Covariance Fixups and Testing

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In ENDF we trust…

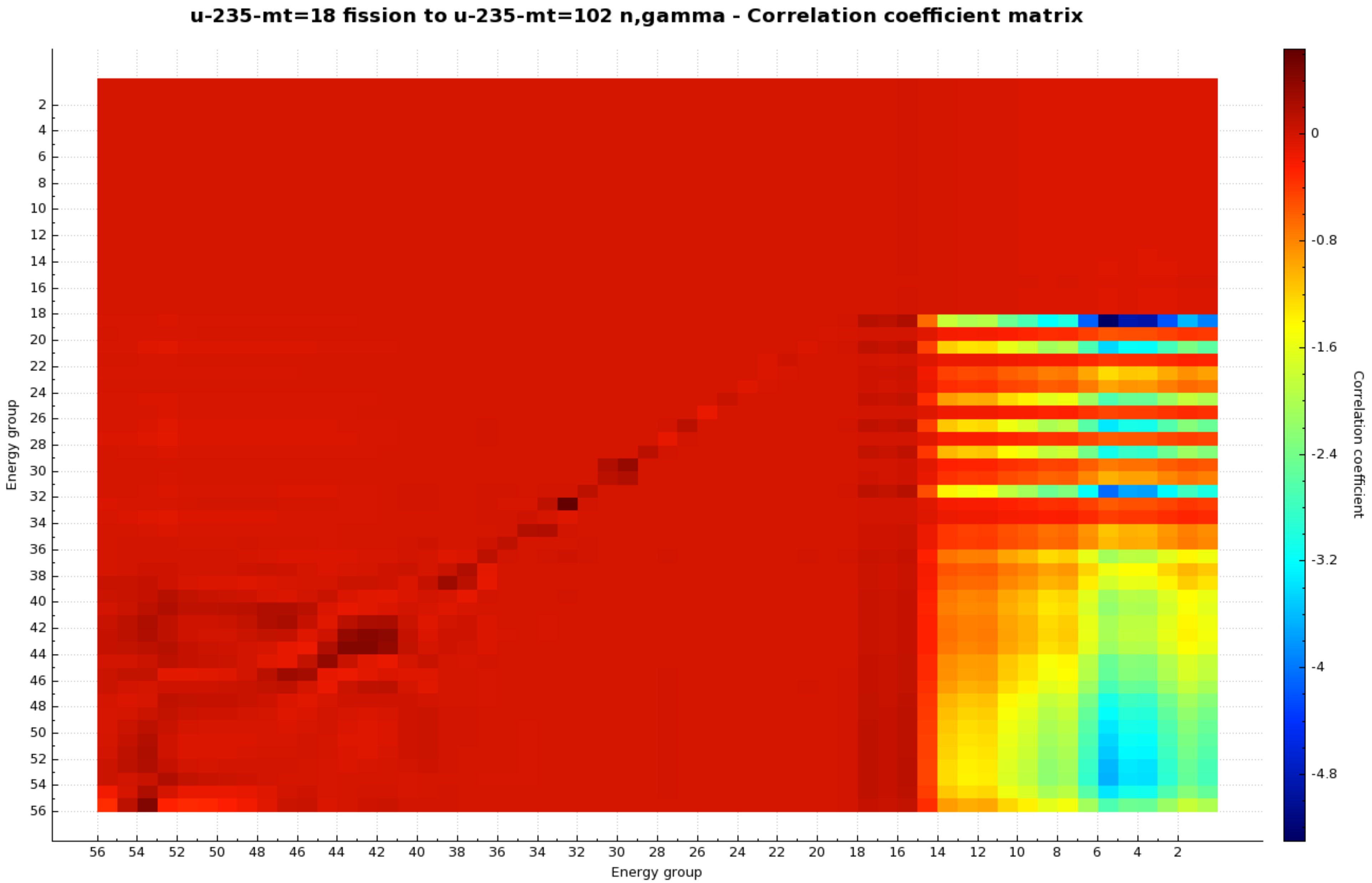
- Covariance data are a recurring problem
  - Last minute changes let mathematically incorrect covariance matrices slip into ENDF-8
  - Limited precision of ENDF format makes it difficult to ensure that matrices (when processed) do not lead to mathematically illegal values

Covariance, what's the worst that could happen?

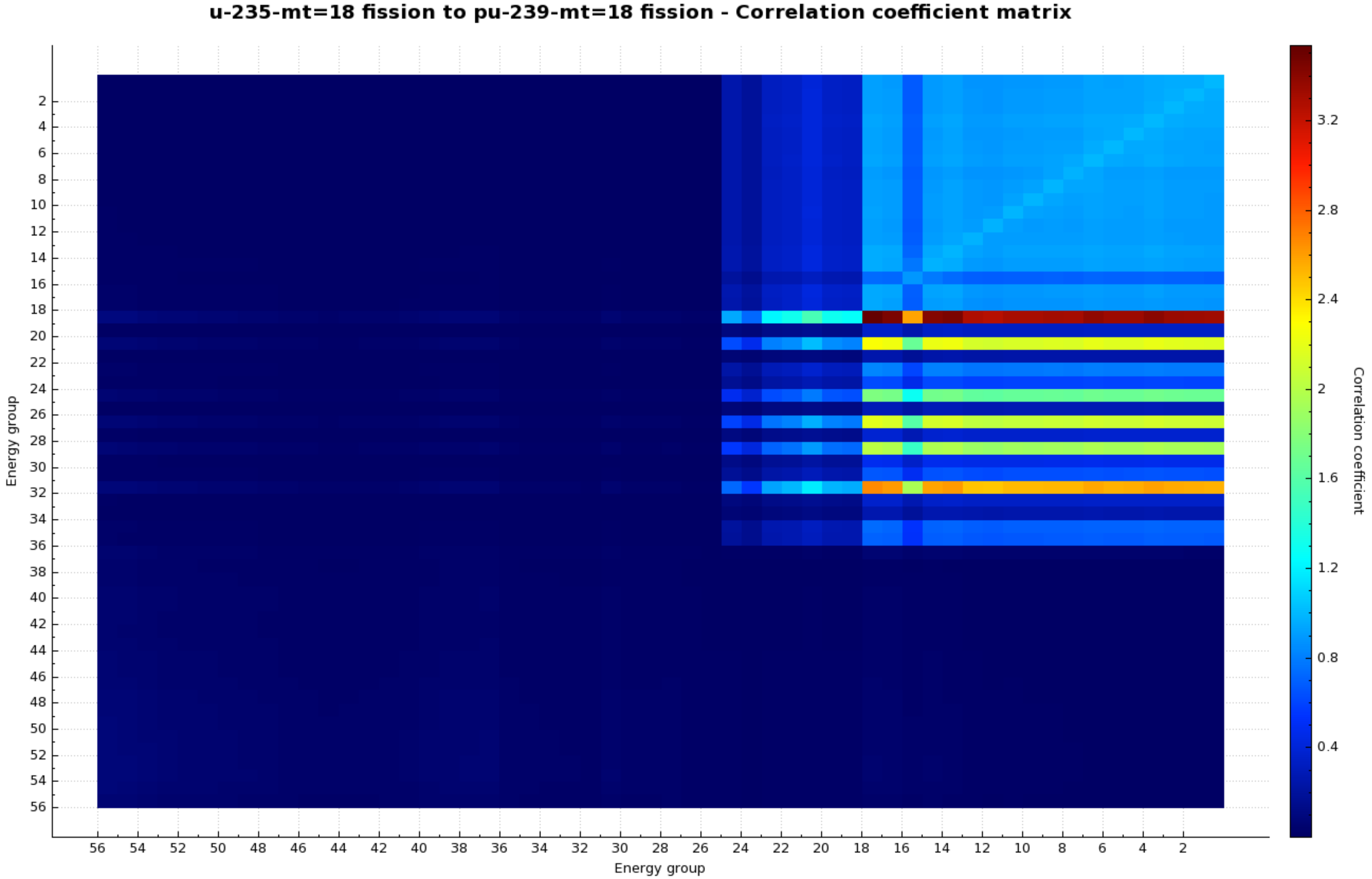
- The ENDF format itself is an impediment due to precision issues
  - Truncation of correlation/covariance values lead to rank deficient matrices
    - Symmetric, non-singular, real matrices are guaranteed to have (strictly) positive, real eigenvalues; correlation matrices of cross sections are an example of such matrices

- Occasionally, errors in the data or processing occur
  - ENDF-8 U-235 gives some pretty pictures…

Mathematically incorrect covariance matrices



Mathematically incorrect covariance matrices



Example

Take a mathematically legal correlation matrix

$$C = \begin{pmatrix} 1 & -0.2145 & 0.1384 & -0.5355 \\ & 1 & -0.9137 & 0.1328 \\ & & 1 & -0.0770 \\ & & & 1 \end{pmatrix}$$

All elements are between -1 and +1

Eigenvalues are: 0.0830, 0.4611, 1.3891, 2.0669

Suppose the matrix below was the correlation matrix intended

$$C = \begin{pmatrix} 1 & -0.2145 & 0.1384 & -0.5355 \\ & 1 & -0.9137 & 0.1328 \\ & & 1 & -0.0770 \\ & & & 1 \end{pmatrix}$$

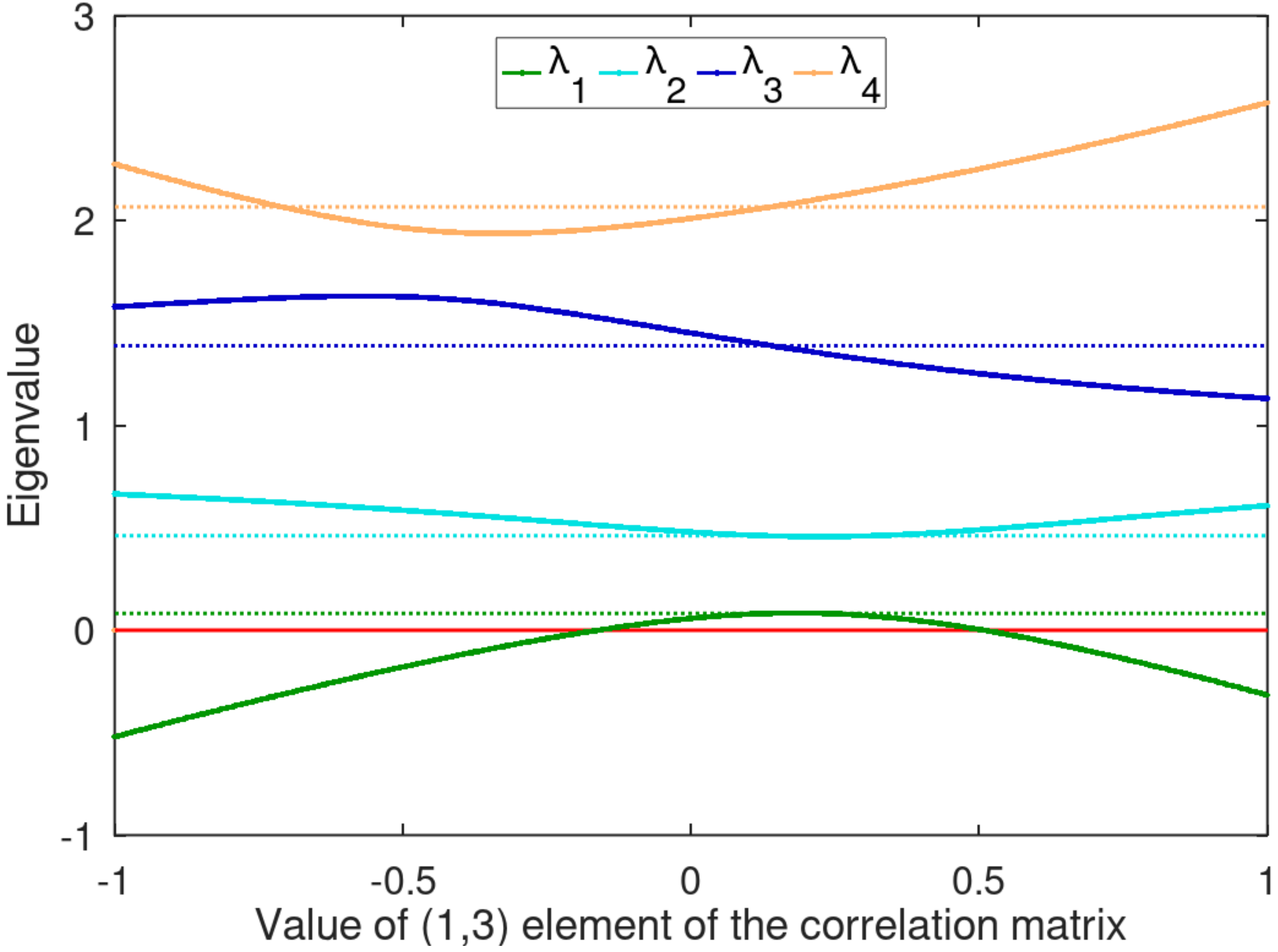
However, due to unknown reasons, the (1,3) element is messed up and the matrix below is what is reported in ENDF

$$C' = \begin{pmatrix} 1 & -0.2145 & 1.4 & -0.5355 \\ & 1 & -0.9137 & 0.1328 \\ & & 1 & -0.0770 \\ & & & 1 \end{pmatrix}$$

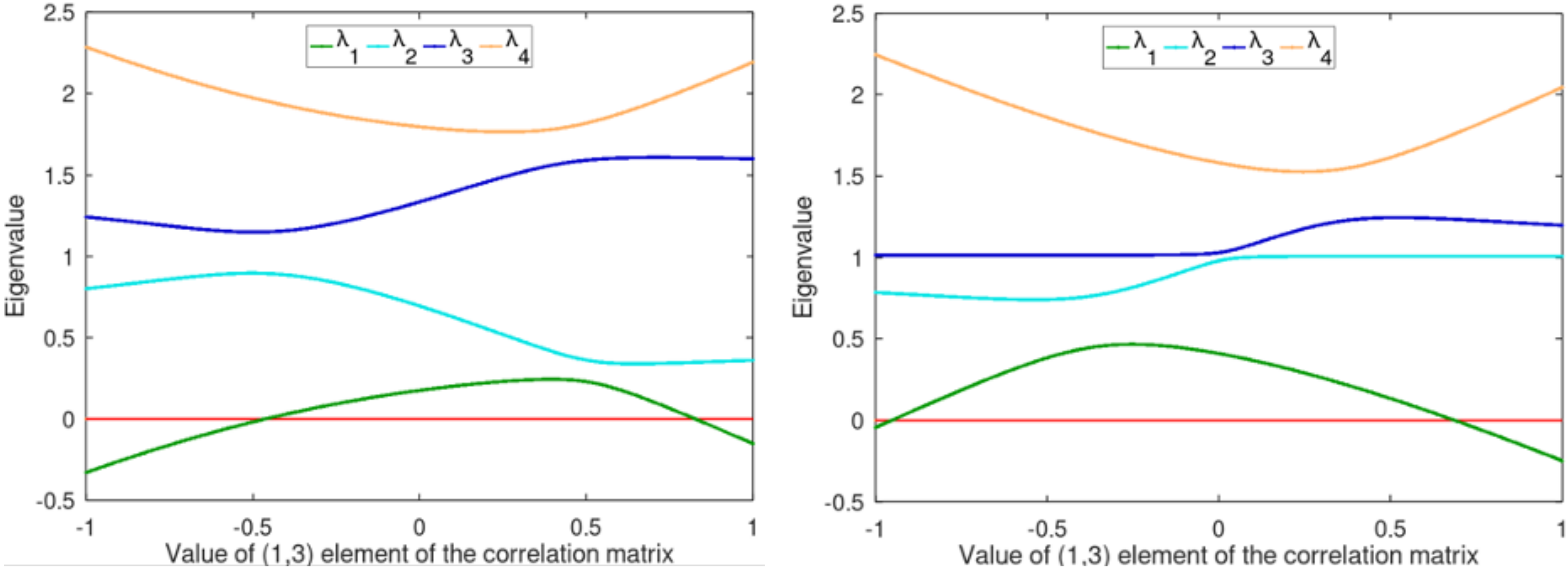
The new eigenvalues are, -0.6400, 0.6920, 1.0737, 2.8742

The difficult question is, without the knowledge of the intended matrix how can the processing code fix this obvious mistake?

Explore every option for replacing the bad element of the correlation matrix



We repeat this for new legal correlation matrices, conclusions are the same



The conclusions for element-wise fix-up of several erroneous values are the same through a proof-by-induction argument

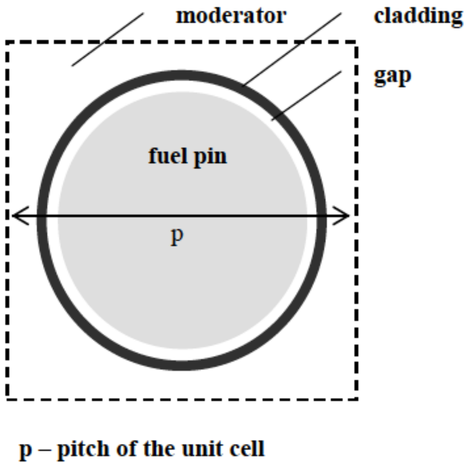
There are other options instead of fixing up only the single erroneous value

Taking the SVD and keeping only the positive eigenvalues is not the best option either because the largest eigenvalue diverges from the largest eigenvalue of the “intended” matrix as the value of the ”erroneous” element grows large

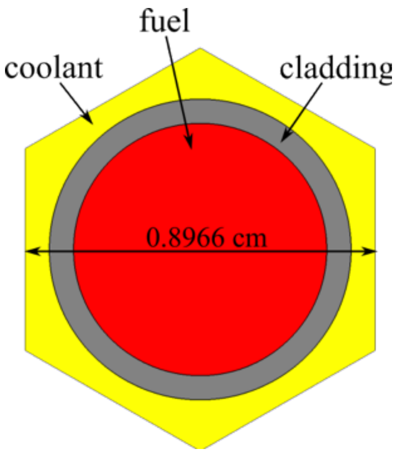
How do we fix mathematically incorrect covariances?

- If it is a minor roundoff problem, we bump the values back into the valid range, and report it (as in SCALE 6.2)
- If an egregious error (outside of precision) is detected for **ANY** matrix element, PUFF and COGNAC (AMPX covariance modules) will now:
  - Set self correlation matrices to the identity matrix
  - Set cross correlation matrices to the zero matrix
- In practice, this has only affected a small subset of isotopes in the ENDF-8 covariance library

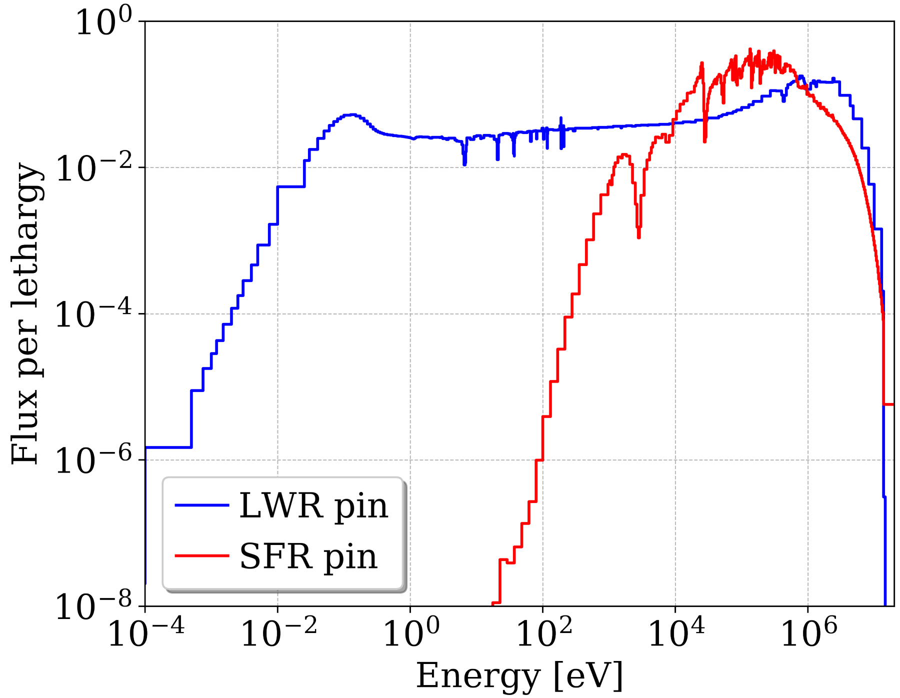
Test models and tools



Light Water Reactor (LWR) pin*:
- UO_2 fuel, 4.85 wt % ^{235}U
- Zircaloy-4 cladding
- Water coolant



Sodium-cooled Fast Reactor (SFR) pin:
- U-TRU-Zr fuel, 18.98 wt.% TRU
- HT-9 steel cladding
- Sodium coolant



Neutron flux

Applied SCALE 6.3 beta tools and data:
- Neutron transport: **NEWT**, 2-dimensional deterministic code
- Uncertainty/sensitivity analysis: **TSUNAMI-2D**, perturbation theory
- Cross section library: 252-group LWR, 302-group SFR

* K. Ivanov et al., *Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I)*. NEA/NSC/DOC(2013)7 (2016).

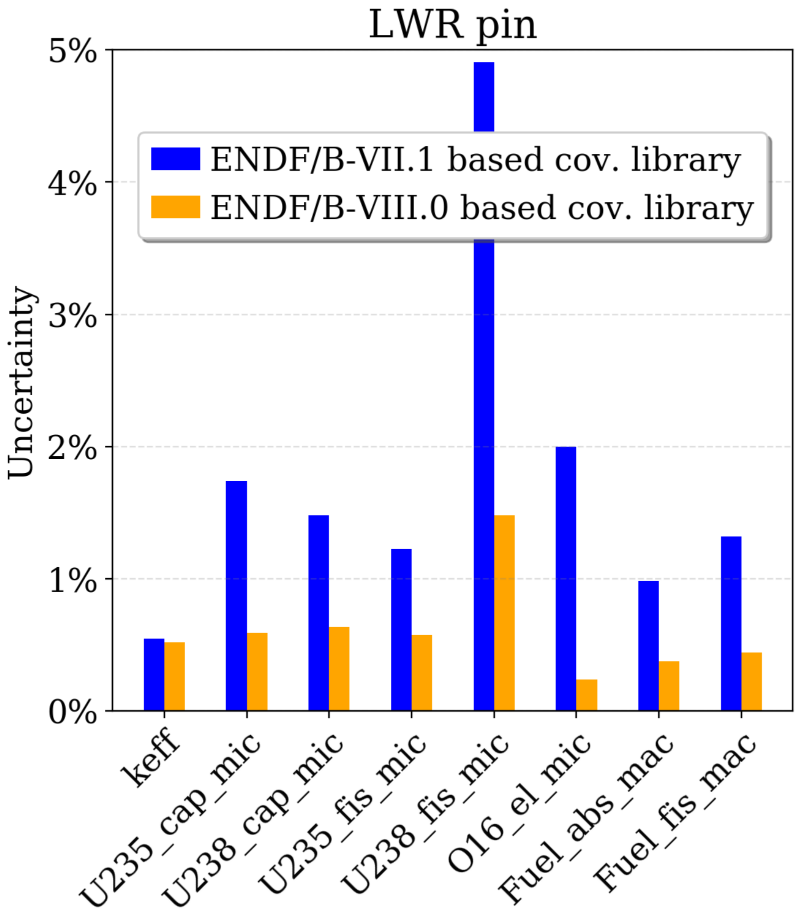
Impact of the ENDF/B-VIII.0 covariance matrix corrections

Relevant differences of uncertainties, σ, when using the original vs. the corrected data

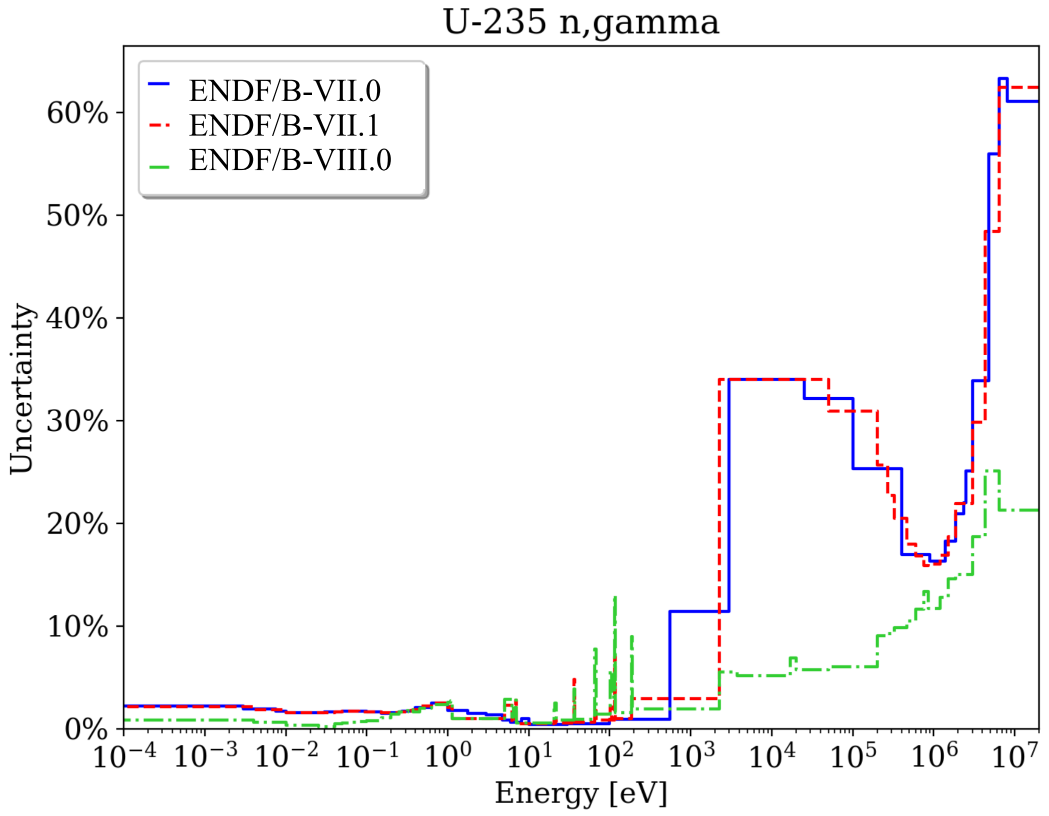
		σ_1, *original*	σ_2, *corrected*	$\frac{\sigma_2}{\sigma_1} - 1$	*Additional contribution to* σ_1, *not observed for* σ_2
LWR pin	k_{eff}	0.523%	0.517%	-1.05%	^{235}U fis – ^{238}U fis: 0.054% ^{235}U fis – ^{235}U n,g: 0.052%
	U235_cap_mic	0.589%	0.553%	-6.16%	^{235}U fis – ^{235}U n,g: 0.205%
	U238_fis_mic	1.478%	1.463%	-1.01%	^{235}U fis – ^{238}U fis: 0.212%
	Fuel_fis_mac	0.444%	0.437%	-1.46%	^{235}U fis – ^{235}U n,g: 0.078%
SFR pin	*keff*	1.085%	1.052%	-3.06%	^{238}U fis – ^{239}Pu fis: 0.257%
	U238_fis_mic	2.737%	2.618%	-4.38%	^{238}U fis – ^{239}Pu fis: 0.797%
	Fuel_fis_mac	1.101%	0.982%	-10.82%	^{238}U fis – ^{239}Pu fis: 0.481% ^{235}U fis – ^{239}Pu fis: 0.118%
	Fuel_abs_mac	1.044%	1.022%	-2.09%	^{238}U fis – ^{239}Pu fis: 0.207%

- Small impact on total output uncertainties, noticeable impact on individual contributions
- Correction leads to decrease of all observed output uncertainties
- Differences need to be considered when comparison uncertainty analyses (e.g. OECD/NEA uncertainty analysis benchmark activities)

Comparison of ENDF/B-VII.1 and ENDF/B-VIII.0 results

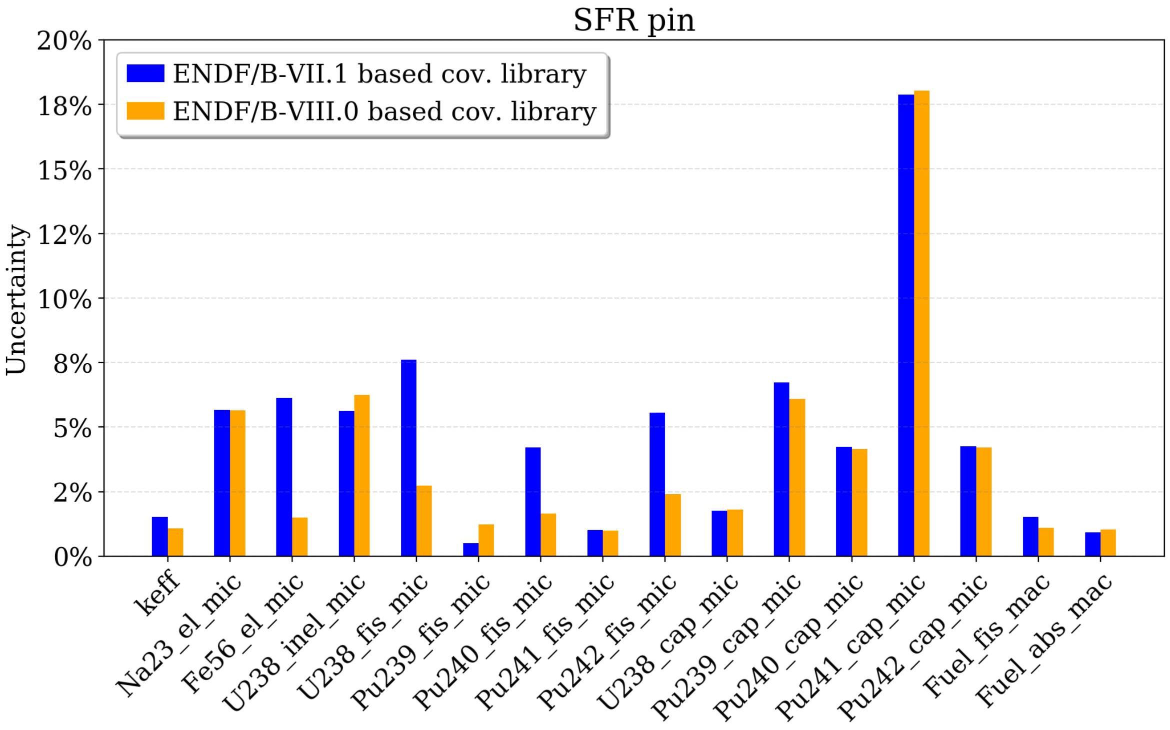


LWR output uncertainties: eigenvalue, collapsed 1-group microscopic and macroscopic cross sections

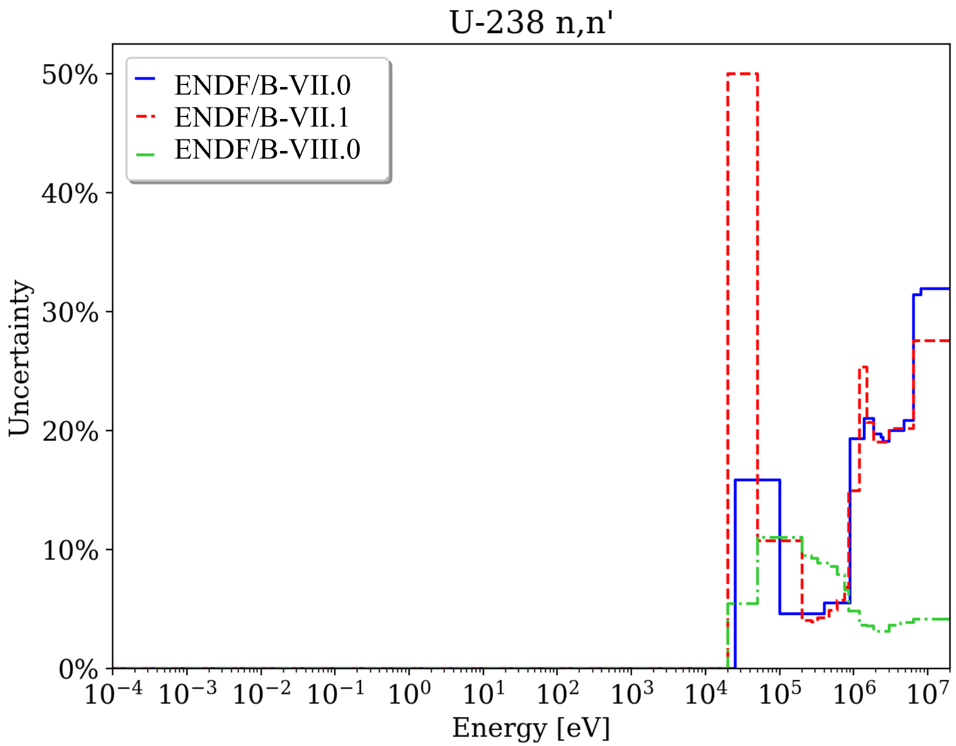


Example of relevant nuclear data uncertainty impacting LWR results

Comparison of ENDF/B-VII.1 and ENDF/B-VIII.0 results



SFR output uncertainties: eigenvalue, collapsed 1-group microscopic and macroscopic cross sections



Example of relevant nuclear data uncertainty impacting SFR results

- Large differences for various output uncertainties due to uncertainty updates of for many important nuclide reactions
- Analysist like me can be surprised by increased uncertainties in new ENDF/B releases

Acknowledgements

- Thanks to our sponsors, NCSP and NRC
- Thanks to Vlad Sobes for initial vision
- Thanks to Marco Pigni for making this all moot by repairing the U-235 ENDF-8 file error