Covariance Testing at Oak Ridge National Laboratory

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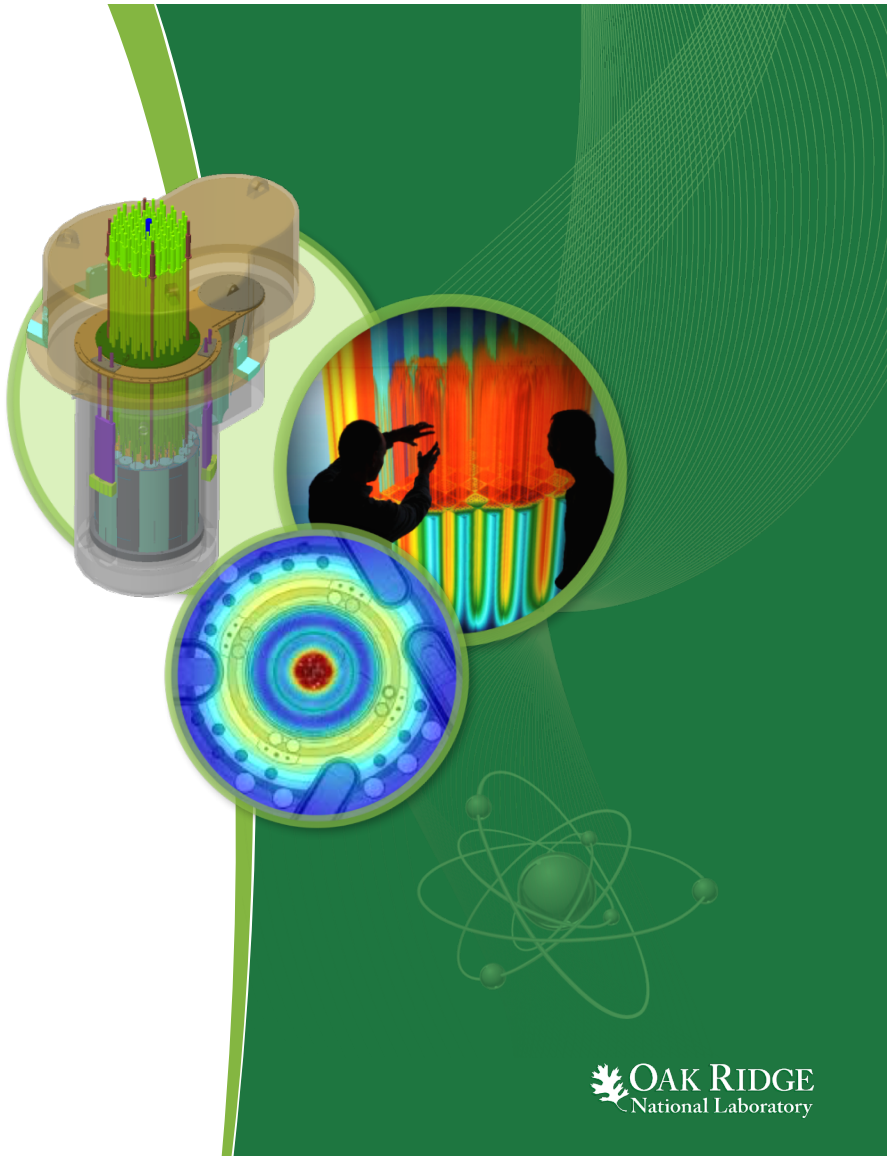

CSEWG

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Introduction

- Covariance processing of ENDF/B-VIII.0 Beta 5
- Differences between ENDF/B-VIII.0 Beta 5 and ENDF/B-VII.1 covariance matrices
- Propagation to k_{eff} values
- C_k (similarity) comparison

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
  - Modified ENDF/B-VII.1 ^{239}Pu, ^{235}U nubar and H capture uncertainties; these are prerelease ENDF/VIII.0 rev. 632, 631 and 611
  - Chi uncertainties processed from new ENDF/B-VII.1 file 35
  - 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 use only the following reactions: 1, 2, 4, 16, 18, 102, 103, 104, 105, 106, 107, 452, 455, 456. Therefore, this presentation concentrates on those reactions. Future libraries will contain all cross section data for use in the CE sampler.

Processing of ENDF/B-VIII.0 Beta 5

- Process the cross section data at 293 K
- Using PUFF and a Maxwellian-1/E-fission-1/E flux, generate the covariance matrices for 56 groups
- Using COGNAC, apply our usual correction (extend uncertainties to lower-energy groups; correct correlation and relative uncertainties that are larger than 1
- Compare with ENDF/VII.1 covariance data (for comparison only; use the cross section data from ENDF/VII.1)
- Make two covariance libraries:
  - Library **ENDF/B-VIII.0 Beta 5 Covariance Library** contains only data from ENDF/B-VIII.0 Beta 5
  - Library **ENDF/B-VIII.0 Beta 5 Covariance Library with SCALE 6.2** contains data from ENDF/B-VIII.0 Beta 5 plus all covariance matrices from the SCALE 6.2 library not already present in ENDF/B-VIII.0 Beta 5

Redundant covariance matrices

If desired, PUFF calculates redundant covariance matrices (and all cross correlations) if they are not given in ENDF

- 452 not given (but 455 and 456): $^{242}Am^{m}$, ^{243}Am, ^{237}Np, ^{240}Pu, ^{241}Pu, ^{234}U, ^{236}U
- 455 not given (but 452 and 456 and cross section data for 455): ^{238}Pu, ^{239}Pu
- 4 not given: ^{12}C, ^{55}Mn, ^{232}Th, ^{235}U, ^{238}U, ^{180}W, ^{182}W, ^{183}W, ^{184}W
- 1 not given for 37 nuclides

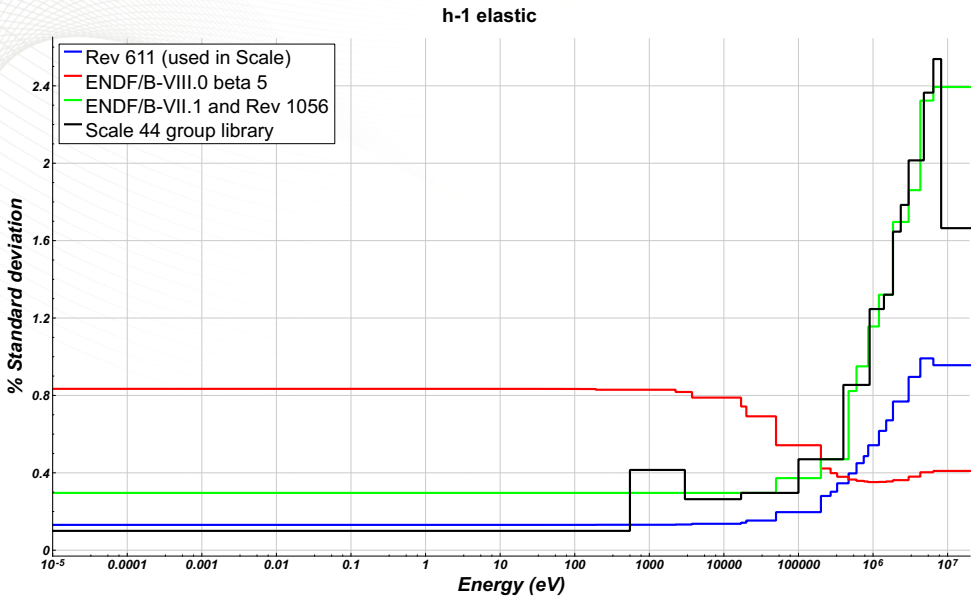
SCALE does not use 1 directly. Only SAMPLER uses 455 and 456.

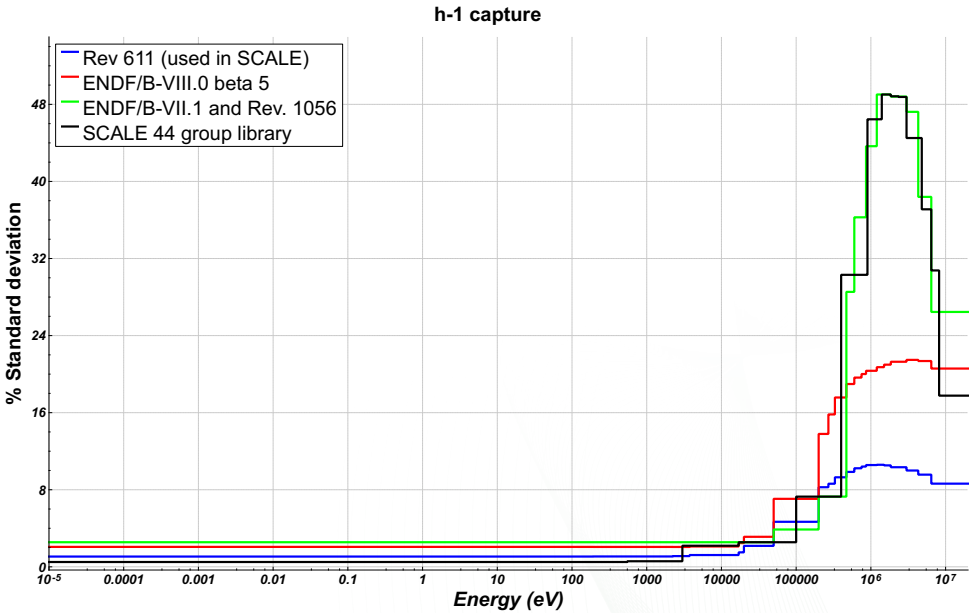
Covariance with substantial differences

Comparing ENDF/VII.0 and ENDF/VIII.0 Beta 5, the following covariance matrices show large differences in at least one energy range:

- ^{10}B (elastic, n-alpha), ^{16}O (elastic, n-alpha), ^{56}Fe (elastic, n-n', capture, n-p), ^{182}W (elastic, capture), ^{183}W (elastic), ^{184}W (elastic, capture), ^{186}W (elastic, capture), ^{197}Au (capture), ^{233}U (nubar [prompt, delayed, and total], fission, capture, elastic), ^{235}U (total nubar, elastic, fission, capture), ^{238}U (fission, total nubar, elastic, capture), ^{239}Pu (total nubar, fission, elastic, capture), ^{240}Pu (elastic), ^{2}H (elastic), ^{1}H (elastic, capture)
- ^{103}Rh, 147Pm, ^{149}Sm, 151Sm, ^{155}Eu were changed by ORNL to be consistent with ATLAS values in thermal range

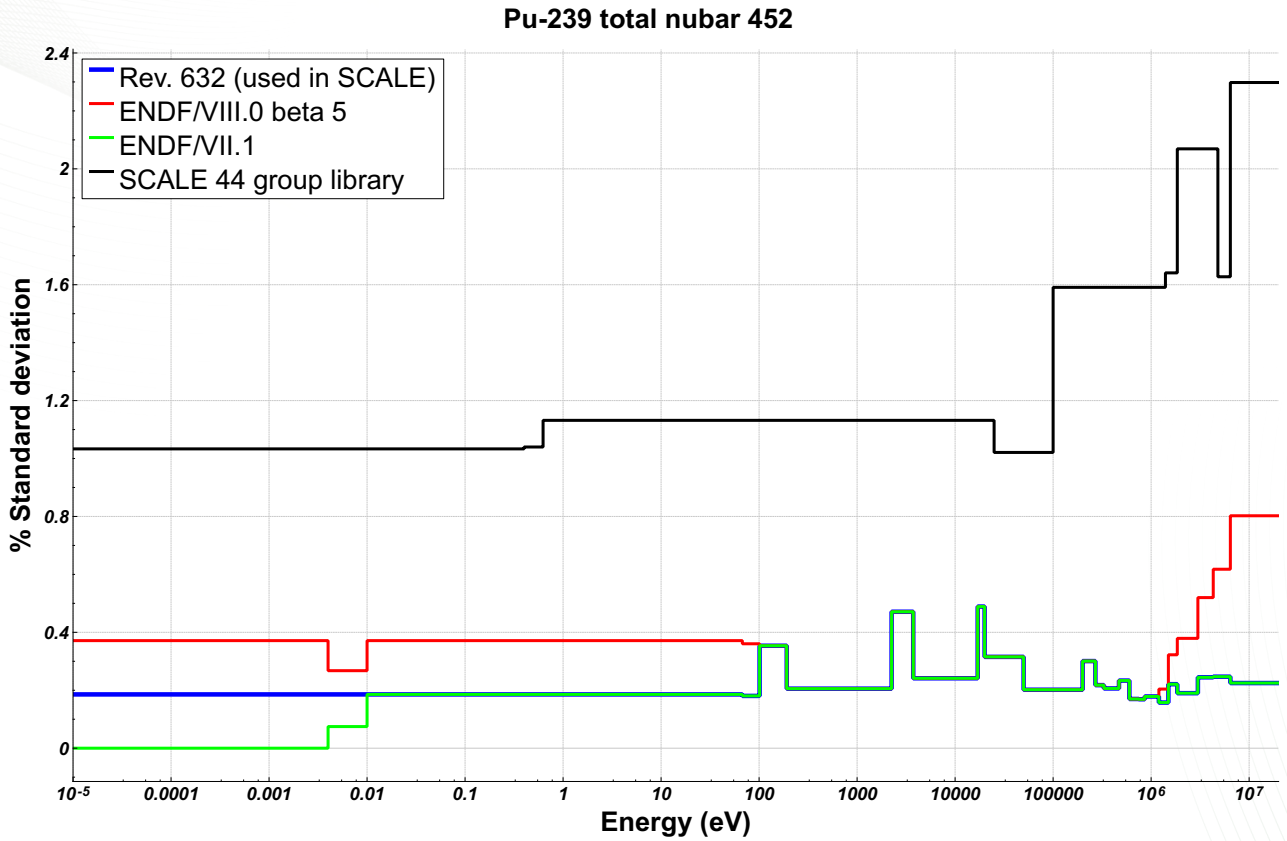
^{1}H changes



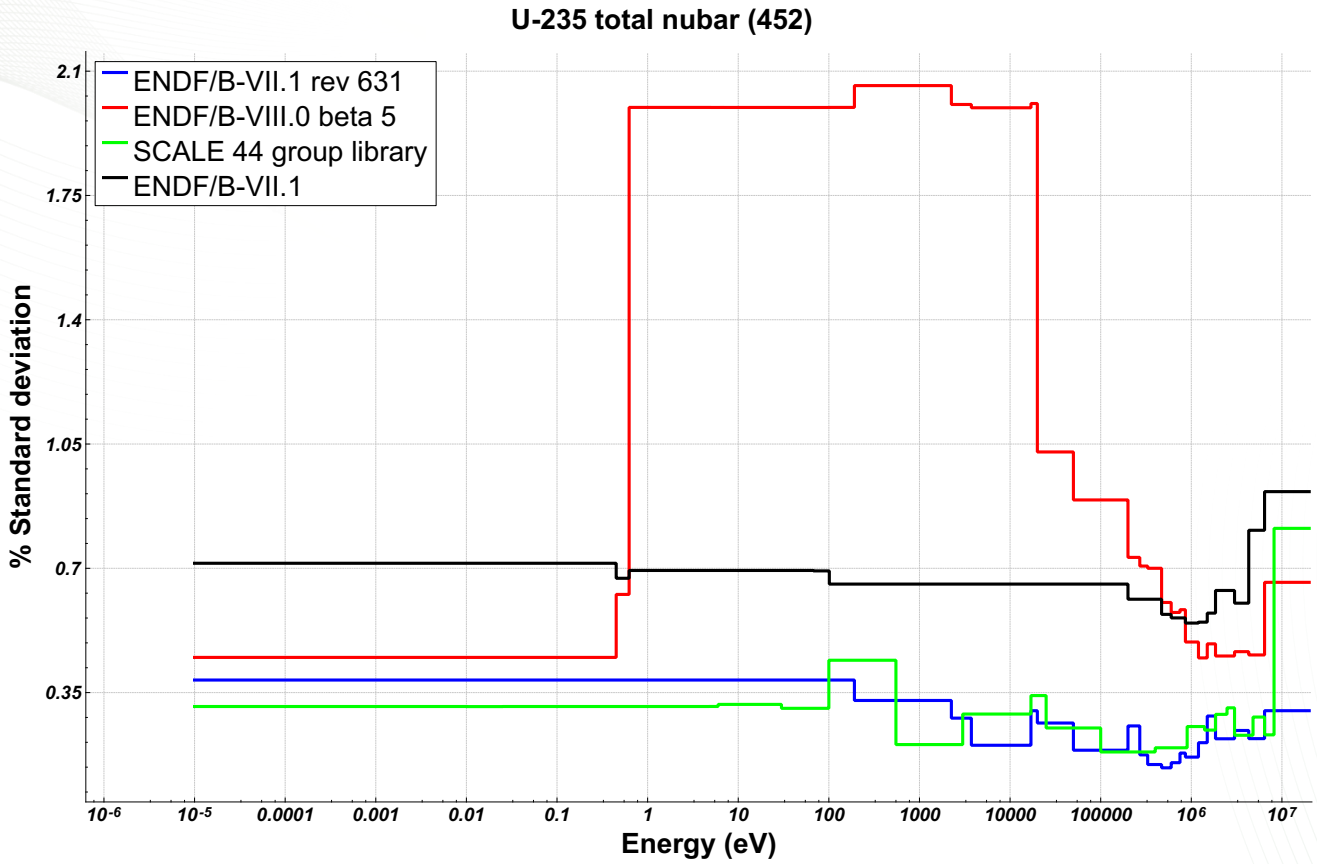


SCALE also uses ^{1}H uncertainty in the thermal region of ^{1}H bound in H_2O and other moderators with ^{1}H as the major scatterer

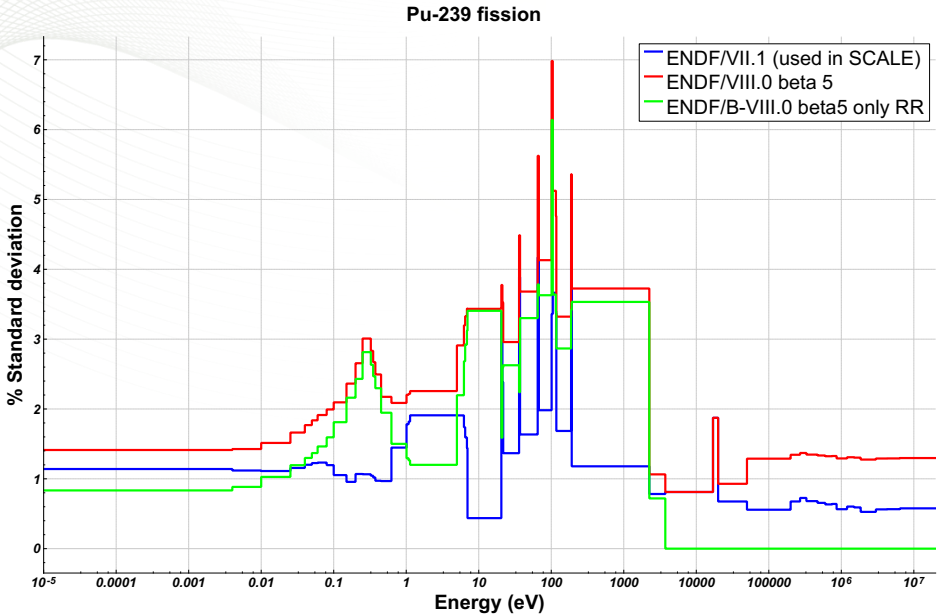
^{239}Pu nubar changes

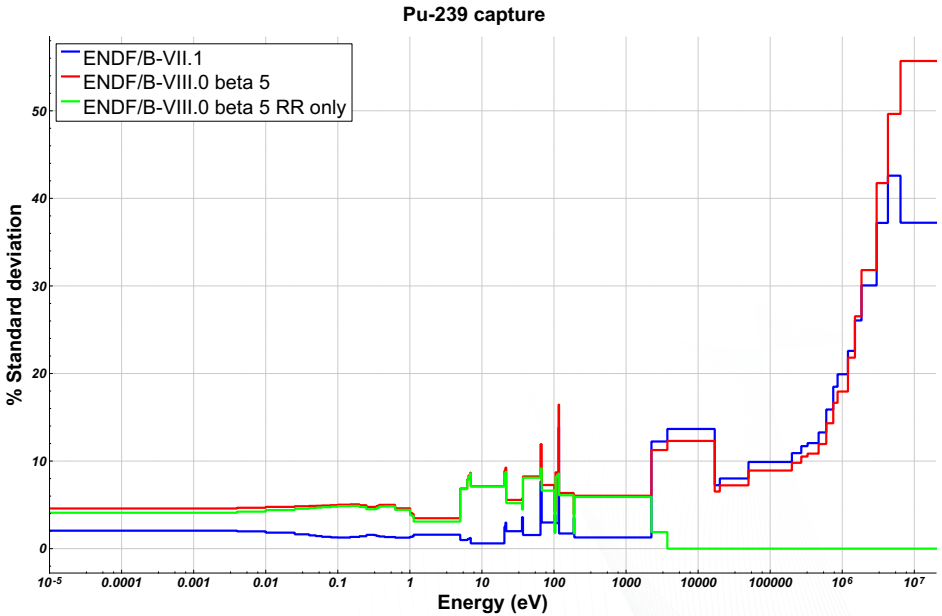


^{235}U nubar



^{239}Pu



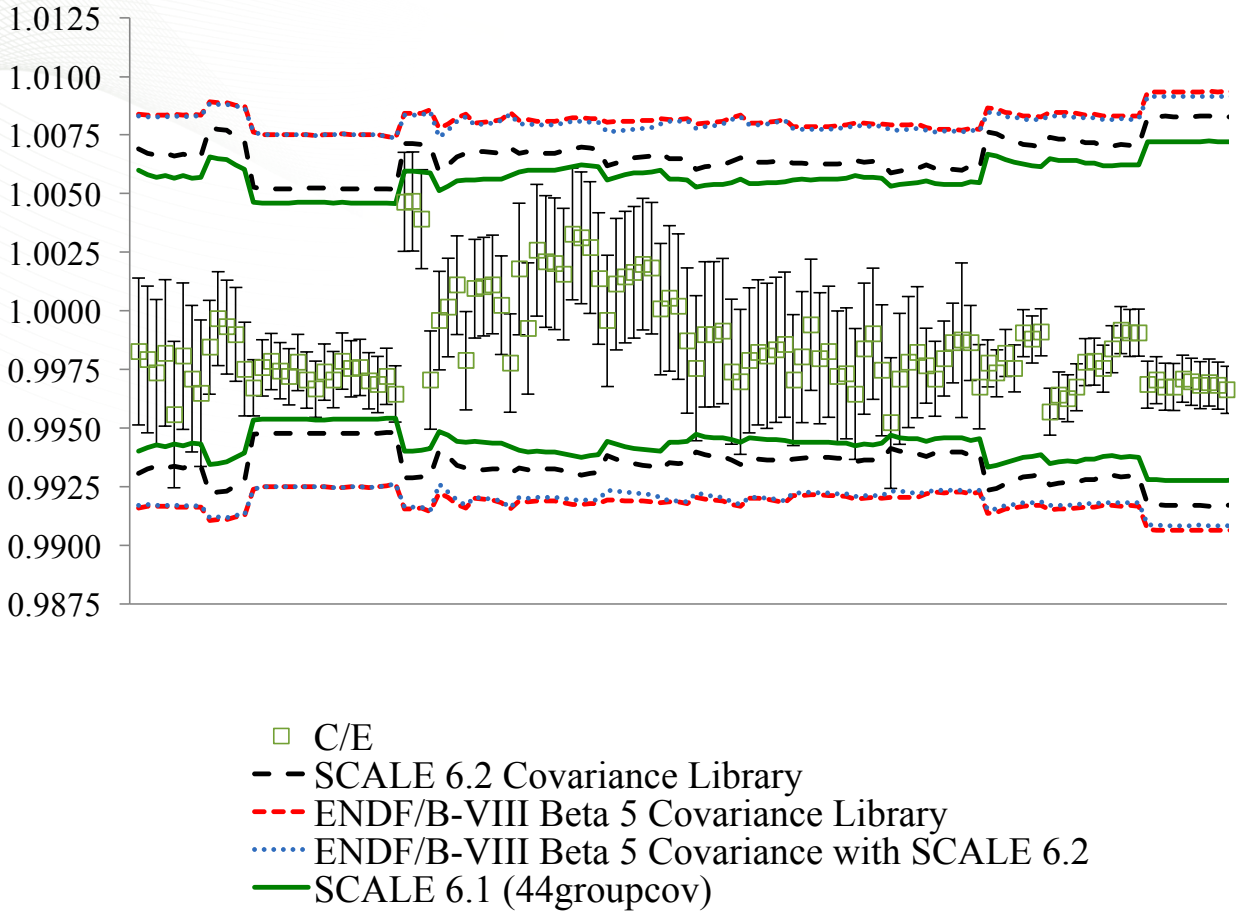


In the resolved range, there is a covariance matrix from resonance parameters (JEFF data, adapted slightly by Marco Pigni) and File 33 covariance information

Covariance testing in SCALE

- Sensitivity data used for testing were generated in SCALE 6.1 using ENDF/VII.0 cross section data
  - Covariance library contains relative uncertainty; thus it should be applicable to the current library
  - Results support that testing is effective even with old sensitivity data because they are stationary with respect to the data changes—change one thing at a time!
- Two categories are compared:
  - Uncertainty in k_{eff} due to cross section covariance data
    - TSUNAMI-IP will calculate k_{eff} uncertainty resulting from covariance data
    - Covariance patching turned off for data testing ("uncert" and "values" keywords in parameters block)
    - Covariances propagated with sensitivities to determine uncertainty in k_{eff}
  - c_k (similarity) of a reference set of experiments with reference applications

LEU-COMP-THERM

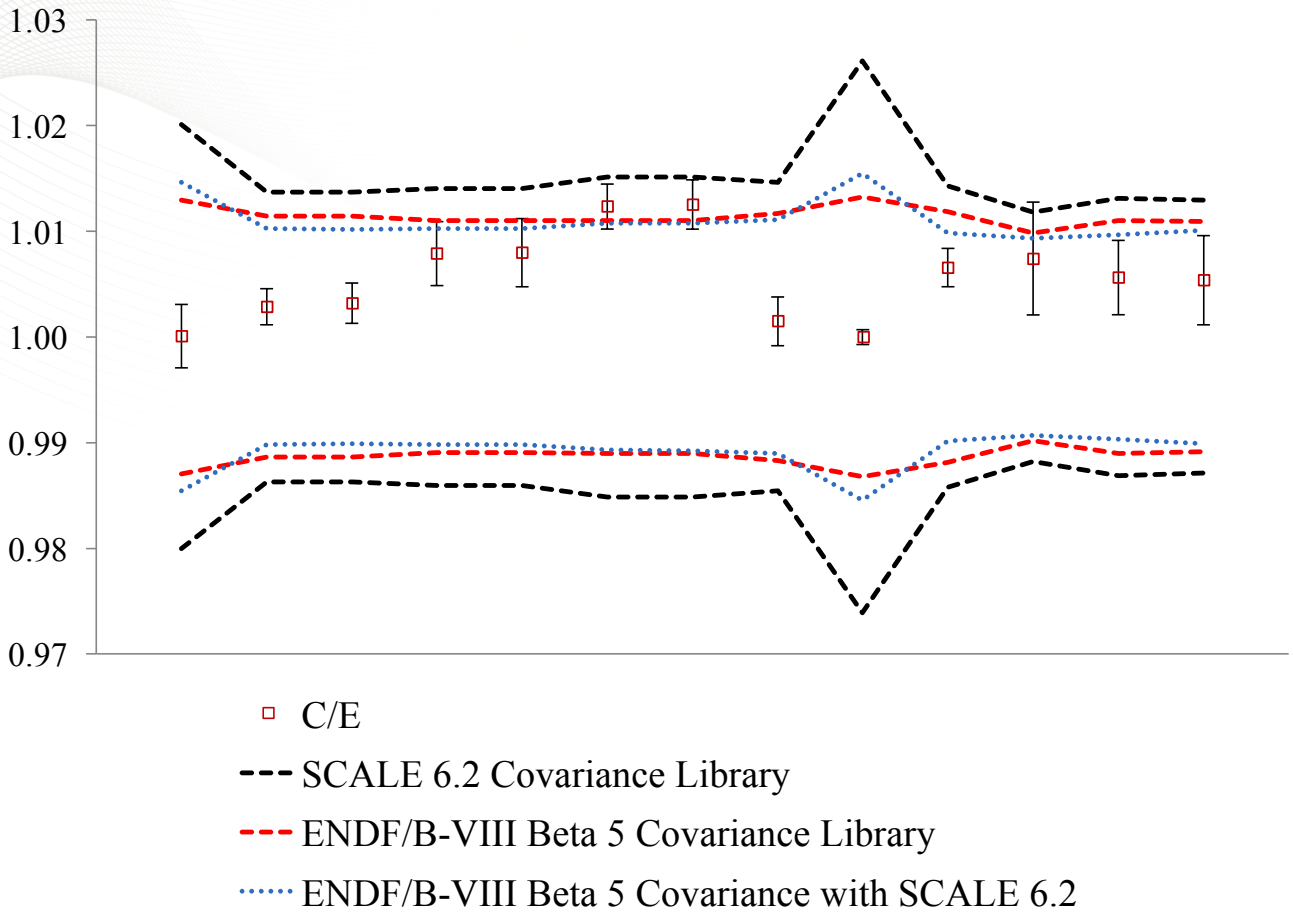


Larger error bands than for Scale 6.2 covariance library. Traced to ^{1}H capture and ^{235}U nubar.

SCALE 6.2 uses the lower ENDF/B-VII.2 preliminary data, as shown on previous slide.

In systems with soluble B, the change in covariance data in ^{10}B data also contributes to the difference between Scale 6.2 and Beta 5 results.

MIX-COMP-FAST



Difference between ENDF/B-VIII Beta 5 with and without SCALE 6.2 covariance data is due to a cross correlation between ^{238}U elastic and (n,n').

ENDF/VII.1 defines elastic as 1 – 4 – 16 – 17 – 18 – 102. This introduces the (2,4) correlation.

ENDF/B-VIII Beta 5 gives an explicit covariance matrix for 51. A correlation between (2,51) is given, but SCALE does not use it and PUFF ignores, creating redundant 4.

c_k (similarity) assessment

- Purpose:
  - Calculate c_k parameter for each experiment in a reference set compared with multiple spent fuel storage/transportation applications
  - What is c_k?
    - Correlation coefficient between an experiment and an application based on shared nuclear data uncertainty

Uncertainty matrix: $\mathbf{C_{kk}} = \mathbf{S_k} \mathbf{C_{\alpha\alpha}} \mathbf{S_k^T}$ given:

$$\mathbf{C_{\alpha\alpha}} \equiv \left[\frac{\mathrm{COV}(\alpha_m, \alpha_p)}{\alpha_m \alpha_p} \right], \; m = 1, 2, \ldots, M; \; p = 1, 2, \ldots, M$$

Covariance data

$$\mathbf{S_k} \equiv \left[\frac{\alpha_m}{k_i} \frac{\partial k_i}{\partial \alpha_m} \right], \; i = 1, 2, \ldots, I; \; m = 1, 2, \ldots, M$$

Sensitivity data

c_k (corr. coef.): $c_k = \dfrac{\sigma_{ij}^2}{(\sigma_i \sigma_j)}$ where:

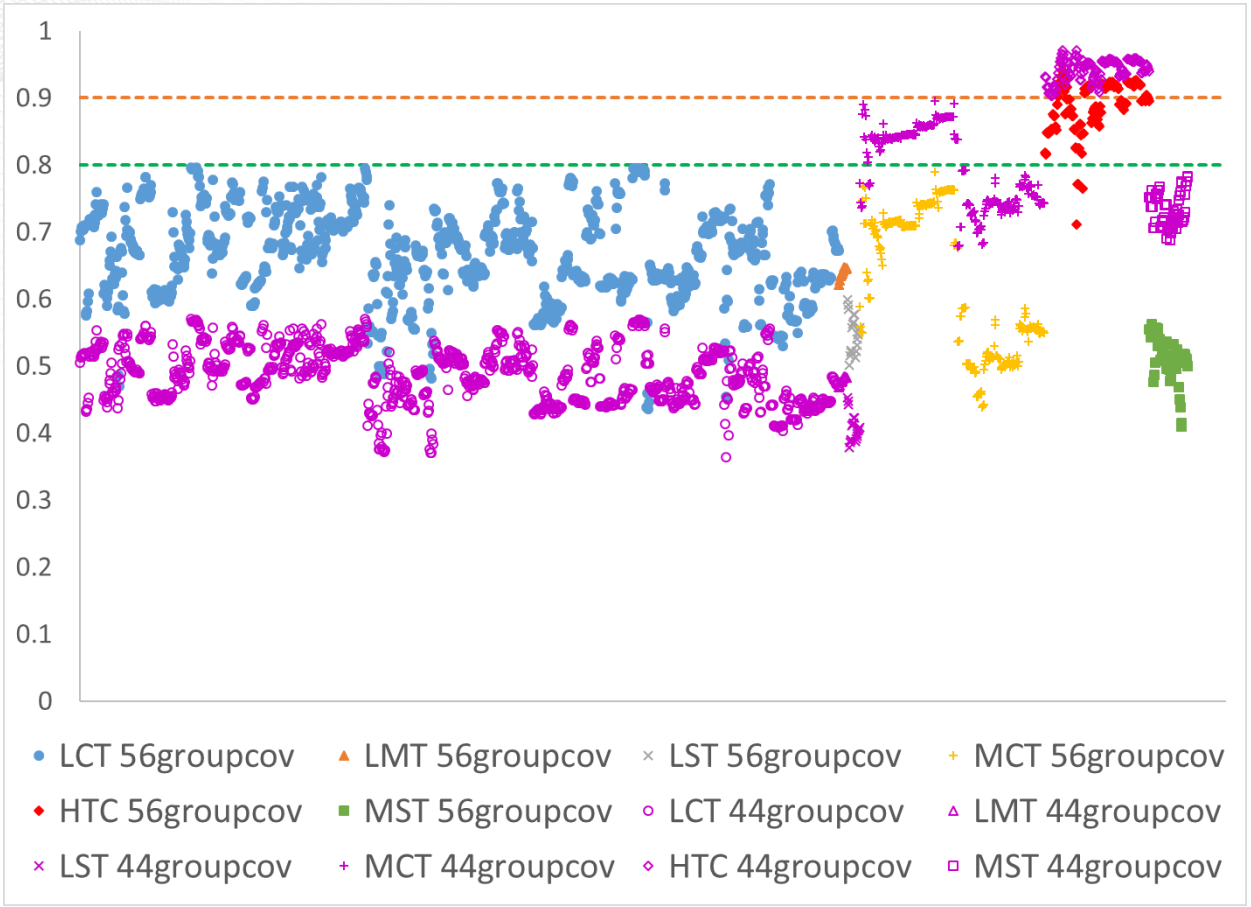
σ_{ij}^2 is off-diagonal term of $\mathbf{C_{kk}}$ matrix (aka covariance)

σ_i and σ_j are square root of diagonal terms (aka standard deviations)

c_k (similarity) assessment (2)

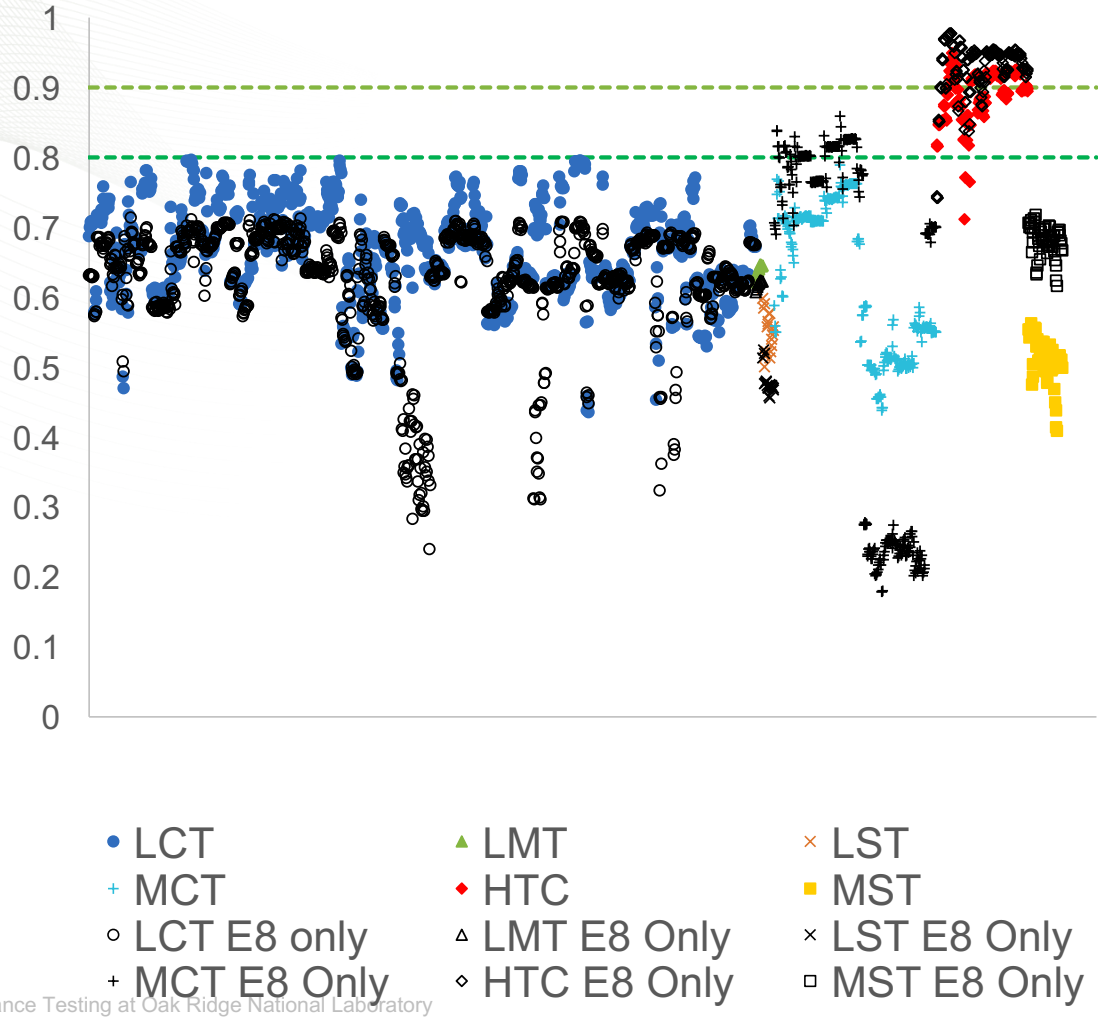
- Purpose (continued):
  - How is it useful in covariance testing?
    - c_k can indicate which covariance data are important in determining similarity
    - Results should be logical results of materials in systems
    - Especially helpful for comparison of primary fissile species uncertainty data
- Methodology:
  - TSUNAMI-IP calculates c_k-provided sensitivity data files for each application and experiment
  - "c" and "values" keywords in parameter block
  - "c_long" is also helpful because it provides the c_k contribution from each element in the covariance matrix

c_k results—historical context: SCALE 6.1 to SCALE 6.2



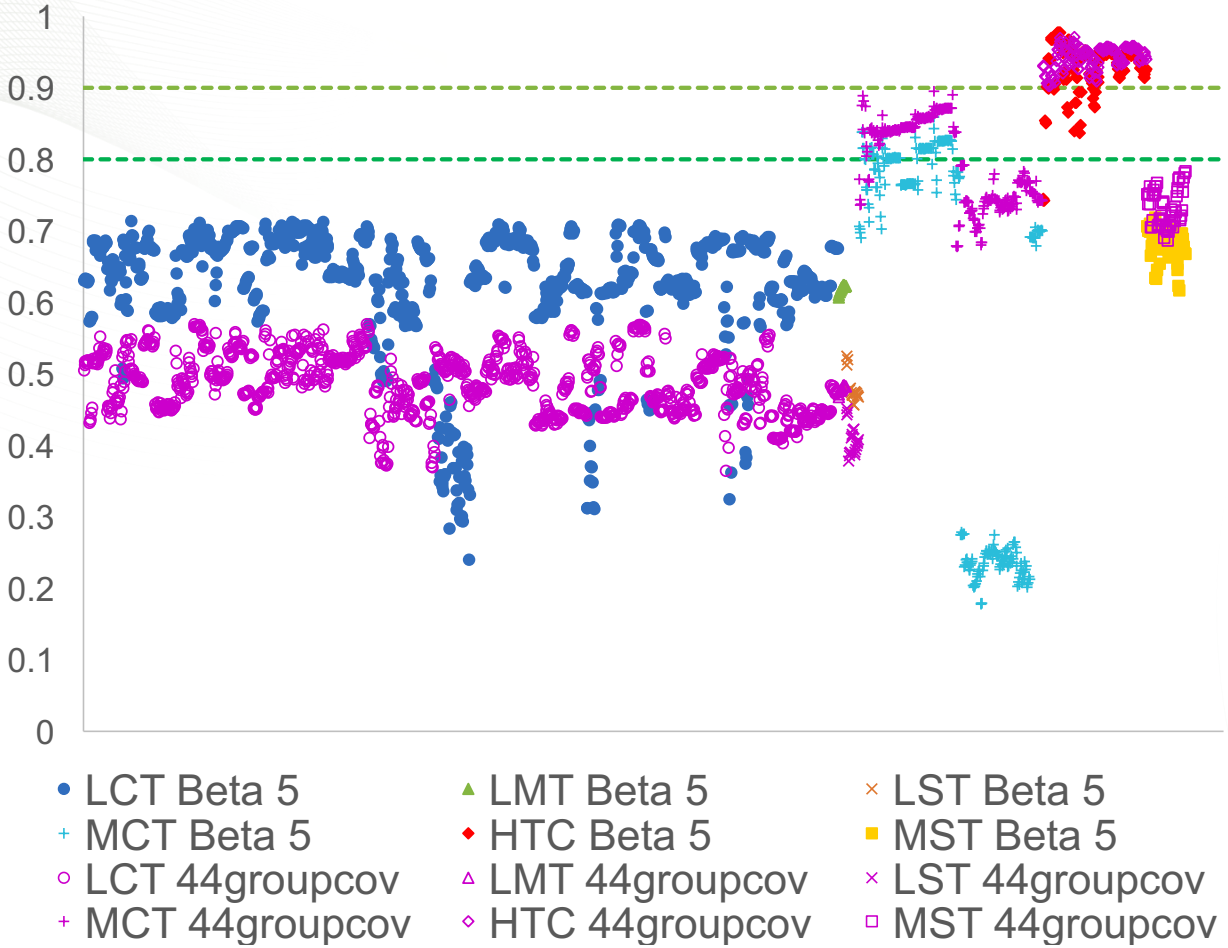
- 1643 unique critical experiments compared with pressurized-water reactor (PWR) spent nuclear fuel cask with fuel at representative discharge burnup
- SCALE 6.1 (purple)
- SCALE 6.2 (various)
- This change caused significant turmoil for use of c_k to select similar experiments for validation

c_k results—SCALE 6.2 & ENDF/B-VIII Beta 5 Plus



- SCALE 6.2 (various)
- ENDF/B-VIII plus SCALE data (black)
- Low c_k values for MCT are due to h-poly, as it currently is not associated with the uncertainty in ^{1}H

c_k results—SCALE 44 group library & ENDF/B-VIII



- 44 group library (various)
- ENDF/B-VIII plus SCALE data (pink)
- The balance has shifted back toward MCTs for PWR fuel, and more LCTs get over the 0.9 bar for peak reactivity. Also, the c_ks are a little better for the HTCs in both systems

Summary

- Substantial differences exist between ENDF/VII.1 and ENDF/B-VIII.0 Beta 5 covariance data
- ^{235}U nubar, ^{239}Pu, and ^{1}H covariance data have all increased and were previously identified by ORNL as being very large
- Uncertainty bands have historically been too wide, and they still tend to increase and not decrease with each new release
- Inappropriate uncertainty bands undermine the usefulness of S/U methods for criticality safety validation, reactor physics uncertainty quantification, and depletion calculation uncertainty quantification