 18, 102, 103, 104, 105, 106, 107, 452, 455, 456

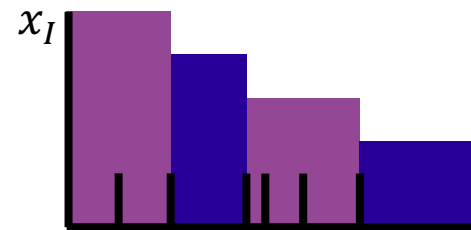
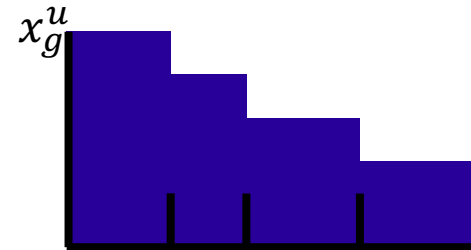
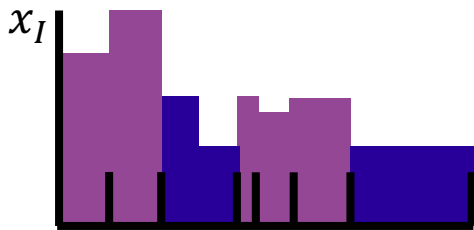
Generating a union grid for use in PUFF



PUFF options for cross section data

Point-wise covariances in ENDF are often given as relative uncertainties; therefore, the cross section is needed on the union grid

- The cross section is given in point-wise form
- The multigroup (MG) cross section can be correctly group-averaged on a union grid

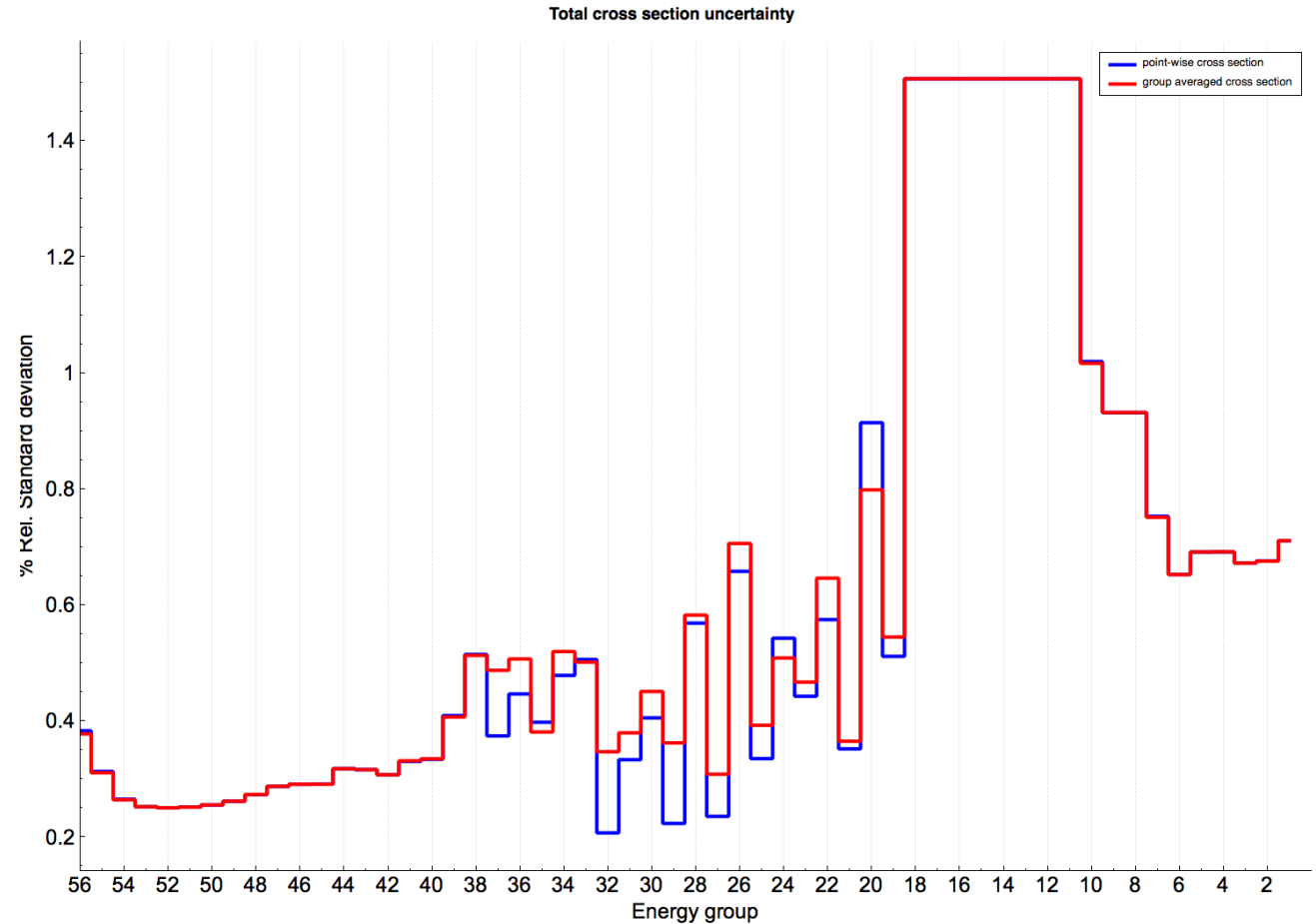


The cross section is given in MG form: the best approach is to assume the same cross section on the union grid

- The same applies for the flux
- PUFF allows both options for cross section and flux

Cross section options for ^{235}U

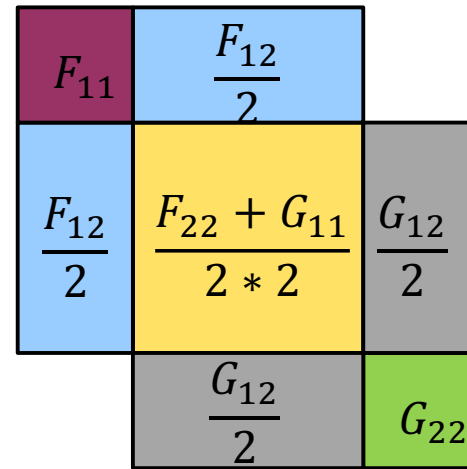
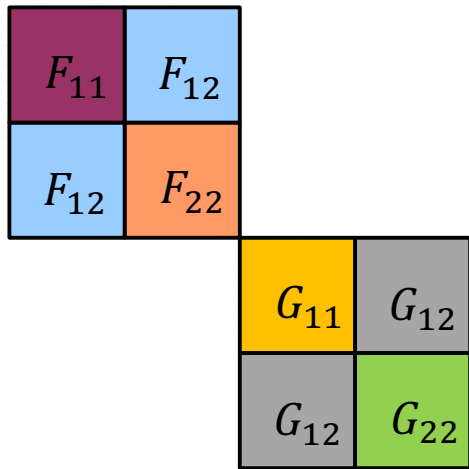
- Uncertainties can vary if they are processed with point-wise cross section data or MG cross section data
- If comparing with other codes (for example NJOY), ensure that the same options are used
- Currently, point-wise cross section is the default option for PUFF and NJOY



Collapsing to user groups

Matrix collapse
(includes flux)

$$\frac{\sum \phi_i \phi_j M_{ij}}{\sum \phi_i \sum \phi_j}$$

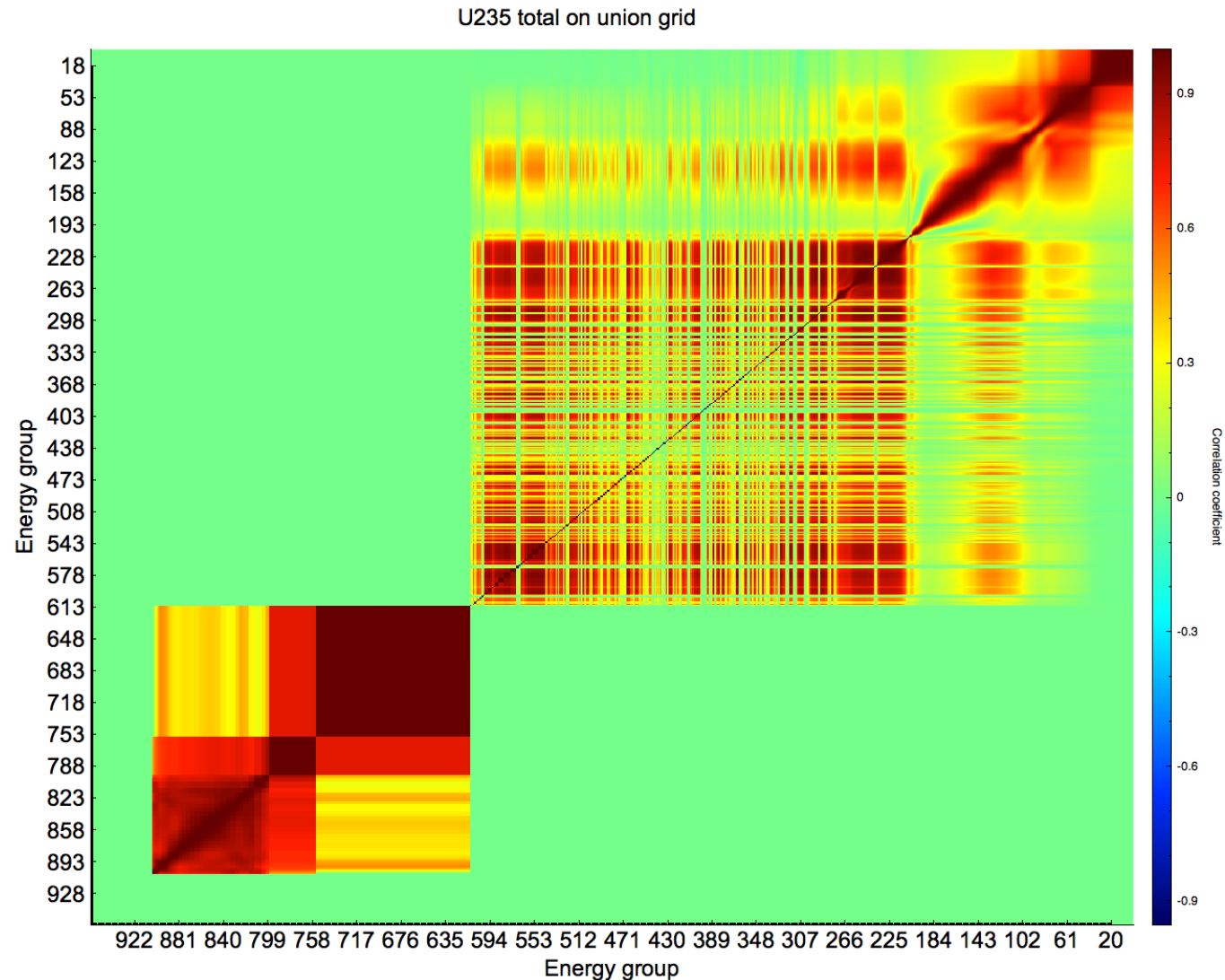


Assuming flux is 1
on each union group

- Collapsing to user groups is done on absolute covariance matrix
- Constrained matrices (chi matrices) collapse without flux
- Gaussian error propagation does not include flux, but cross section collapse also includes flux

Cross material covariance matrices

- Some ENDF files contain cross material covariance matrices
- PUFF saves a COVERX file on the union grid for each material
- If processing ENDF files with cross covariance materials, PUFF can use the above file to retrieve the cross section data and covariance matrices needed
- This step is not automated, and additional PUFF runs must be set up manually before binding the final library



Covariance data on the evaluator grid

PUFF has an option to view each of the cross section covariance matrices in an ENDF file on the evaluator grid

Explicit matrices

=====

mat1= 125 mt1= 2, mat2= 125 mt2= 2

Energy bounds

1 1.00000e-05
2 1.00000e+05
3 5.00000e+05
4 1.00000e+06
5 2.00000e+06
6 4.00000e+06
7 6.00000e+06
8 8.00000e+06
9 1.00000e+07
10 1.20000e+07
11 1.40000e+07
12 1.60000e+07
13 1.80000e+07
14 2.00000e+07

	column	1	2	3	4	5	6	7	8
1		8.77542e-06	1.38849e-05	2.79801e-05	3.88661e-05	5.25229e-05	6.77747e-05	7.46362e-05	7.52854e-05
2		1.38849e-05	2.21044e-05	4.46560e-05	6.20404e-05	8.38345e-05	1.08156e-04	1.19094e-04	1.20119e-04
3		2.79801e-05	4.46560e-05	9.03092e-05	1.25482e-04	1.69565e-04	2.18749e-04	2.40870e-04	2.42937e-04
4		3.88661e-05	6.20404e-05	1.25482e-04	1.74360e-04	2.35628e-04	3.03993e-04	3.34743e-04	3.37618e-04
5		5.25229e-05	8.38345e-05	1.69565e-04	2.35628e-04	3.18450e-04	4.10889e-04	4.52472e-04	4.56393e-04
6		6.77747e-05	1.08156e-04	2.18749e-04	3.03993e-04	4.10889e-04	5.30241e-04	5.83960e-04	5.89030e-04
7		7.46362e-05	1.19094e-04	2.40870e-04	3.34743e-04	4.52472e-04	5.83960e-04	6.43158e-04	6.48730e-04
8		7.52854e-05	1.20119e-04	2.42937e-04	3.37618e-04	4.56393e-04	5.89030e-04	6.48730e-04	6.54433e-04
9		7.06024e-05	1.12637e-04	2.27794e-04	3.16594e-04	4.27988e-04	5.52378e-04	6.08404e-04	6.13741e-04
10		6.12297e-05	9.76802e-05	1.97555e-04	2.74561e-04	3.71159e-04	4.79053e-04	5.27657e-04	5.32291e-04
11		4.77550e-05	7.61838e-05	1.54077e-04	2.14138e-04	2.89474e-04	3.73630e-04	4.11541e-04	4.15170e-04
12		3.07354e-05	4.90329e-05	9.91668e-05	1.37822e-04	1.86313e-04	2.40475e-04	2.64883e-04	2.67219e-04
13		1.07019e-05	1.70763e-05	3.45412e-05	4.80018e-05	6.48884e-05	8.37560e-05	9.22628e-05	9.30925e-05
	column	9	10	11	12	13			

```
=puff_iv  
point=32 master=21  
out=1 uncol=16 detail=true  
mat=9228  
ngrp=56  
endf=11  
flux=12 matwt=99 mtwt=2099  
end
```

Resonance parameter covariance matrices

- ENDF can give covariance matrices for the resonance parameters

$$\langle \Delta P_k, \Delta P_l \rangle$$

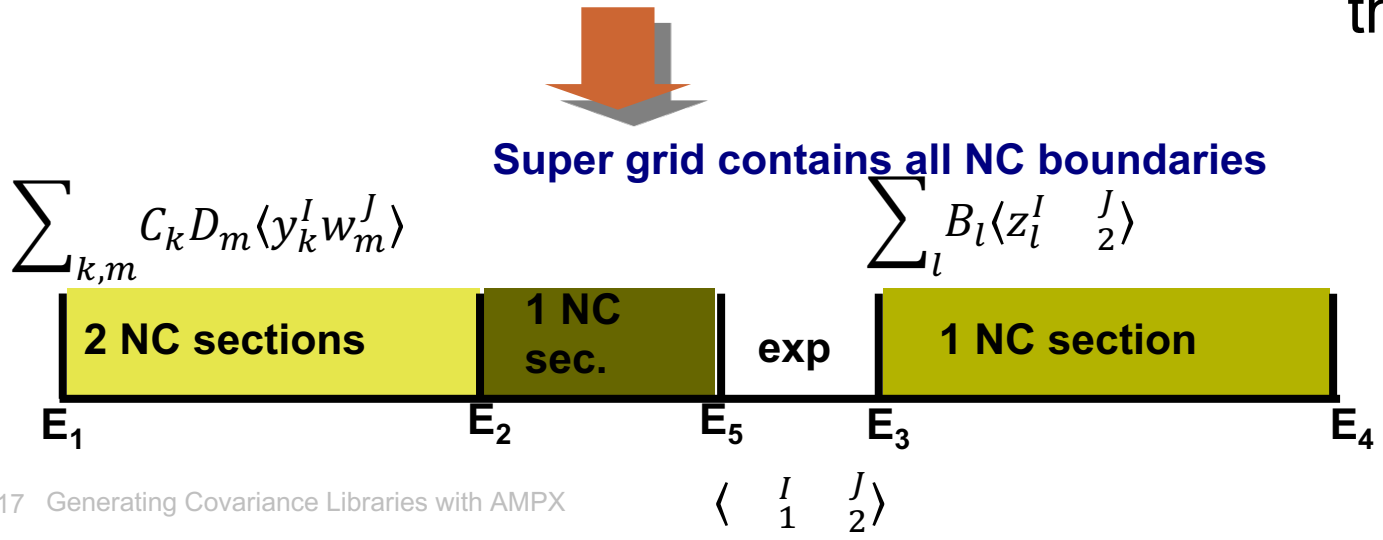
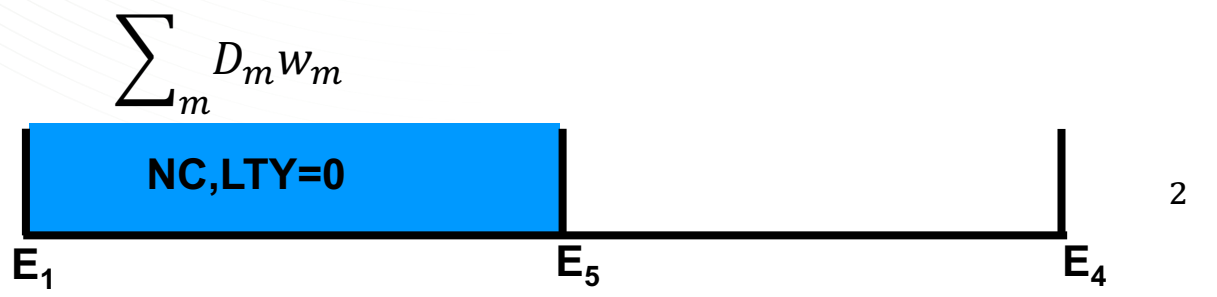
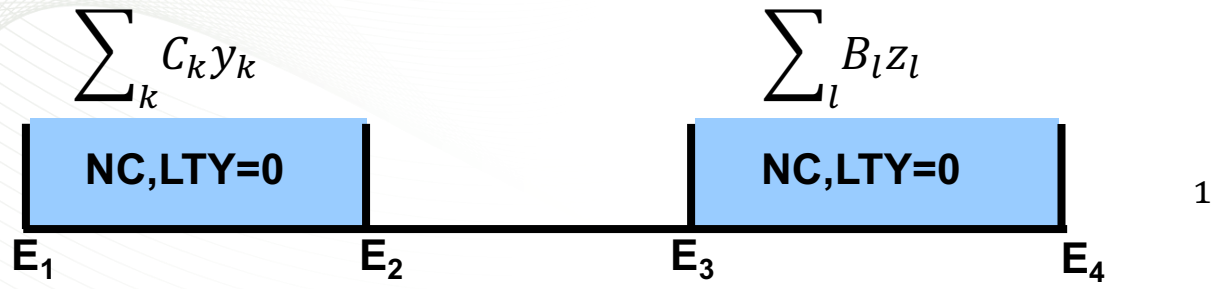
- SCALE requires covariance matrices with respect to cross section, so the resonance parameters' covariance must be propagated to the cross section
- The sensitivity of the cross section is group averaged as follows:

$$D_{Ik}^m = \frac{1}{\phi_I} \int_I \varphi \frac{\partial \sigma_m}{\partial P_k} dE$$

- This is performed analytically using SAMRML. Integration is performed by fourth order Runge-Kutta. All resonance formalisms are converted to “R-Matrix Limited Format” in order to use SAMRML
- The group-averaged cross section covariance is:

$$\langle \Delta \sigma_I^m, \Delta \sigma_J^n \rangle = \sum_{kl} D_I^m \langle \Delta P_k, \Delta P_l \rangle D_J^n$$

Derived covariance matrices in ENDF



- ENDF can give covariance matrices as derived: for example, the total is the sum of all other reactions in a given energy range
- This implies many additional matrices as there is a cross correlation between the derived reaction and all reactions from which it is derived
- PUFF automatically generates these cross matrices

Redundant cross section

- For a redundant cross section (total or total inelastic), ENDF does not always give covariance information
- If the partials are given, PUFF generates the covariance matrix for the redundant cross section, including all the cross correlation that this implies
- This is especially important for total inelastic cross sections, as it is often not given in ENDF, but the covariance matrix is used in SCALE

Conclusion

- PUFF can be used to generate covariance libraries for SCALE
- If using the same group bounds as an existing SCALE covariance library, covariance matrices from that library can be imported
- cognac applies some corrections
- covcomp allows to compare two covariance