

SCALE/AMPX Sensitivity and Uncertainty Analysis Capabilities and Data

Presented to:

OECD NEA Working Party on Evaluation Cooperation (WPEC) Subgroup 44 on Investigation of Covariance Data in General Purpose Nuclear Data Libraries

OECD/NEA Headquarters, Paris, France

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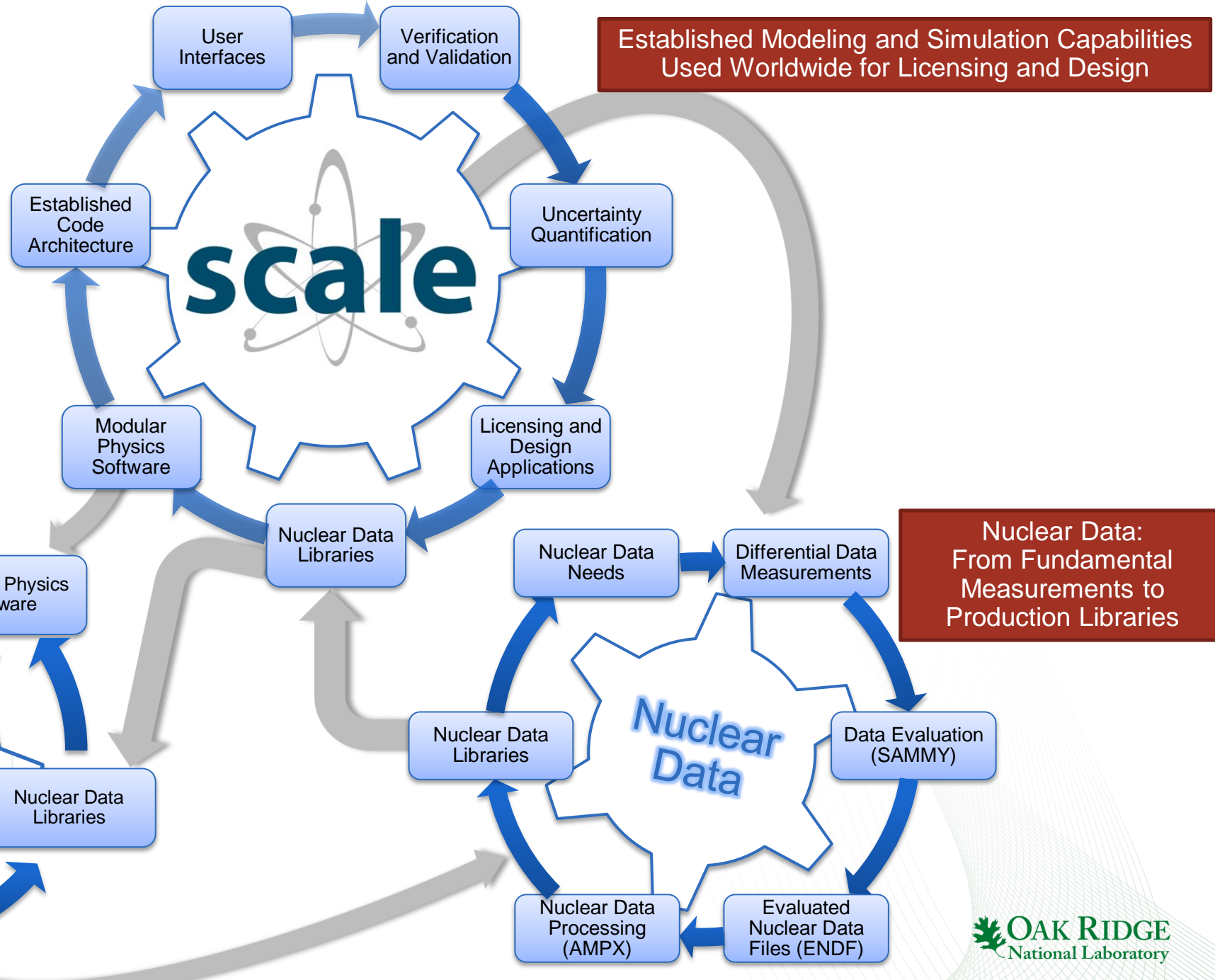
William J. Marshall

Dorothea Wiarda

ORNL is managed by UT-Battelle
for the US Department of Energy



Modeling and Simulation Tools for Neutronics and Shielding Analysis

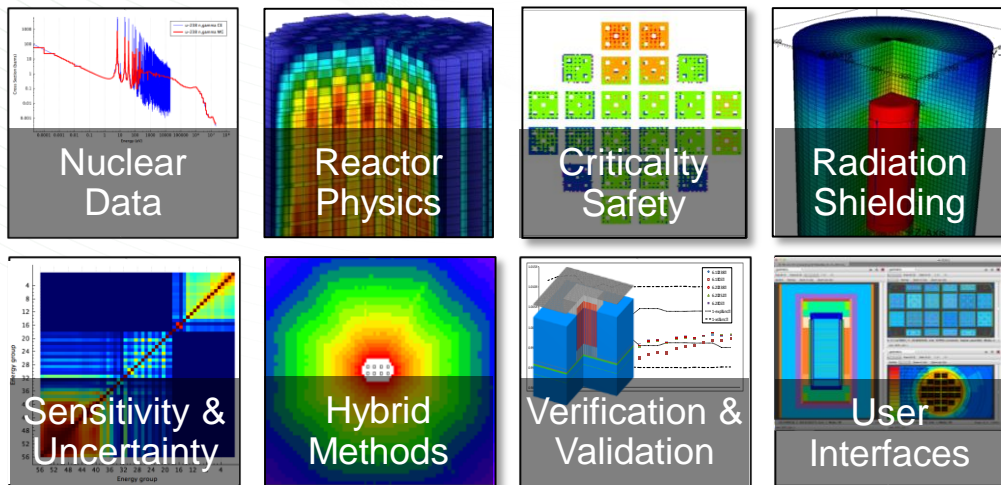


SCALE Code System

Neutronics and Shielding Analysis Enabling Nuclear Technology Advancements

<http://scale.ornl.gov>

Practical Tools Relied Upon for Operations and Regulation



Global Distribution: 8000 Users in 56 Nations

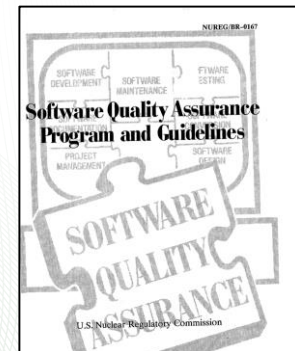
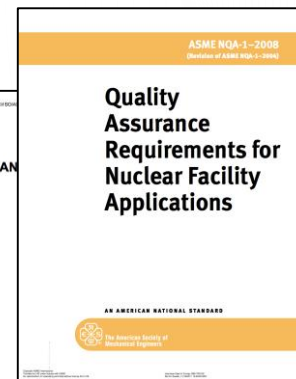
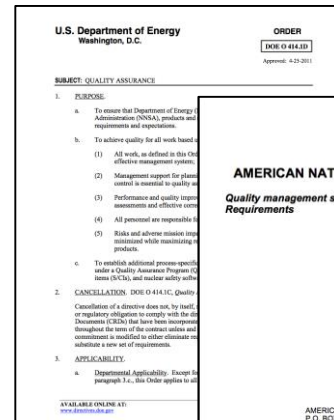


Professional Training for Practicing Engineers and Regulators

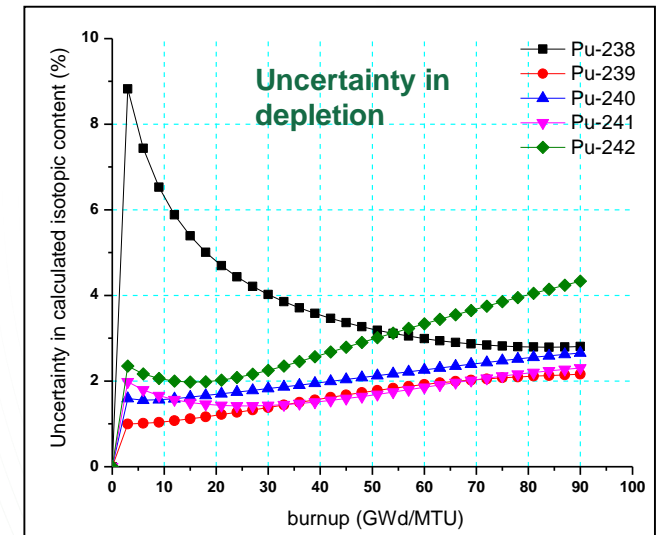
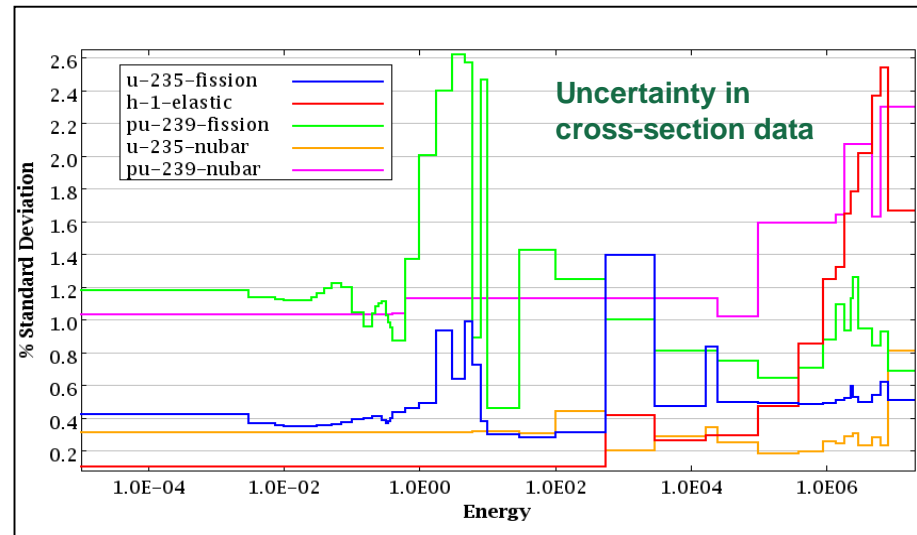
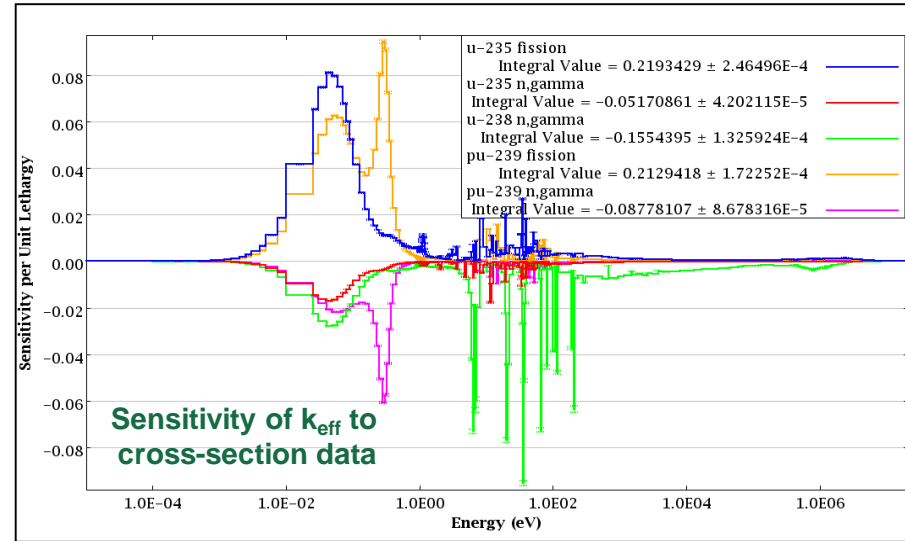
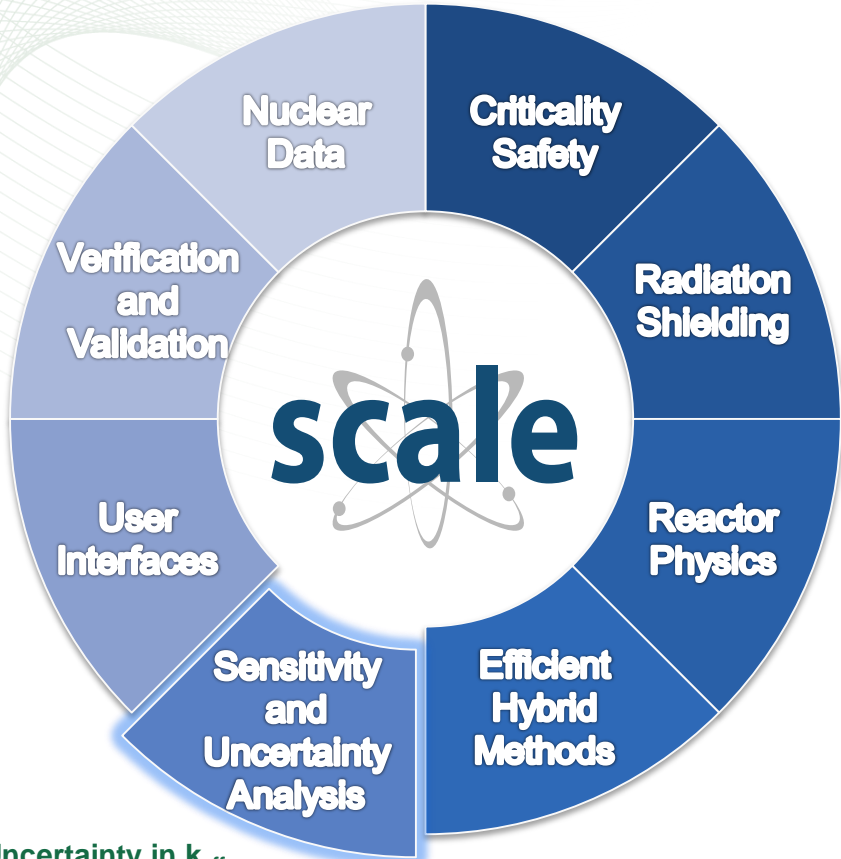


FY16 Statistics:
 12 week-long courses
 1 conference tutorial
 150 participants from 15 nations

Robust Quality Assurance Program Based on Multiple Standards



Sensitivity and Uncertainty Analysis

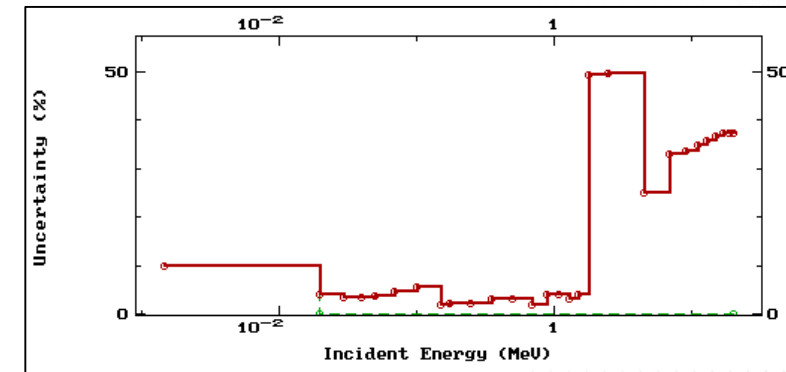
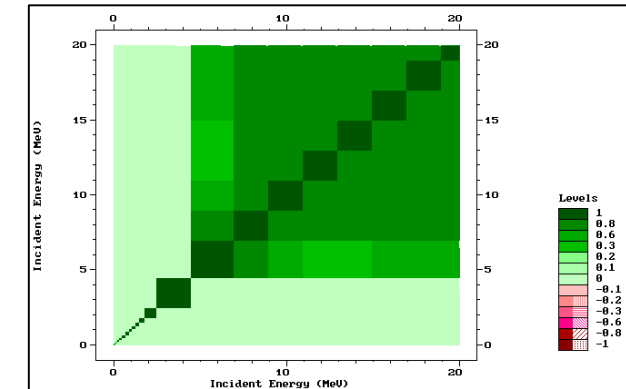
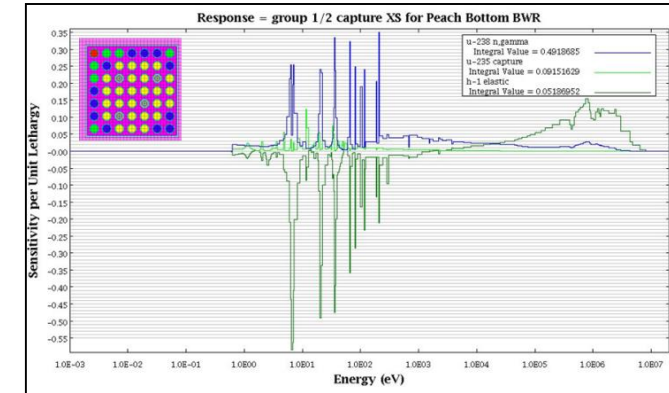


Uncertainty in k_{eff}

| Covariance Matrix | | Unc. in % dk/k |
|---------------------------|---------------------------|-----------------------------|
| Nuclide-Reaction | Nuclide-Reaction | Due to this Matrix |
| ²³⁹ Pu nubar | ²³⁹ Pu nubar | $4.0032E-01 \pm 2.5625E-06$ |
| ²³⁸ U n,gamma | ²³⁸ U n,gamma | $1.9457E-01 \pm 1.2387E-05$ |
| ²³⁹ Pu fission | ²³⁹ Pu fission | $1.5501E-01 \pm 1.0838E-05$ |
| ²³⁵ U nubar | ²³⁵ U nubar | $1.3981E-01 \pm 5.0038E-07$ |
| ²³⁹ Pu fission | ²³⁹ Pu n,gamma | $1.2261E-01 \pm 4.3564E-06$ |

Sensitivity and Uncertainty Enhancements

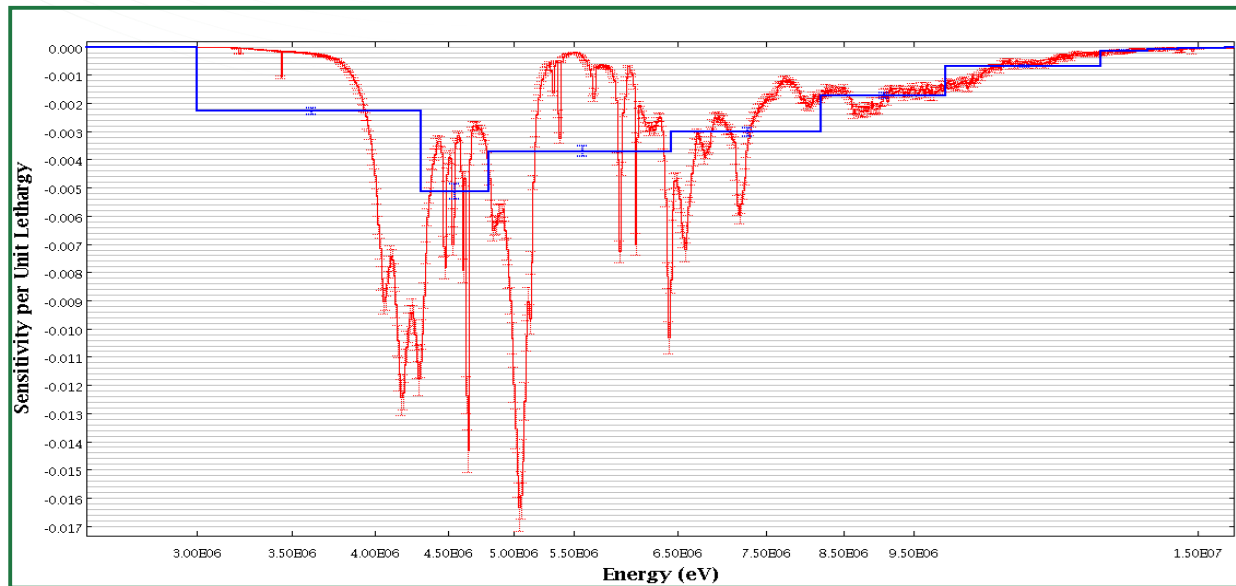
- Sensitivity computations with continuous-energy Monte Carlo for eigenvalue and GPT responses “CE-TSUNAMI”
- New statistical sampling code “Sampler” for general UQ of Scale MG Sequences
- Covariance data
 - Neutron cross section covariance library based on ENDF/B-VII.1 and previous SCALE 6.1 data
 - New fission product yield covariances
 - New decay data covariances
 - New gamma yield covariances
- Calculation of experimental correlation coefficients with Sampler



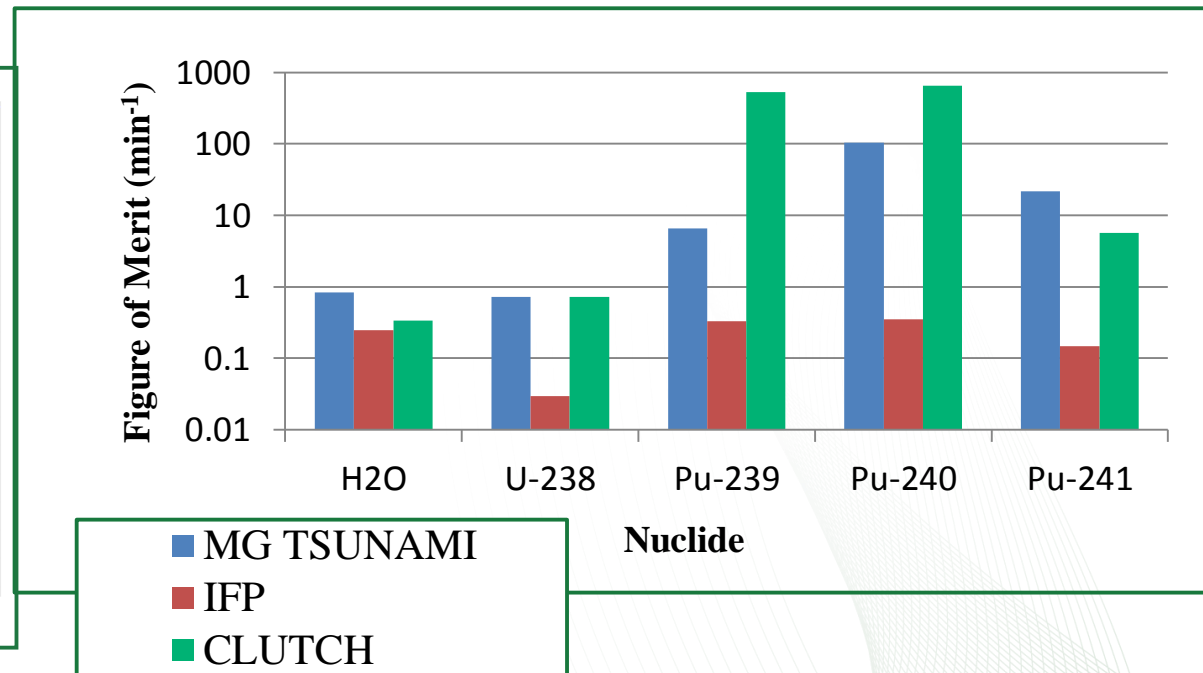
Continuous-energy TSUNAMI-3D

- In SCALE6.2 the multigroup TSUNAMI-3D code has been extended to perform continuous-energy (CE) sensitivity coefficient calculations.
 - This work involved the development of the CLUTCH sensitivity method, a new and efficient approach for calculating eigenvalue sensitivity coefficients.

O-16 Capture Sensitivity 238-group VS Microgroup CLUTCH



MIX-COMP-THERM-004-001 FoM Comparison



C. M. Perfetti, B. T. Rearden, and W. R. Martin, "SCALE Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations," *Nucl. Sci. Eng.* **182**(3), 332-353 (2016).

CE TSUNAMI-3D Sensitivity Capabilities use High-Fidelity Monte Carlo Methods

H-1 Elastic Scatter Sensitivity

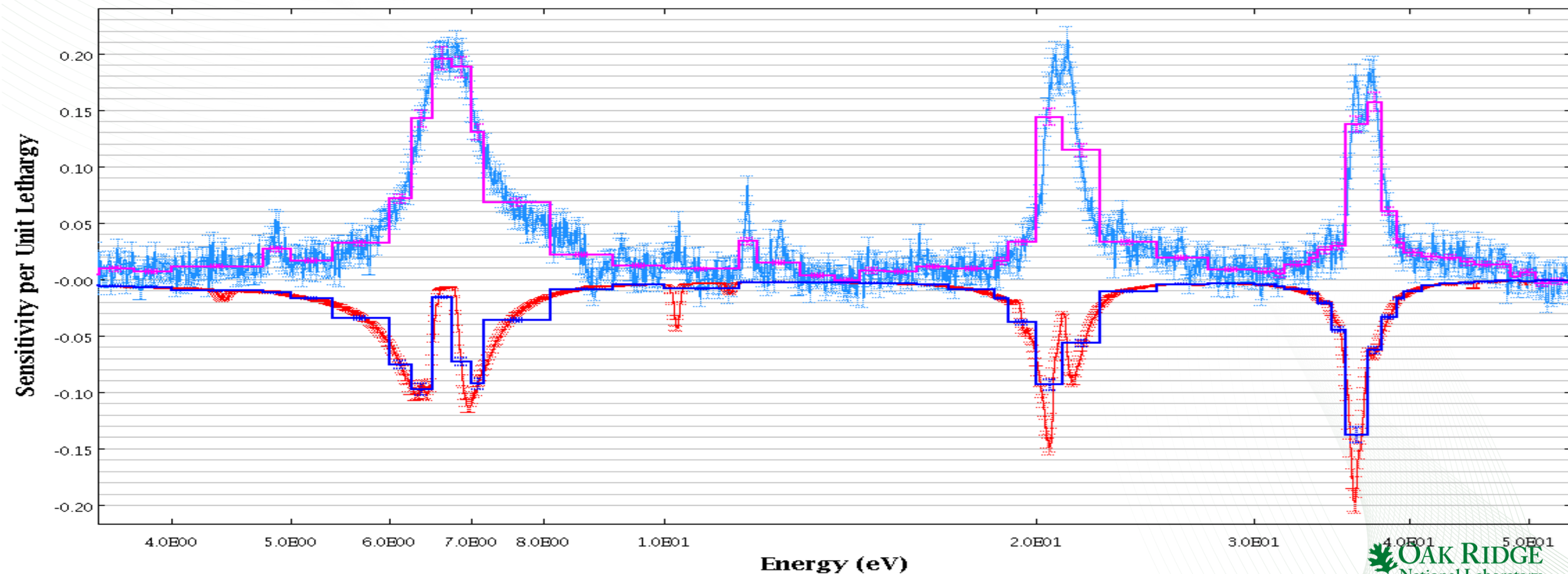
238-group CLUTCH VS

Microgroup CLUTCH

U-238 Capture Sensitivity

238-group CLUTCH VS

Microgroup CLUTCH



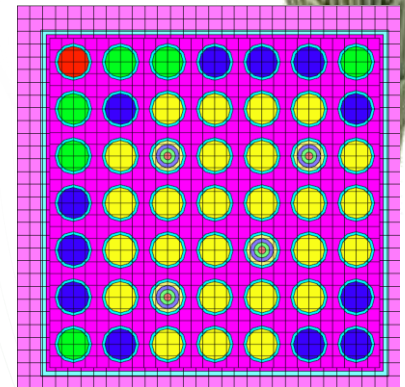
Generalized Perturbation Theory

- Recent developments have enabled the calculation of generalized response sensitivity coefficients using high-fidelity, continuous-energy Monte Carlo methods.
- Generalized Perturbation Theory (GPT) calculates sensitivity coefficients for any system response that can be expressed as the ratio of reaction rates.

$$R = \frac{\langle S_1 f \rangle}{\langle S_2 f \rangle}$$

- Applications for GPT sensitivity/uncertainty analysis include:
 - Relative powers
 - Isotope Conversion Ratios
 - Multigroup Cross Sections
 - Experimental Parameters

| NUMBER | EXPERIMENT | Type | Format | Value | Xsec Uncert |
|--------|---------------|------|----------|-----------|-------------------|
| 1 | k_infinity | keff | Relative | 1.1083E+0 | 4.98551E-1 % dk/k |
| 2 | fission_grp_1 | gpt | Relative | 1.9155E-3 | 6.91925E-1 % dR/R |
| 3 | fission_grp_2 | gpt | Relative | 2.7748E-2 | 3.23440E-1 % dR/R |
| 4 | absorpt_grp_1 | gpt | Relative | 7.1637E-3 | 8.36728E-1 % dR/R |
| 5 | absorpt_grp_2 | gpt | Relative | 5.3702E-2 | 2.38082E-1 % dR/R |
| 6 | cornerrod_fpf | gpt | Relative | 1.1458E+0 | 1.67147E-1 % dR/R |



GPT Calculations in CE TSUNAMI-3D

- The generalized importance function for a response can be expressed as the sum of two terms: the intra-generation effect term and the inter-generational effect term.
 - The **intra-generation** effect describes how much importance a neutron generates after an event occurs.
 - The **inter-generational** effect describes the importance that is generated by the daughter fission neutrons of the original particle.

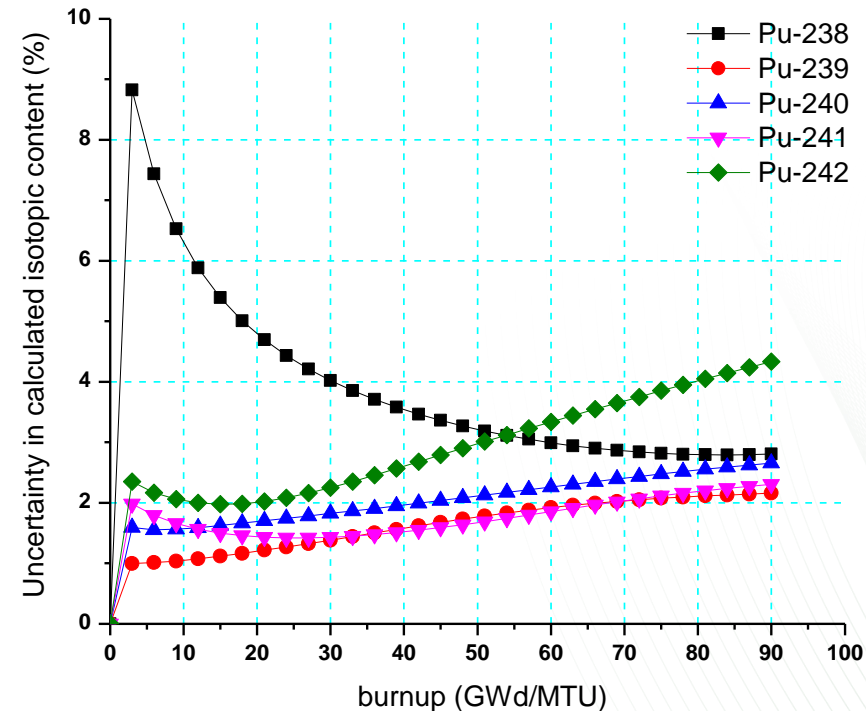
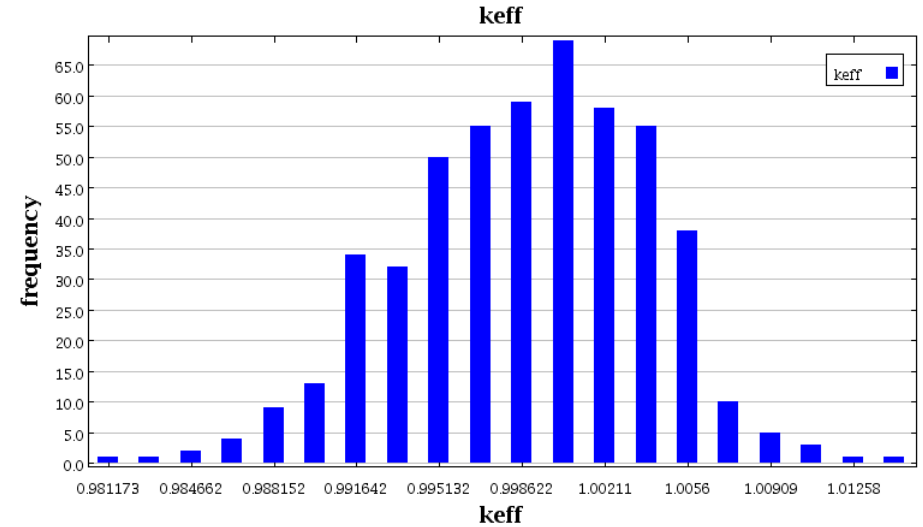
$$\Gamma^\dagger(\tau_s) = \frac{1}{Q_s} \left\langle \frac{1}{R} \frac{\partial R}{\partial \phi}(r) \phi(\tau_s \rightarrow r) \right\rangle + \frac{\lambda}{Q_s} \left\langle \Gamma^\dagger(r) P(r) \phi(\tau_s \rightarrow r) \right\rangle$$

- CE TSUNAMI-3D uses the **CLUTCH** sensitivity method to calculate the intra-generation term, and an **Iterated Fission Probability**-based approach to calculate the inter-generational term.

C. M. Perfetti and B. T. Rearden, "Development of a Generalized Perturbation Theory Method for Uncertainty and Sensitivity Analysis Using Continuous-Energy Monte Carlo Methods," *Nucl. Sci. Eng.* **182**(3), 354-368 (2016).

Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

- Sampler provides uncertainty in **any** computed result from **any** SCALE sequence due to uncertainties in:
 - neutron cross sections
 - fission yield and decay data
 - geometry and composition
- Sampler propagates uncertainties through **complex analysis sequences** such as depletion calculations
- **Correlations** between systems are also computed



SCALE 6.0–6.1 Covariance Library (401 materials)

| Data Source | Materials |
|--------------------------------|--|
| ENDF/B-VII.0 | ^{152,154-158,160} Gd, ^{191,193} Ir, ⁷ Li, ⁹⁹ Tc, ²³² Th |
| ENDF/B-VII-p | ¹⁹⁷ Au, ²⁰⁹ Bi, ⁵⁹ Co, ²³ Na, ⁹³ Nb, ⁵⁸ Ni, ²³⁹ Pu, ⁴⁸ Ti, ^{233,235,238} U*, V |
| ENDF/B-VI | ²⁷ Al, ²⁴¹ Am, C, C-graphite, ^{50,52-54} Cr, ⁶⁵ Cu, ¹⁵⁶ Dy, ^{54,56-58} Fe, In, ⁵⁵ Mn, ^{60-62,64} Ni, ²⁰⁶⁻²⁰⁸ Pb, ²⁴² Pu, ^{185,187} Re, ⁴⁵ Sc, Si, ²⁸⁻³⁰ Si, ⁸⁹ Y |
| JENDL 3.3 | ¹¹ B, ^{240,241} Pu |
| JENDL 3.3+BLO | ¹⁶ O |
| SG-26 | ^{234,236} U, ^{242,242m} Am, ²⁴²⁻²⁴⁵ Cm, ²³⁷ Np, ²³⁸ Pu |
| BLO LANL evaluation +JENDL 3.3 | ¹⁰ B, ¹ H, H-ZrH, H-poly, Hfreegas |
| BLO LANL evaluation | ⁶ Li |
| BLO Approximate Data | ²²⁵⁻²²⁷ Ac, ^{107,109,110m,111} Ag, ^{243,244,244m} Am, ^{36,38,40} Ar, ⁷⁴⁻⁷⁵ As, ^{130,132,133,135-138,140} Ba, ^{7,9} Be, Bebound, ^{249,250} Bk, ^{79,81} Br, Ca, ^{40,42-44,46,48} Ca, Cd, ^{106,108,110-114,115m,116} Cd, ^{136,138,139-144} Ce, ²⁴⁹⁻²⁵⁴ Cf, Cl, ^{35,37} Cl, ^{241,246-250} Cm, ^{58,58m} Co, ¹³³⁻¹³⁷ Cs, ⁶³ Cu, ^{158,160-164} Dy, ^{162,64,166-168,170} Er, ²⁵³⁻²⁵⁵ Es, ¹⁵¹⁻¹⁵⁷ Eu, ¹⁹ F, ²⁵⁵ Fm, Ga, ^{69,71} Ga, ¹⁵³ Gd, ^{70,72-74,76} Ge, ^{2,3} H, Dfreegas, ^{3,4} He, Hf, ^{174,176-180} Hf, ^{196,198-202,204} Hg, ¹⁶⁵ Ho, ^{127,129-131,135} I, ^{113,115} In, K, ³⁹⁻⁴¹ K, ^{78,80,82-86} Kr, ¹³⁸⁻¹⁴⁰ La, ^{175,176} Lu, Mg, ²⁴⁻²⁶ Mg, Mo, ^{92,97-100} Mo, ^{14,15} N, ^{94,95} Nb, ^{142-148,150} Nd, ⁵⁹ Ni, ^{235,236,238,239} Np, ¹⁷ O, ³¹ P, ²³¹⁻²³³ Pa, ²⁰⁴ Pb, ^{102,104-108,110} Pd, ^{147,148,148m,149,151} Pm, ¹⁴¹⁻¹⁴³ Pr, ^{236,237,243,244,246} Pu, ⁸⁵⁻⁸⁷ Rb, ^{103,105} Rh, ^{96,98-106} Ru, S, ^{32-34,36} S, ^{121,123-126} Sb, ^{74,76-80,82} Se, ^{144,147-154} Sm, ^{112-120,122-125} Sn, ^{84,86-90} Sr, ^{181,182} Ta, ^{159,160} Tb, ^{120,122-126,127m,128,129m,130} Te, ^{227-230,233,234} Th, Ti, ^{46,47,49,50} Ti, ^{232,237,239-241} U, W, ^{182-184,186} W, ^{123,124,126,128-136} Xe, ^{90,91} Y, Zr, ⁹⁰⁻⁹⁶ Zr |

| | |
|--|--|
| ENDF/B-VII.0: evaluated covariance data released with ENDF/B-VII.0 | JENDL-3.3: evaluated covariance data in JENDL-3.3 |
| ENDF/B-VII-p: recently evaluated data proposed for future release of ENDF/B-VII.1 | BLO approximate data: lo-fi covariances from BLO project (Brookhaven, Los Alamos, ORNL) |
| ENDF/B-VI: evaluated covariance data released with ENDF/B-VI | BLO LANL evaluation: LANL R-matrix evaluation from BLO project |

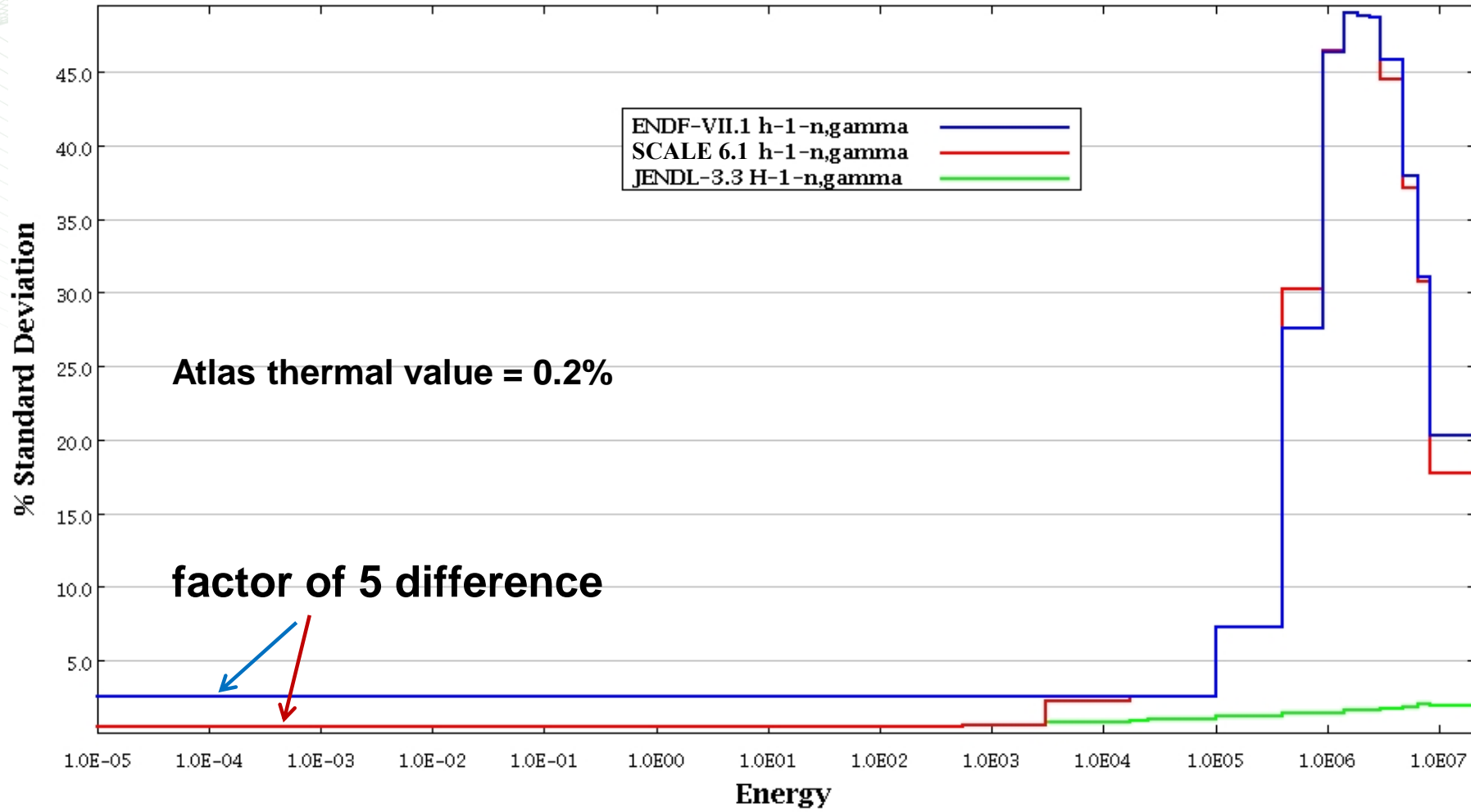
* ²³⁵U thermal nuubar data from JENDL 3.3

SG-26: approximate covariances from WPEC Subgroup-26

ENDF/B-VII.1 Covariance Nuclides

| | | | | | | | |
|------|-------|-------|-------|-------|---------|------------|--------------|
| h1 | ti50 | tc99 | sm151 | pb204 | np235 | bk245 | h-zr2 |
| h2 | cr50 | ru101 | sm152 | pb206 | np236 | bk246 | o-beo |
| he4 | cr52 | ru102 | eu153 | pb207 | np237 | bk247 | o-u2o |
| li6 | cr53 | ru103 | eu155 | pb208 | np238 | bk248 | si28_si2o |
| li7 | cr54 | ru104 | gd152 | bi209 | np239 | bk249 | si29_si2o |
| be9 | mn55 | ru106 | gd153 | ac225 | pu236 | bk250 | si30_si2o |
| b10 | fe54 | rh103 | gd154 | ac226 | pu237 | cf246 | u235_u2o |
| b11 | fe56 | pd105 | gd155 | ac227 | pu238 | cf248 | zr90_zr_zrh |
| c | fe57 | pd106 | gd156 | th227 | pu239 | cf249 | zr91_zr_zrh |
| n15 | co59 | pd107 | gd157 | th228 | pu240 | cf250 | zr92_zr_zrh |
| o16 | ni58 | pd108 | gd158 | th229 | pu241 | cf251 | zr93_zr_zrh |
| f19 | ni60 | ag109 | gd160 | th230 | pu242 | cf252 | zr94_zr_zrh |
| na23 | y89 | i127 | er166 | th231 | pu244 | cf253 | zr95_zr_zrh |
| mg24 | zr90 | i129 | er167 | th232 | pu246 | cf254 | zr96_zr_zrh |
| mg25 | zr91 | xe131 | er168 | th233 | am240 | es251 | h-benzene |
| mg26 | zr92 | xe132 | er170 | th234 | am241 | es252 | benzene |
| al27 | zr93 | xe134 | tm169 | pa229 | am242m1 | es253 | graphite |
| si28 | zr94 | cs133 | tm170 | pa230 | am243 | es254 | h-liquid_ch4 |
| si29 | zr95 | cs135 | w180 | pa232 | cm240 | es254m1 | d-cryo_ortho |
| si30 | zr96 | la | w182 | u230 | cm241 | es255 | h-cryo_ortho |
| cl35 | nb95 | ce141 | w183 | u231 | cm242 | fm255 | d-cryo_para |
| cl37 | mo92 | pr141 | w184 | u232 | cm243 | al_thermal | h-cryo_para |
| k39 | mo94 | nd143 | w186 | u233 | cm244 | fe_thermal | h-solid_ch4 |
| k41 | mo95 | nd145 | ir191 | u234 | cm245 | bebound | |
| ti46 | mo96 | nd146 | ir193 | u235 | cm246 | be-beo | |
| ti47 | mo97 | nd148 | au197 | u236 | cm247 | h-h2o | |
| ti58 | mo98 | pm147 | tl203 | u238 | cm249 | d-d2o | |
| ti49 | mo100 | sm149 | tl205 | np234 | cm250 | h-poly | |

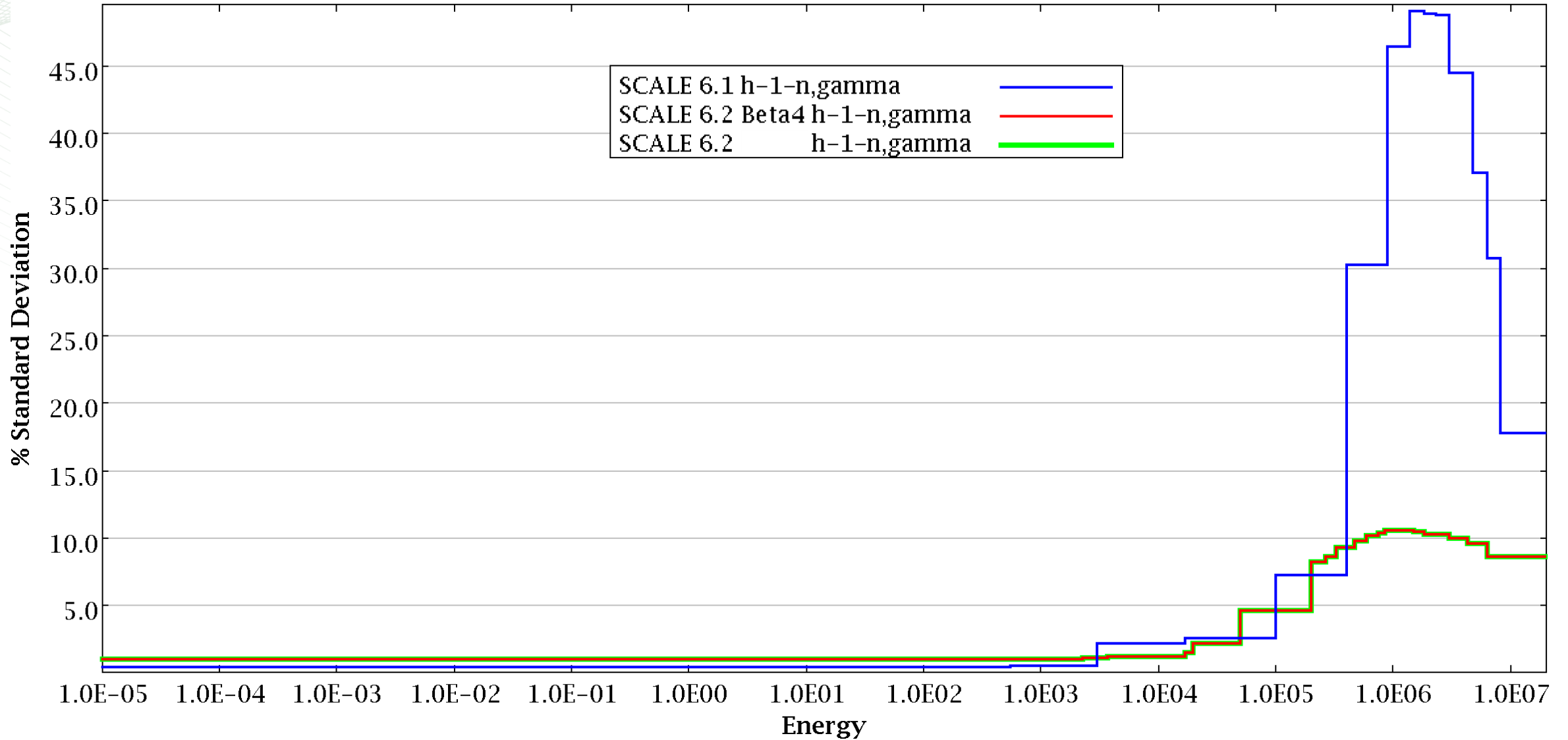
H Capture Uncertainty



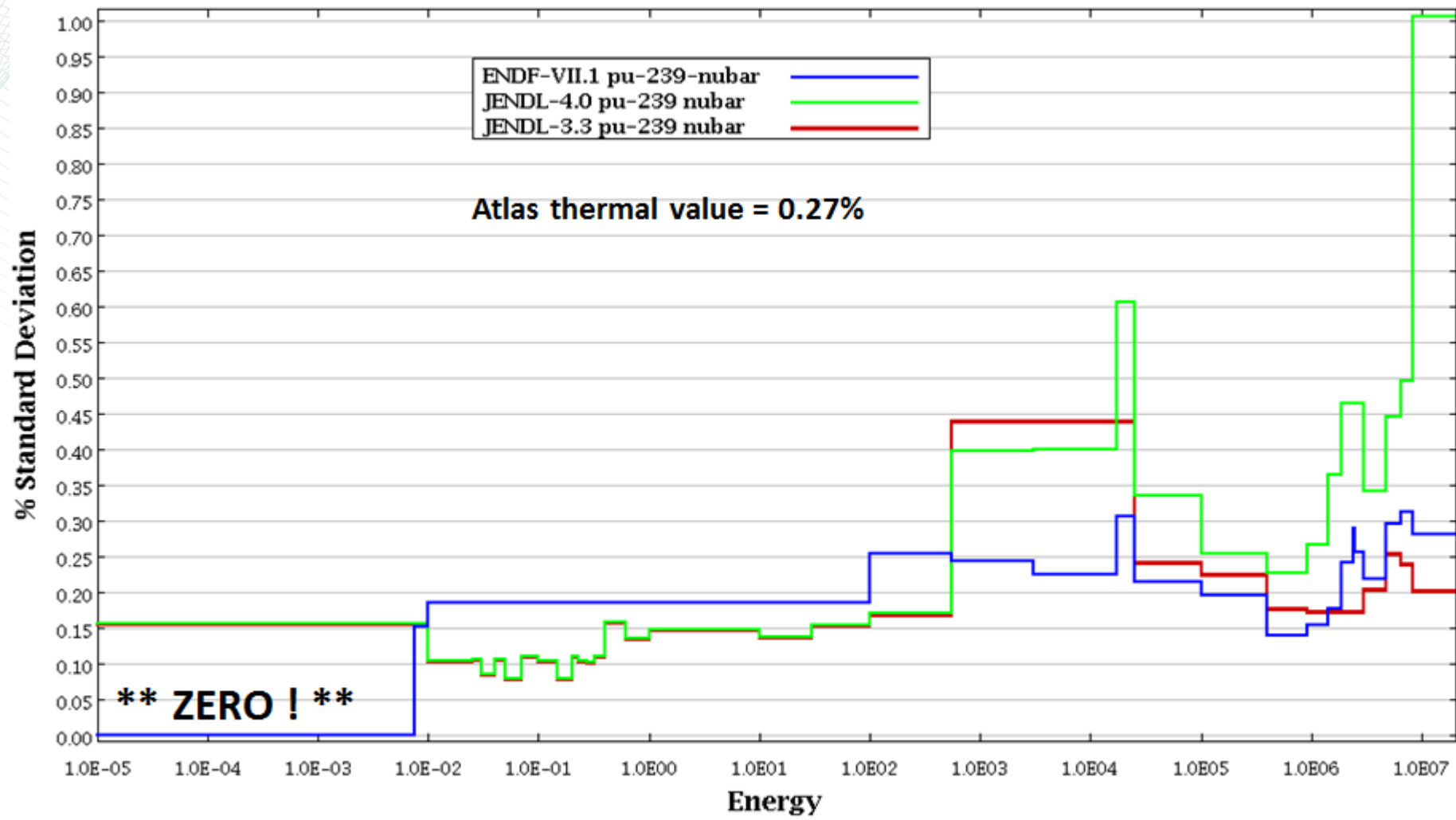
Atlas thermal value = 0.2%

factor of 5 difference

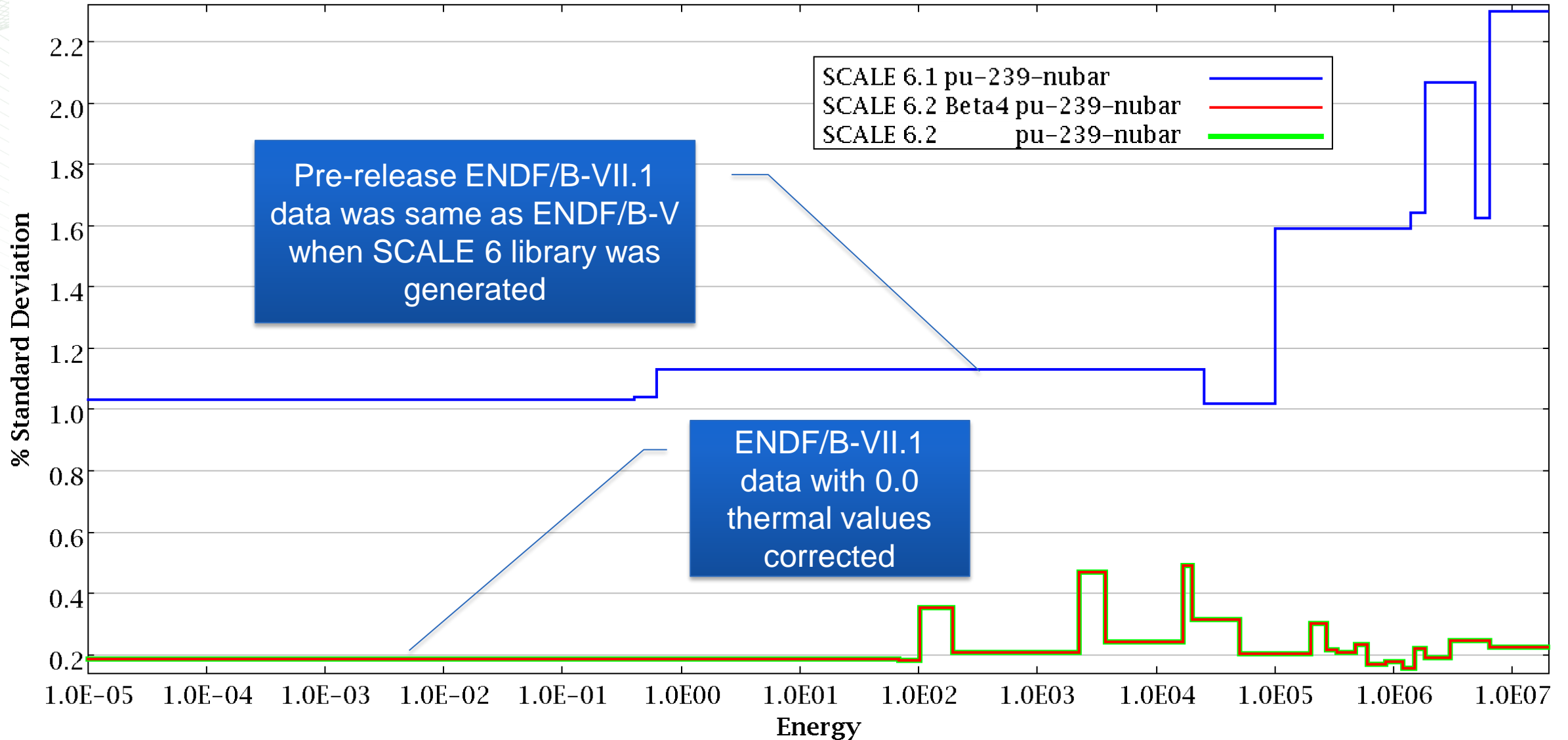
H Capture Uncertainty



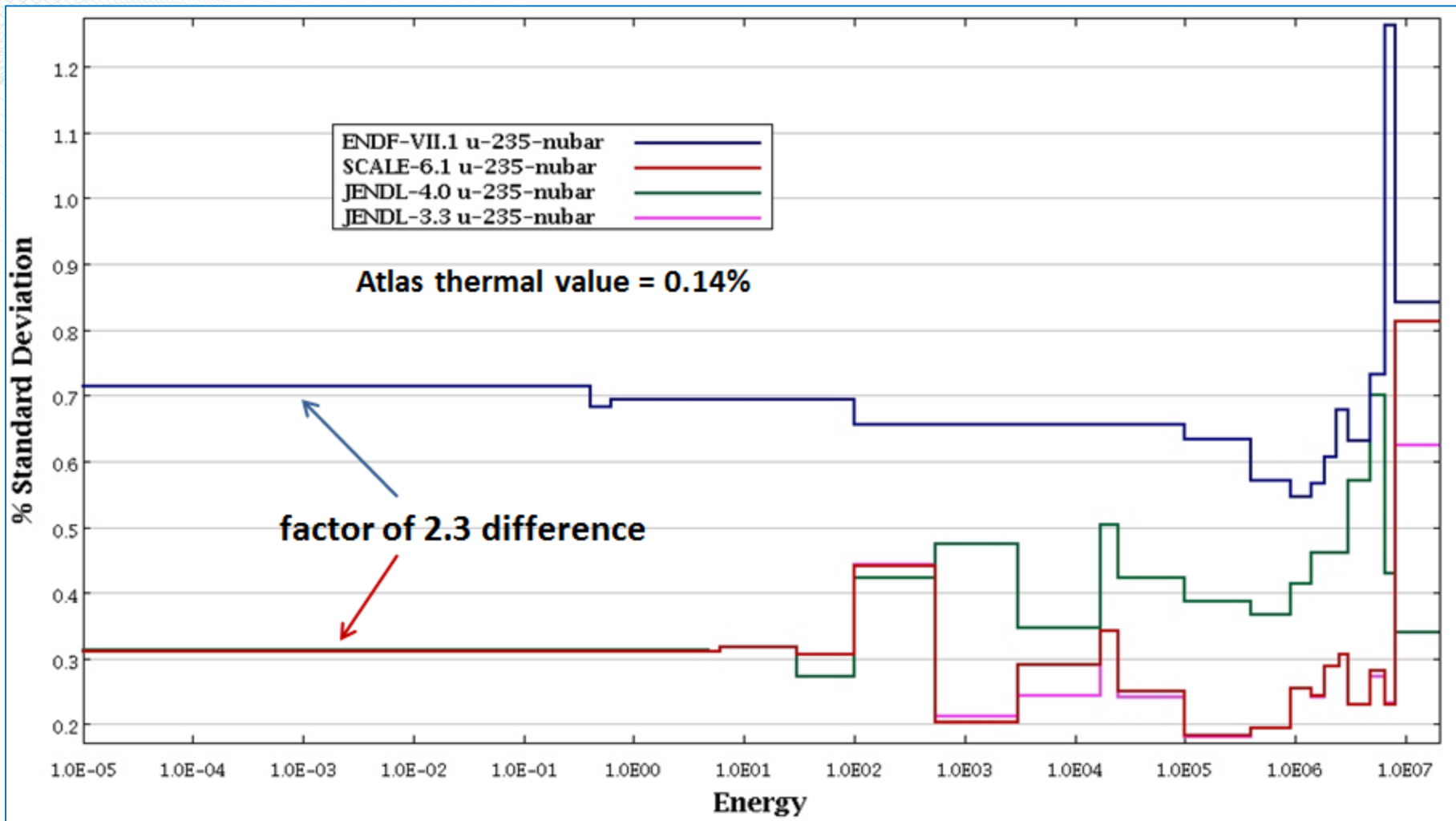
Pu-239 nubar uncertainty



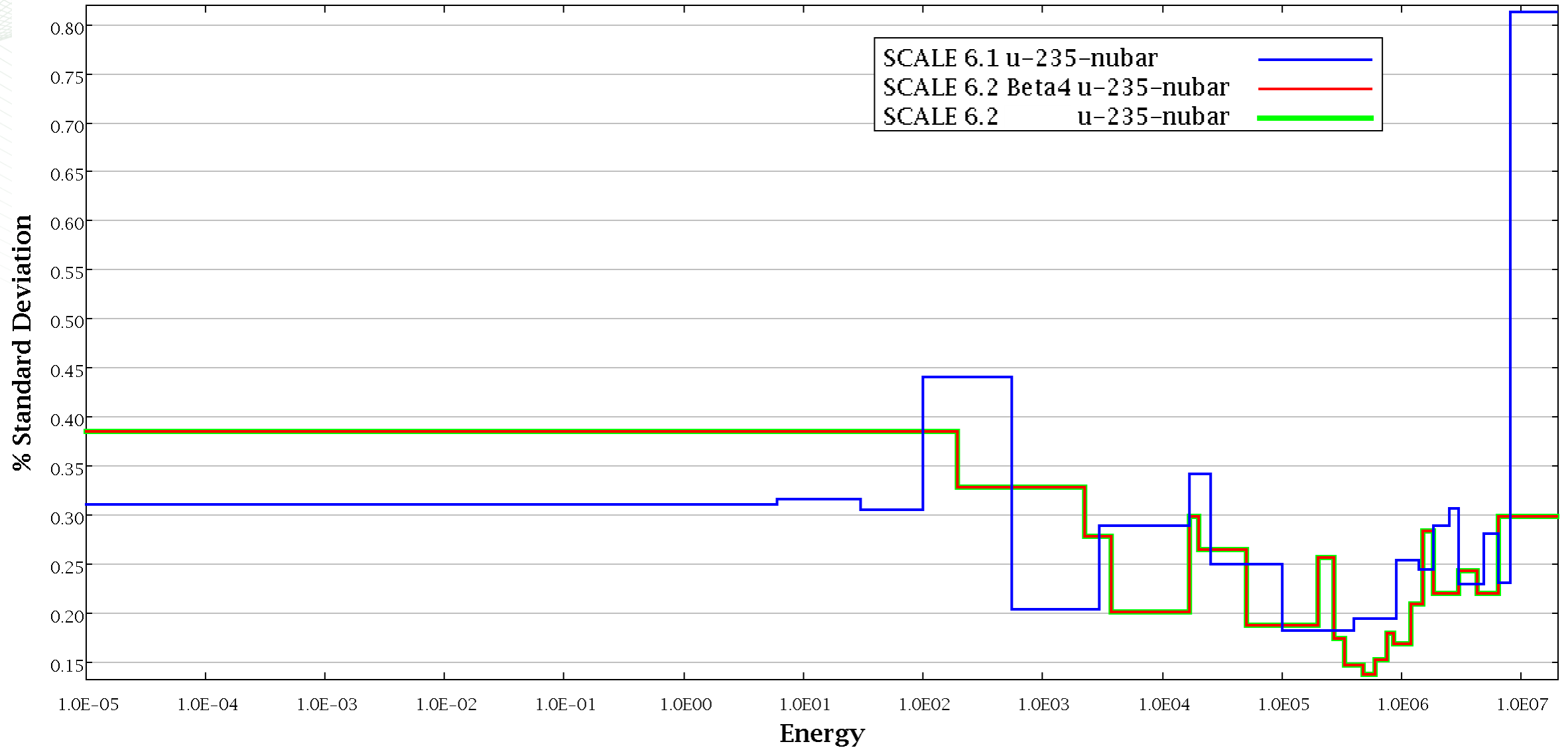
Pu-239 nubar uncertainty



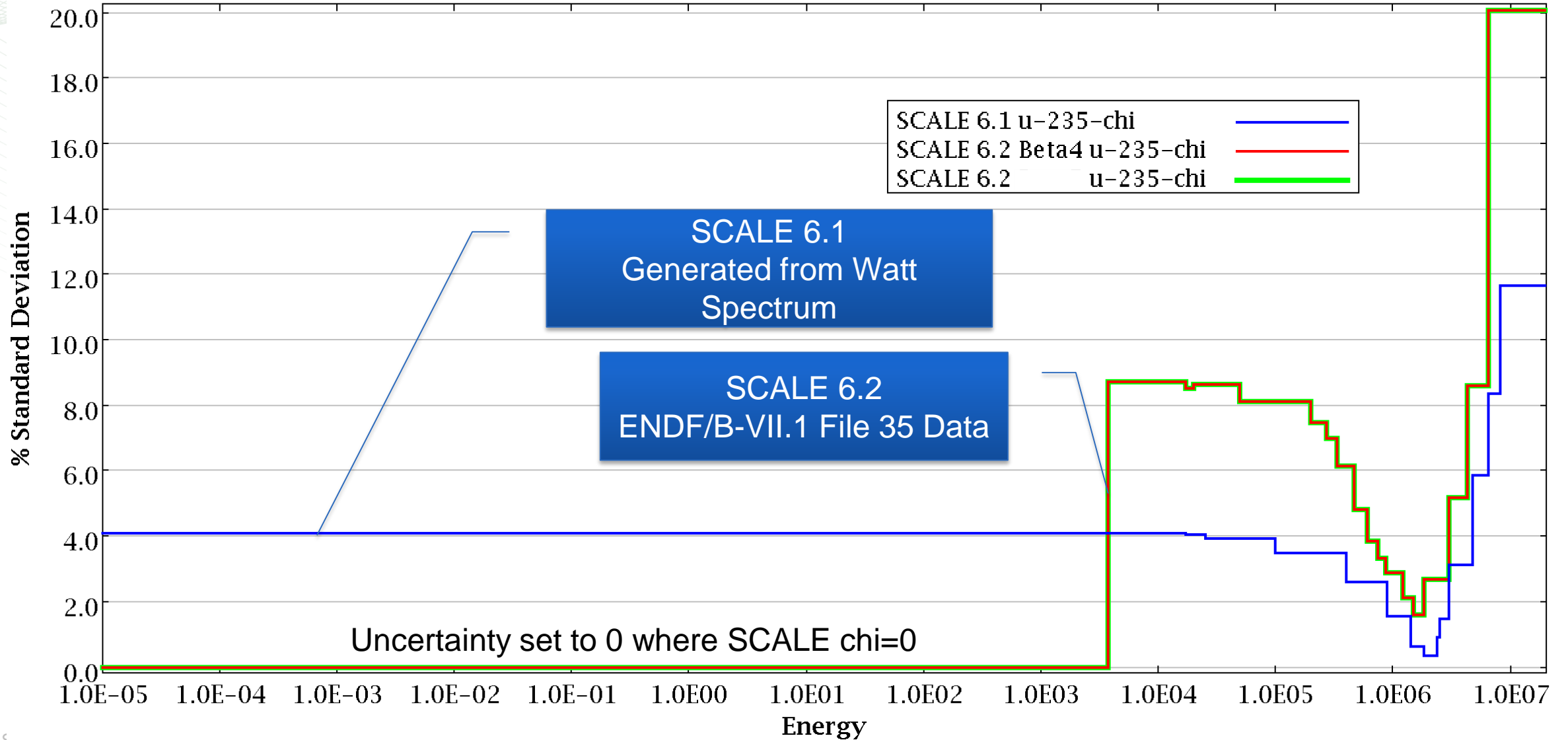
U-235 nubar uncertainty



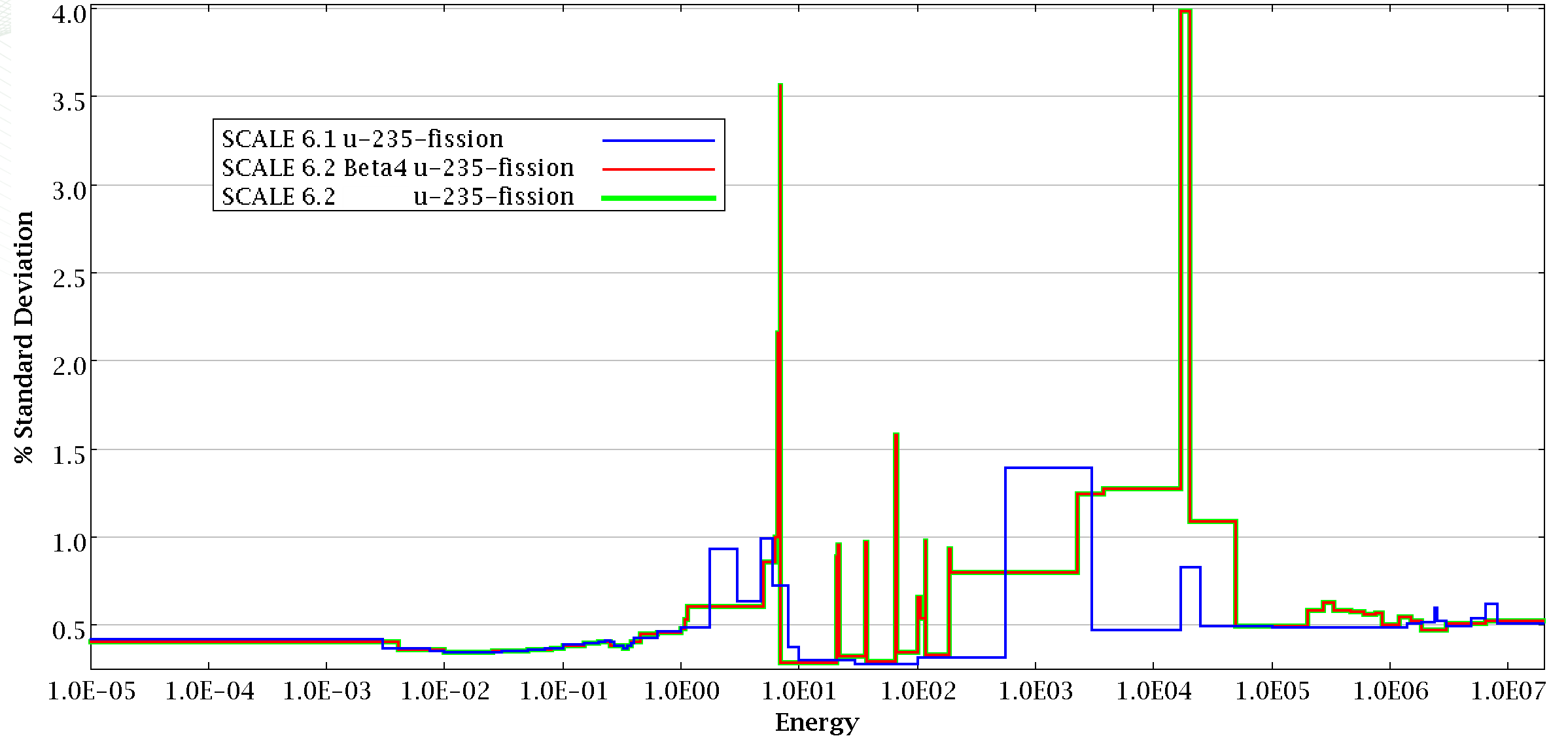
U-235 nubar uncertainty



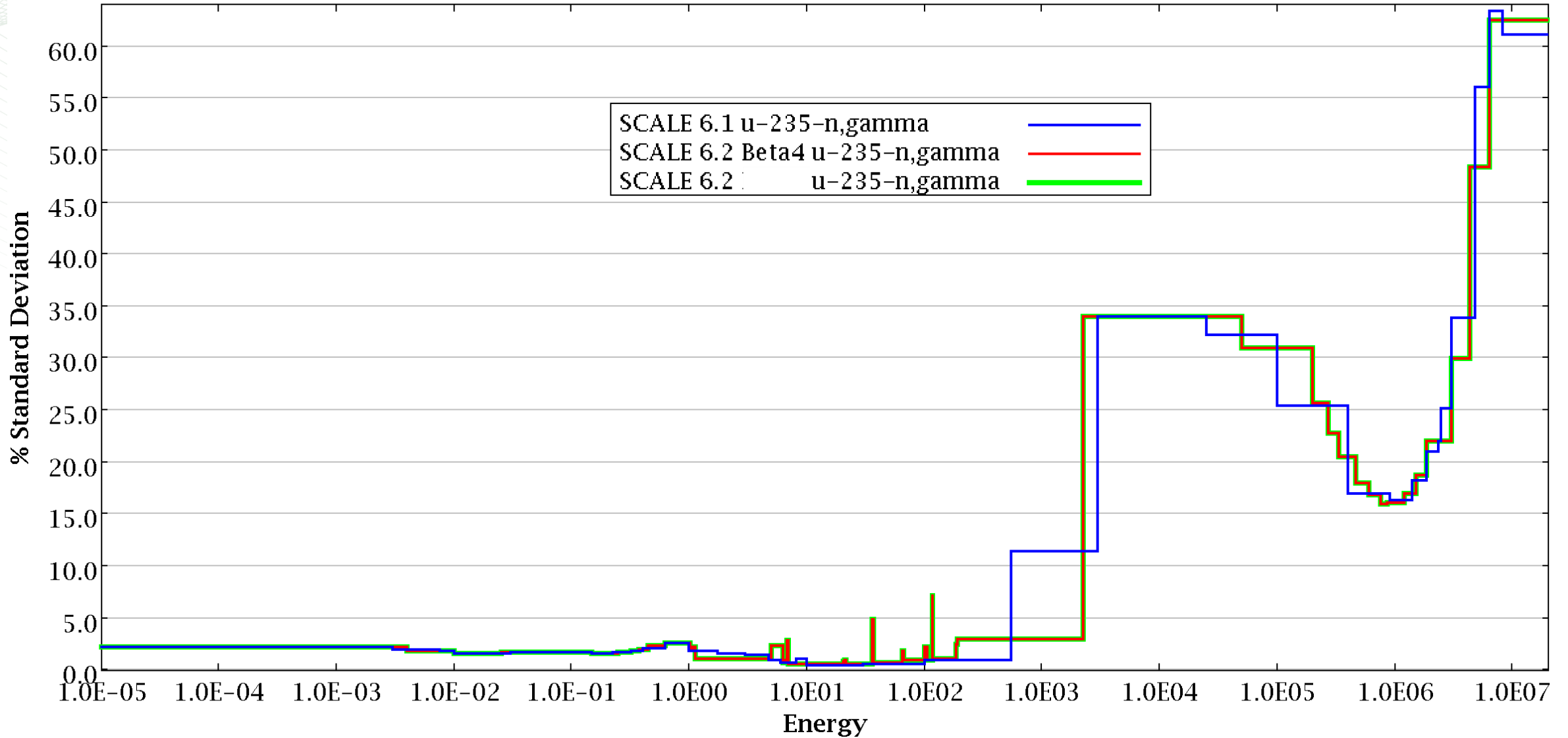
U-235 chi uncertainty



U-235 fission uncertainty

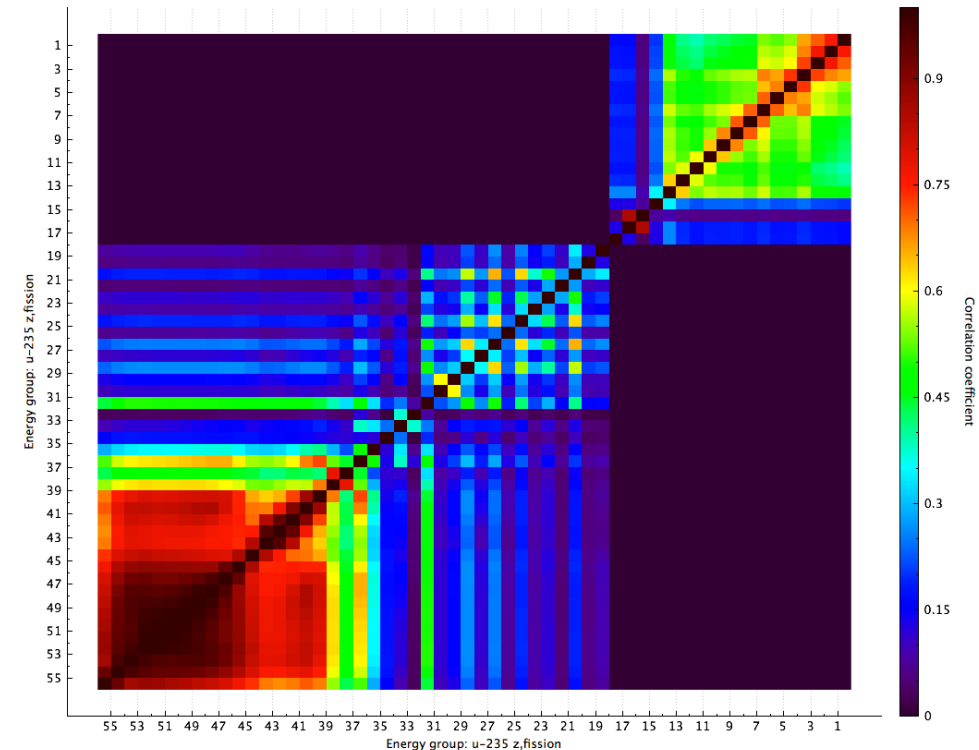
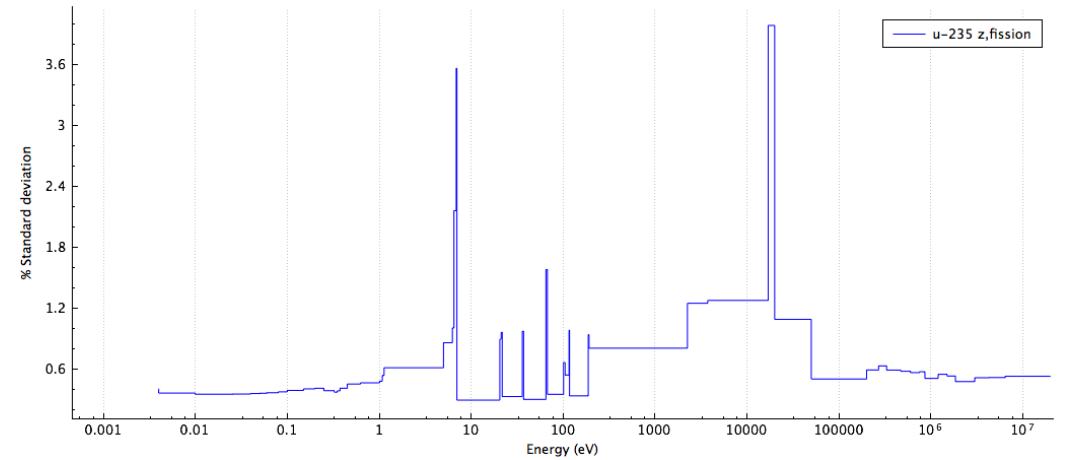


U-235 n,gamma uncertainty



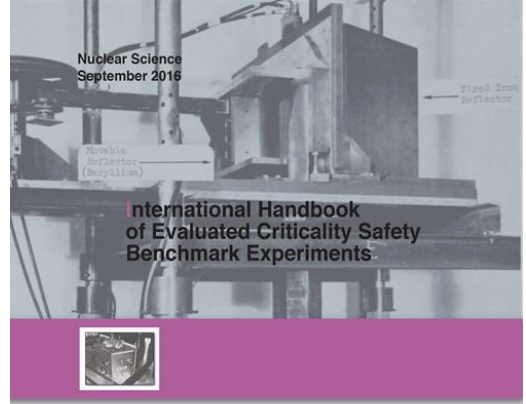
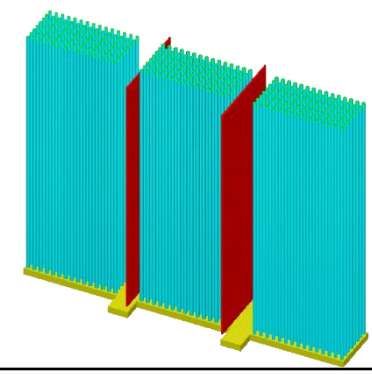
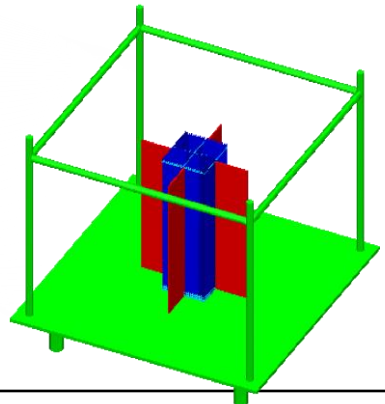
SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes
- SCALE 6.1 data retained for ~215 missing nuclides
- Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF/A repository
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 and from JENDL 4.0 (minor actinides)
 - Previous SCALE chi uncertainties were generated from Watt spectrum data and data were missing for minor actinides
- 56- and 252-group energy structures



Validation with critical benchmarks for many types of systems

- 411 configurations from International Criticality Safety Benchmark Evaluation Project (ICSBEP)



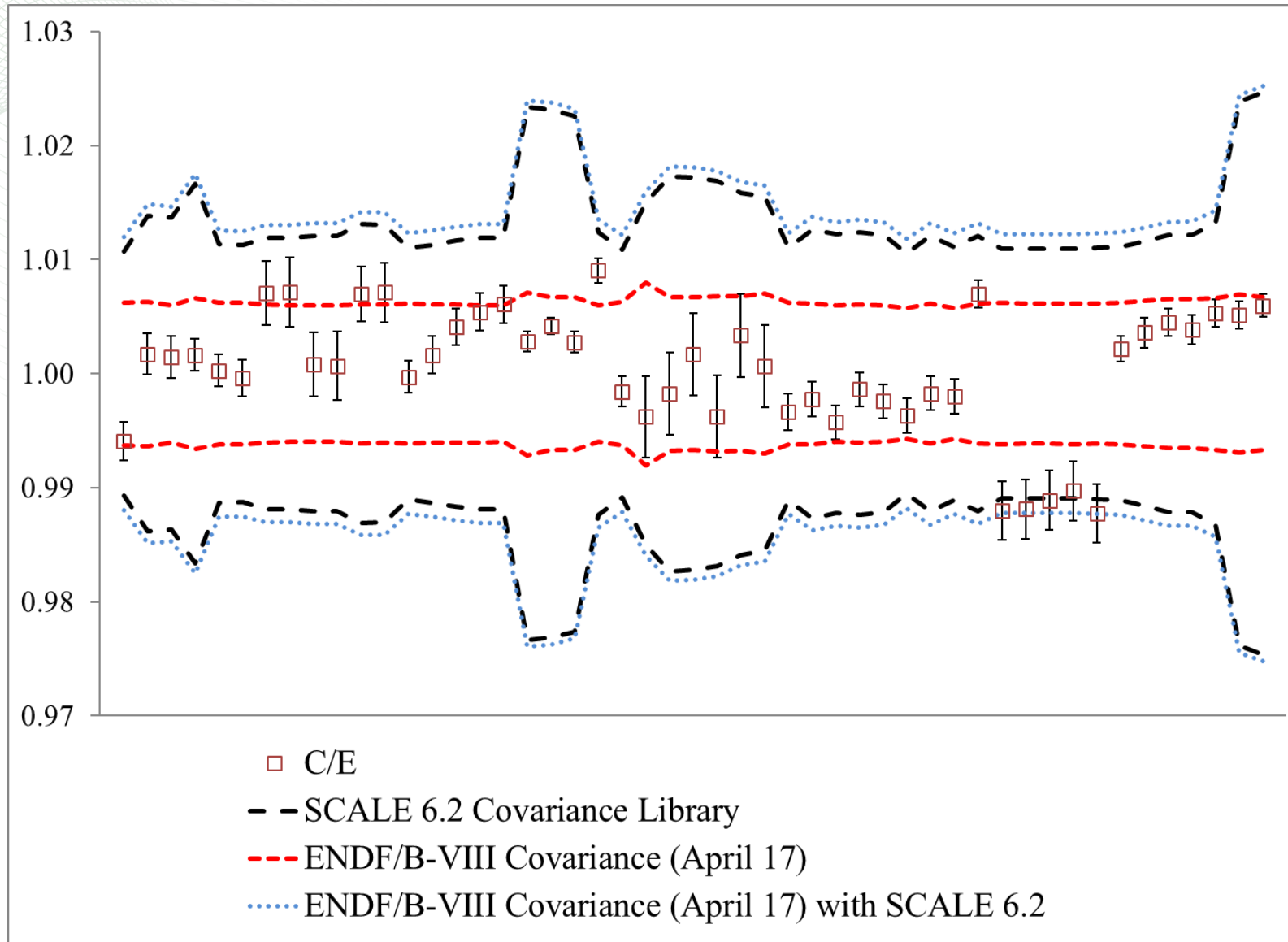
| Sequence / Geometry | Experiment class | ICSBEP case numbers | Number of configurations |
|---------------------|------------------|--|--------------------------|
| CSAS5 / KENO V.a | HEU-MET-FAST | 15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 65 | 18 |
| | HEU-SOL-THERM | 1, 13, 14, 16, 28, 29, 30 | 52 |
| | IEU-MET-FAST | 2, 3, 4, 5, 6, 7, 8, 9 | 8 |
| | LEU-COMP-THERM | 1, 2, 8, 10, 17, 42, 50, 78, 80 | 140 |
| | LEU-SOL-THERM | 2, 3, 4 | 19 |
| | MIX-MET-FAST | 5, 6 | 2 |
| | MIX-COMP-THERM | 1, 2, 4 | 21 |
| | MIX-SOL-THERM | 2 | 3 |
| | PU-MET-FAST | 1, 2, 5, 6, 8, 10, 18, 22, 23, 24 | 10 |
| | PU-SOL-THERM | 1, 2, 3, 4, 5, 6, 7, 11, 20 | 81 |
| CSAS6 / KENO-VI | HEU-MET-FAST | 5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93 | 27 |
| | IEU-MET-FAST | 19 | 2 |
| | MIX-COMP-THERM | 8 | 28 |

- Fissile materials**
 - High-enriched uranium (HEU),
 - Intermediate-enriched uranium (IEU)
 - Low-enriched uranium (LEU)
 - Plutonium (Pu)
 - Mixed uranium/plutonium oxides (MOX)
- Fuel form**
 - Metal (MET),
 - Fissile solution (SOL)
 - Multi-material composition (e.g. fuel pins – COMP)
- Neutron spectra**
 - Fast
 - Thermal

Cross section uncertainty for critical experiments

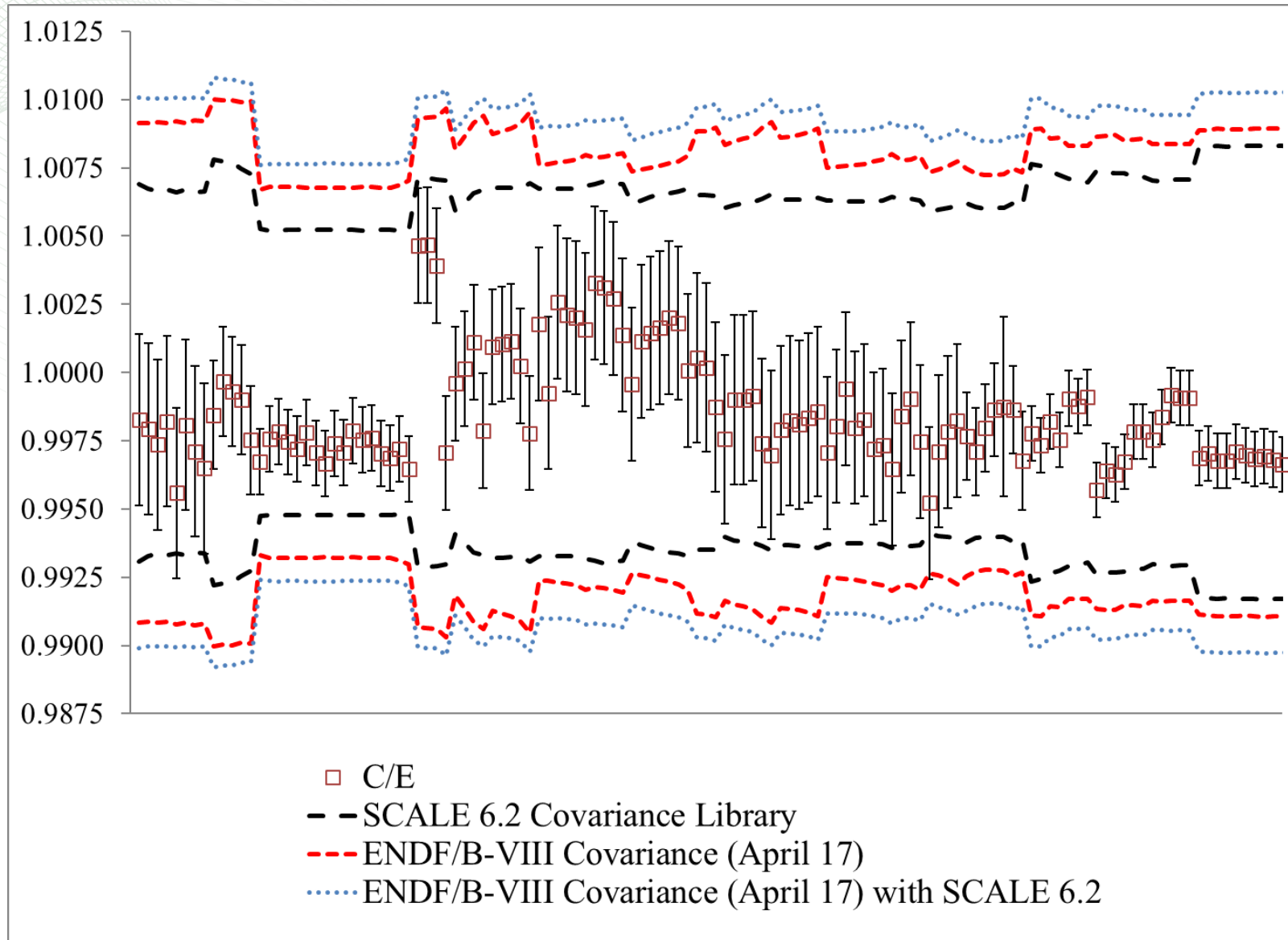
- Purpose:
 - Generate k_{eff} uncertainty due to covariances for critical experiments in VALID library maintained at ORNL
 - Compare variability of predictions with resulting uncertainty band
 - Plots frequently presented by Mark Williams, Brad Rearden, and others
- Methodology:
 - TSUNAMI-IP will calculate 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}
 - Detailed uncertainty edit can also be generated for each element in the covariance matrix

Results (1): HEU-MET-FAST



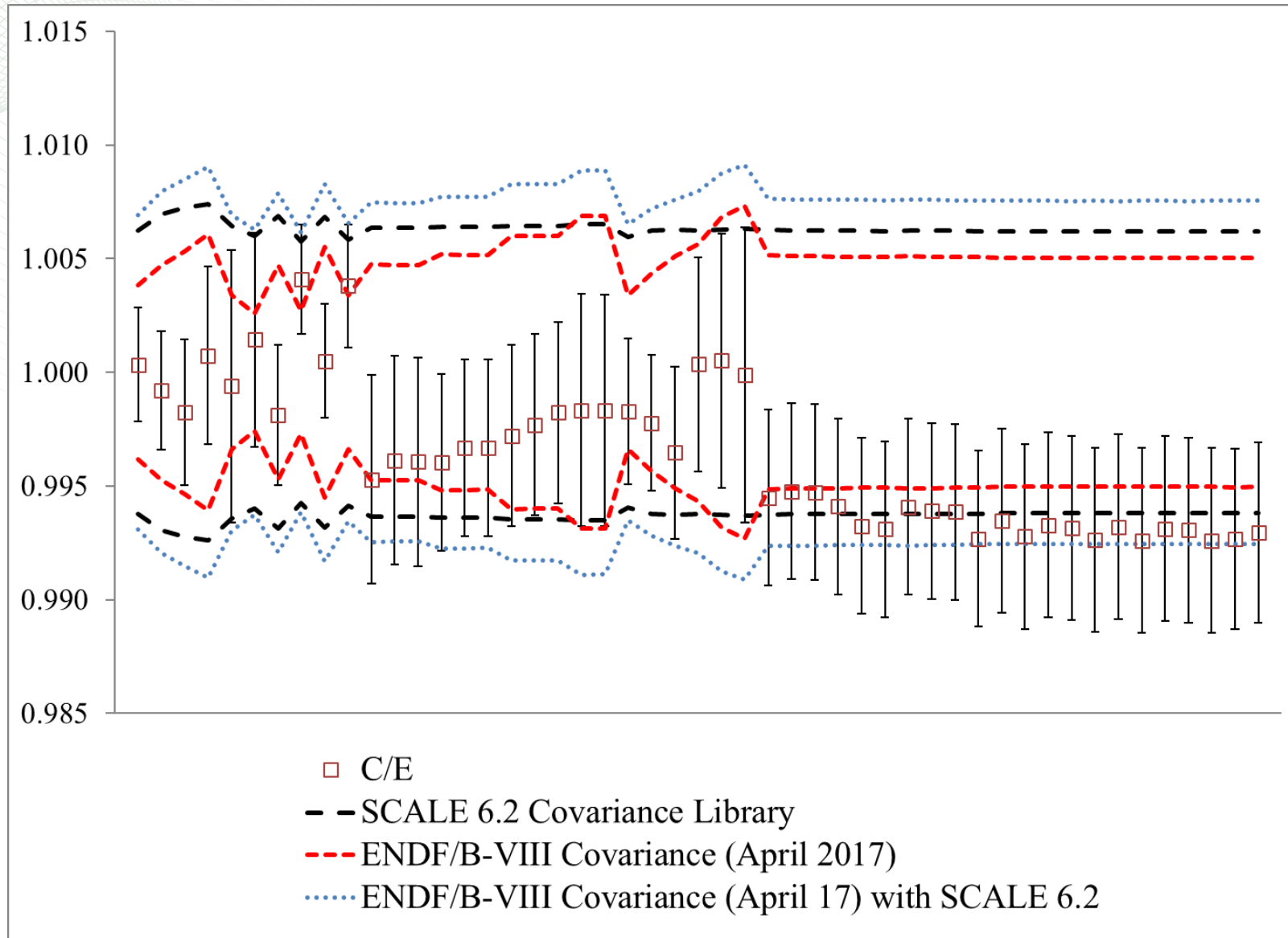
- 49 critical configurations
- C/E plotted for 252-group ENDF/B-VII.1 library
- Error bar is 1σ experimental uncertainty
- X variable is case number: no attempt to find trends
- HMF cases have generally not shown much impact in either ENDF/B-VII.1 or ENDF/B-VIII

Results (2): LEU-COMP-THERM



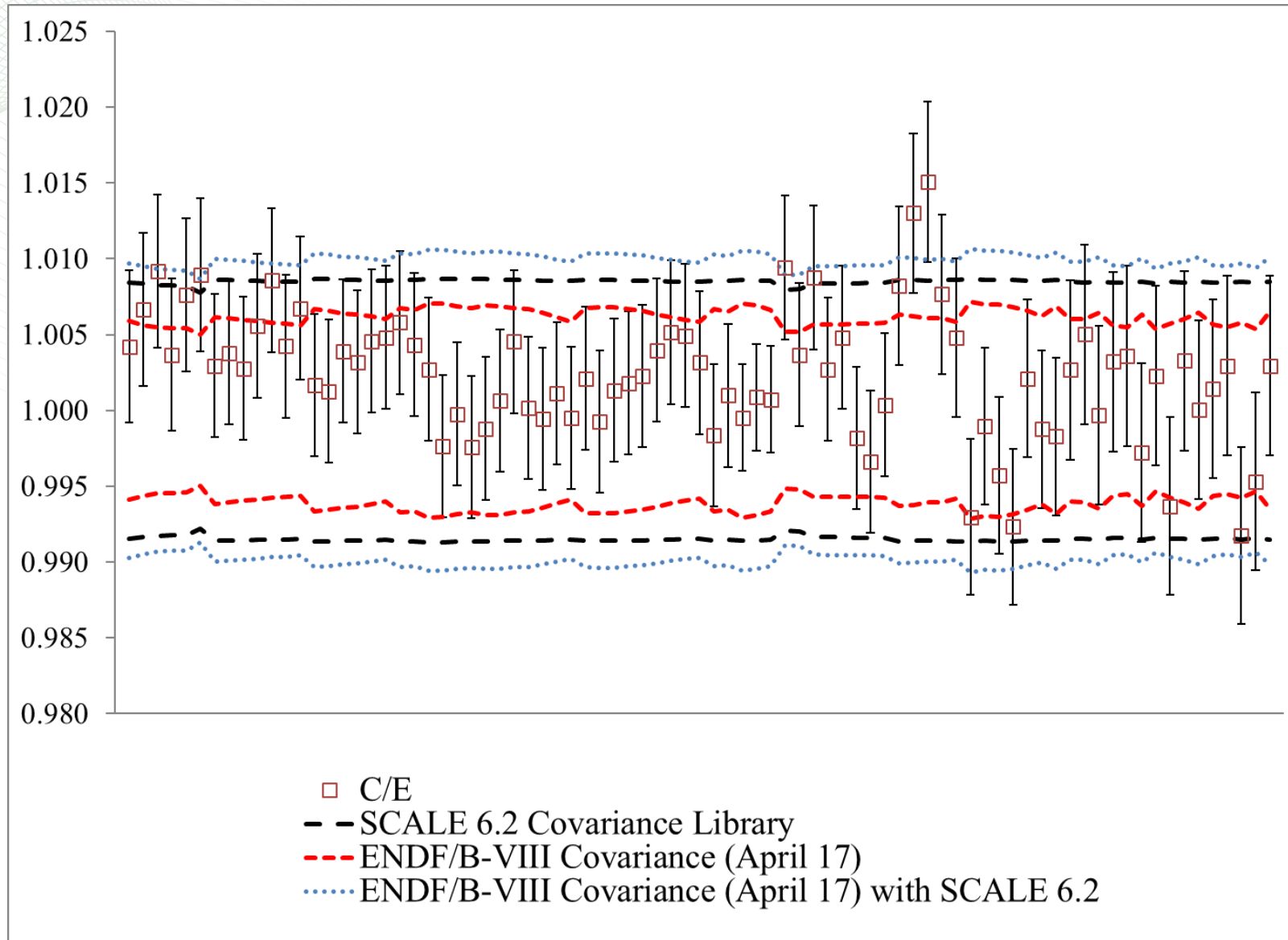
- 140 critical configurations
- C/E and error bar same as previous plot
- Noticeably larger uncertainty band with ENDF/B-VIII than SCALE 6.2.1
- Traced to ^{235}U nubar and ^1H capture and scatter
 - Reintroduction of errors identified in ENDF/B-VII.1 data during preparation and testing of SCALE 6.2 covariance library

Results (3): MIX-COMP-THERM



- 49 critical configurations
- New zigzag in the middle of the data is caused by ^1H capture
- Generally fewer points inside the uncertainty band for Pu-fueled systems in SCALE 6.2 and beyond
 - MCT-008 appears biased low, especially Cases 7-28
- Uncertainty may be creeping back – or is it just the ^1H problem?

Results (4): PU-SOL-THERM



- 81 critical configurations
- ^{239}Pu covariance data missing, so not tested
 - Obviously would have large impact here
- Again, results looked better with ^{239}Pu nuubar from ENDF/B-VII.1
 - Is that unrealistically low?

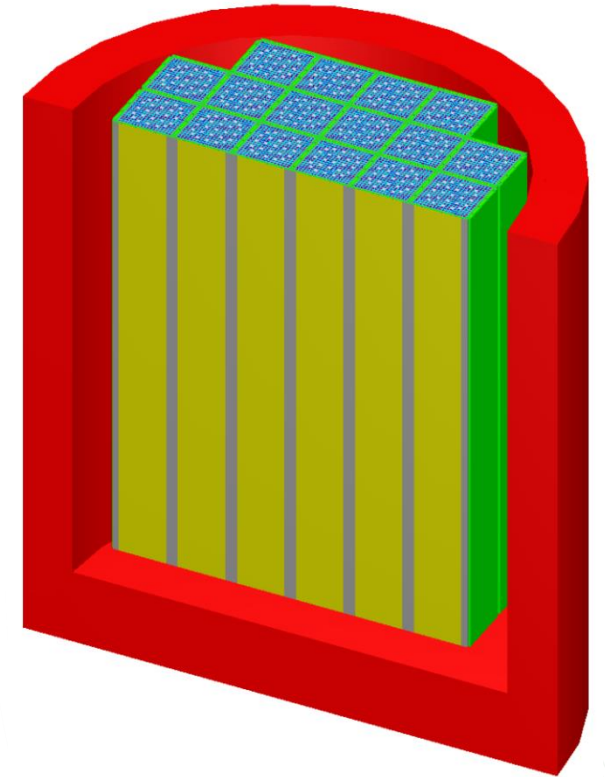
Results (5): Summary Table

| Category | Number of Cases | Avg C/E (CE_V7.1) | Avg Exp Unc | St. Dev. Of C/Es | Avg 1 σ XS Unc | | % of Cases Within | |
|----------|-----------------|-------------------|-------------|------------------|-----------------------|----------|-------------------|------------------|
| | | | | | SCALE 6.2 | E8+SCALE | Exp Unc Band | E8+SCALE XS Band |
| HMF | 49 | 1.00014 | 194 | 477 | 1366 | 1474 | 24.5 | 100 |
| HST | 52 | 0.99802 | 494 | 588 | 1050 | 1288 | 48.1 | 96.2 |
| IMF | 13 | 1.00329 | 269 | 367 | 1528 | 1591 | 23.1 | 100 |
| LCT | 140 | 0.99956 | 195 | 167 | 677 | 934 | 45.7 | 100 |
| LST | 19 | 0.99866 | 318 | 266 | 716 | 1180 | 63.2 | 100 |
| MCT | 49 | 0.99649 | 400 | 337 | 633 | 768 | 46.9 | 100 |
| PMF | 10 | 1.00020 | 204 | 128 | 586 | 584 | 80.0 | 100 |
| PST | 81 | 1.00302 | 497 | 420 | 850 | 995 | 72.8 | 95.1 |

The cross section uncertainty band is TOO WIDE! The experimental uncertainty band is in generally good agreement with the variation seen in the critical experiments.

Criticality Analysis for Used Nuclear Fuel (UNF)

- UNF contains many actinides and fission products
- A limiting condition on UNF cask storage is sub-criticality margin
- NRC allows “burnup credit” for burned fuel and certain FP nuclides
- Uncertainties are important consideration
 - SCALE 6.1 used in S/U for U.S. NRC



NRC Interim Staff Guidance 8, Revision 3

Division of Spent Fuel Storage and Transportation
Interim Staff Guidance - 8
Revision 3

Issue: Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transportation and Storage Casks

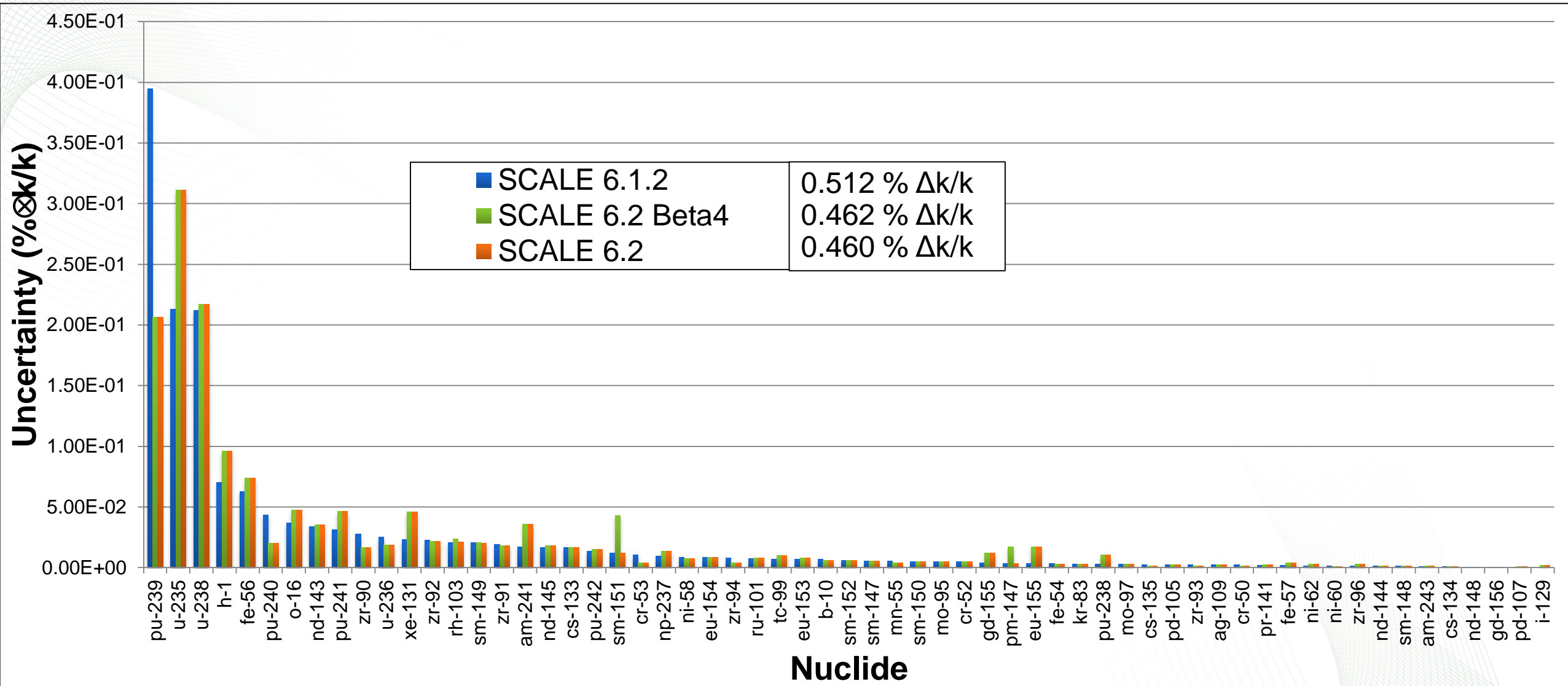
Introduction:

Title 10 of the Code of Federal Regulations (10 CFR) Part 71, *Packaging and Transportation of Radioactive Material*,¹ and 10 CFR Part 72, *Licensing Requirements for the Independent Storage of Spent Nuclear Fuel, High-Level Radioactive Waste, and Reactor-Related Greater Than Class C Waste*,² require that spent nuclear fuel (SNF) remain subcritical in transportation and storage, respectively. Unirradiated reactor fuel has a well-specified nuclide composition that provides a straightforward and bounding approach to the criticality safety analysis of transportation and storage systems. As the fuel is irradiated in the reactor, the nuclide composition changes and, ignoring the presence of burnable poisons, this composition change will cause the reactivity of the fuel to decrease. Allowance in the criticality safety analysis for the decrease in fuel reactivity resulting from irradiation is termed burnup credit. Extensive investigations have been performed both within the United States and by other countries in an effort to understand and document the technical issues related to the use of burnup credit.

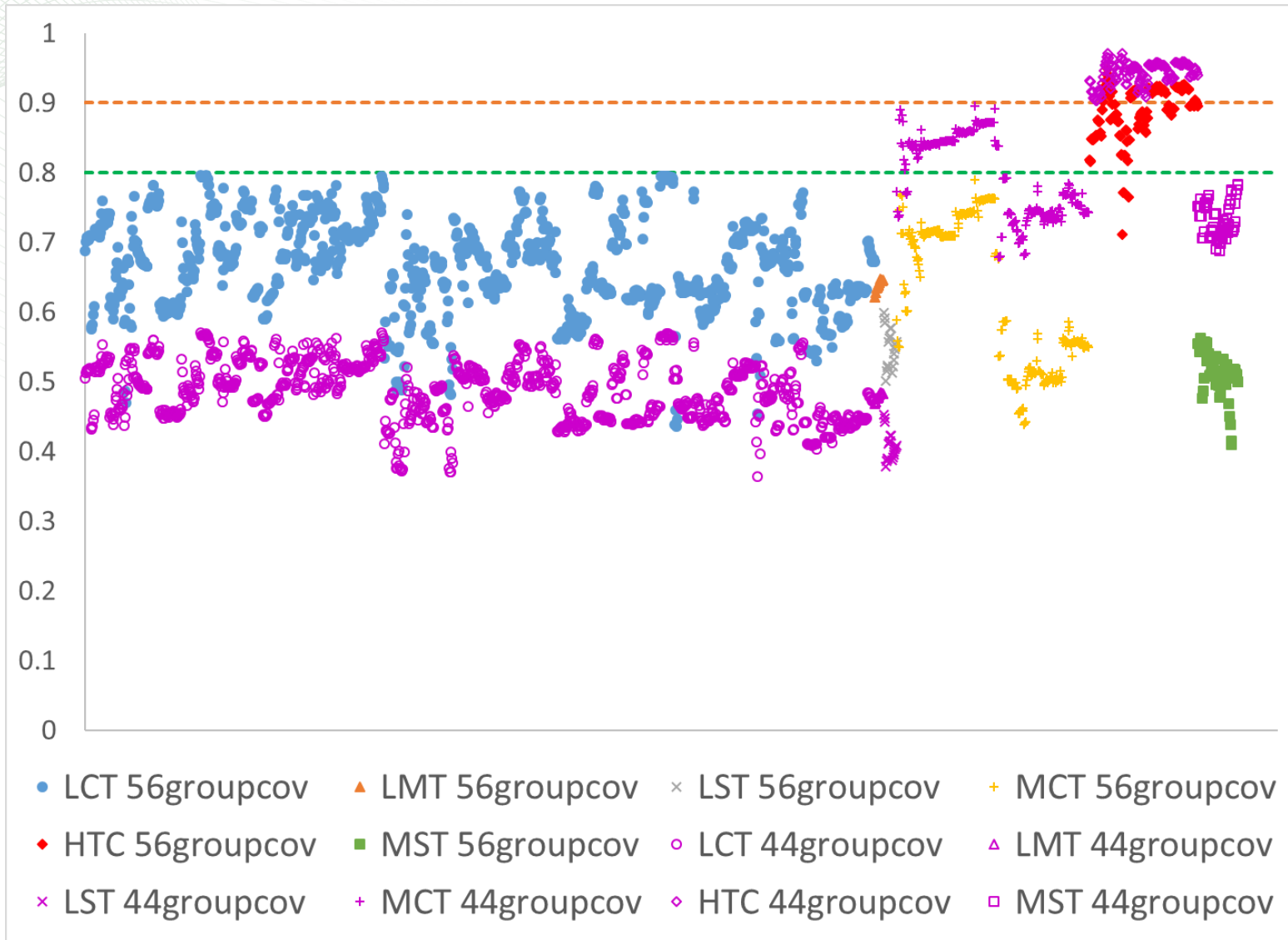
This Interim Staff Guidance (ISG) provides recommendations to the staff for accepting, on a design-specific basis, a burnup credit approach in the criticality safety analysis of pressurized water reactor (PWR) SNF storage and transportation systems. This revision to ISG-8 incorporates the results of burnup credit-related research that has been conducted since Revision 2 (Rev. 2) was published in September 2002. Based on the detailed results of this research and the technical judgment of the U.S. Nuclear Regulatory Commission (NRC) staff, ISG-8, Rev. 3, includes two major changes in the recommendations to staff reviewing burnup credit applications for SNF transportation and storage systems: (1) optional credit for fission product and minor actinide neutron absorbing isotopes in the SNF composition, and (2) misload analyses and additional administrative procedures in lieu of a burnup measurement at the time of loading. This ISG revision also includes an increase in the maximum assembly average burnup recommended for burnup credit.

“In order to achieve an appropriate estimate of the *keff* bias and bias uncertainty due to fission products, ORNL developed a methodology based on the SCALE *Tools for Sensitivity and Uncertainty Methodology Implementation* (TSUNAMI) code, developed as part of the SCALE code system. This methodology uses the nuclear data uncertainty estimated for each fission product cross section known as the cross section covariance data. These data are provided with the ENDF/B-VII cross section library. The TSUNAMI code is used to propagate the cross section uncertainties represented by the covariance data into *keff* uncertainties for each fission product isotope used in a particular application. The theoretical basis of this validation technique is that computational biases are primarily caused by errors in the cross section data, which are quantified and bounded, with a 1σ confidence, by the cross section covariance data. The validity of this theoretical basis is discussed in greater detail in NUREG/CR-7109.”

Top Contributors to Uncertainty for GBC-32

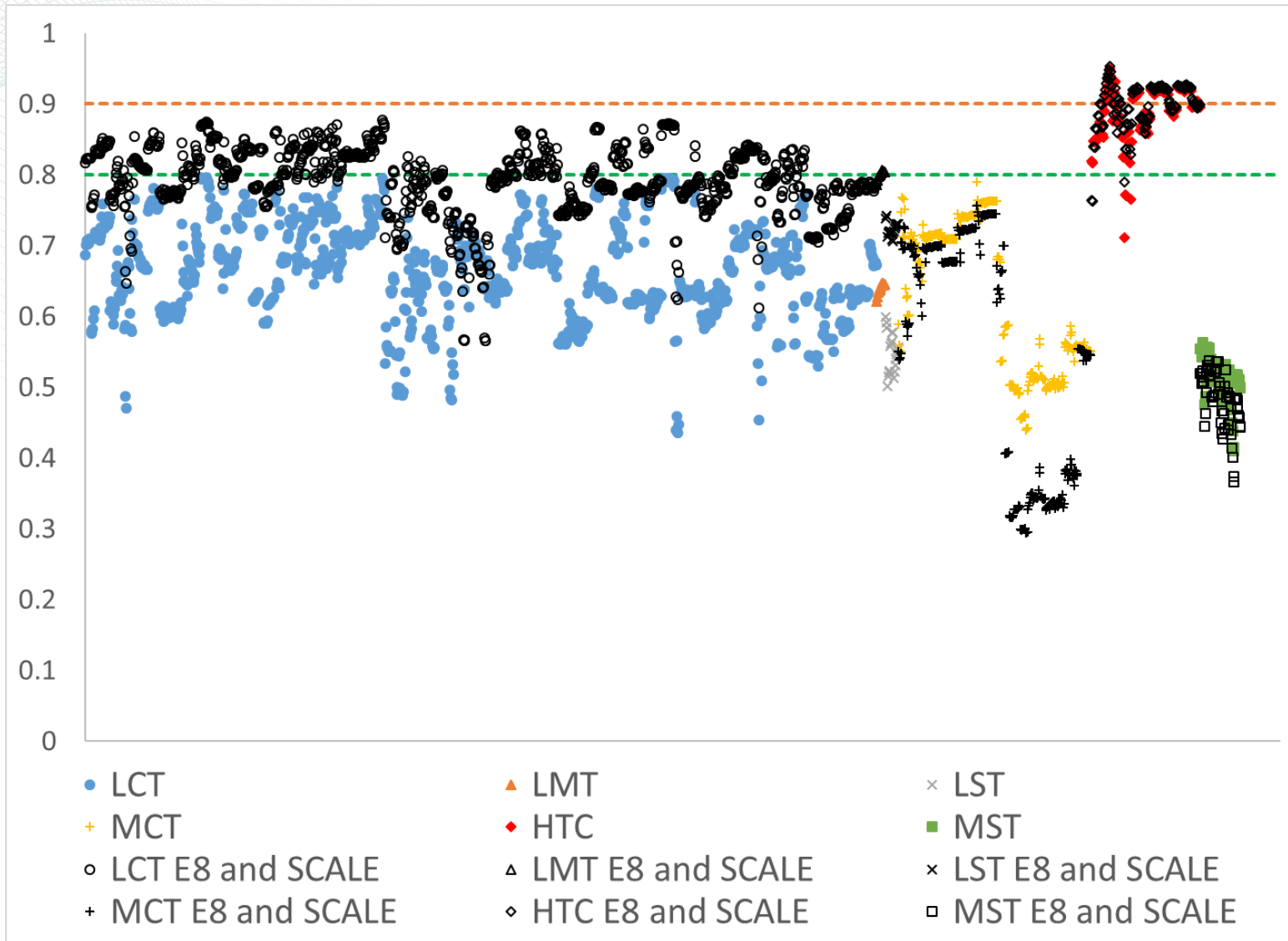


c_k results –SCALE 6.1 to SCALE 6.2



- 1643 unique critical experiments
- PWR SNF 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

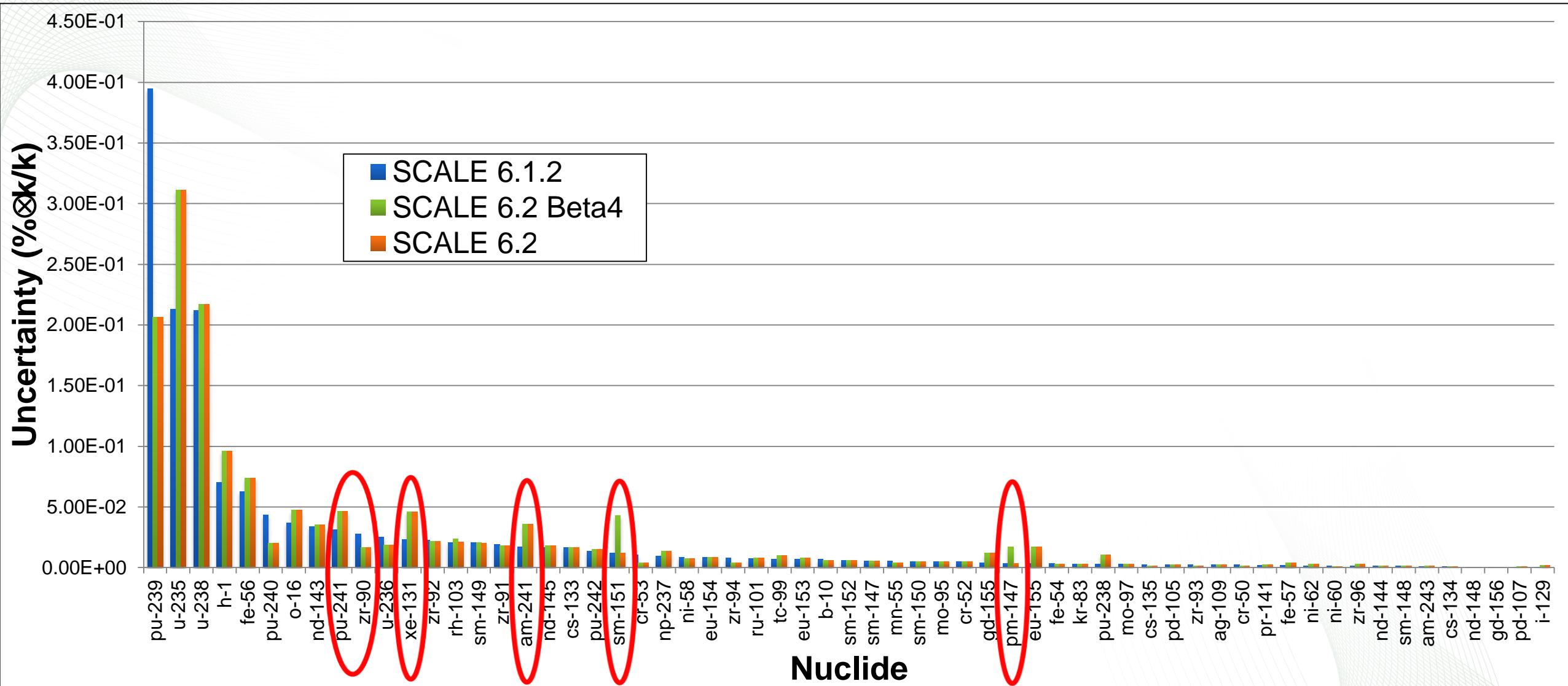


- Same critical experiments and PWR SNF
- SCALE 6.2 (various)
- ENDF/B-VIII plus SCALE data (black)
- This change further reduces MCT systems and increases LCT systems. The result doesn't make sense – LEU can't be representative of SNF.

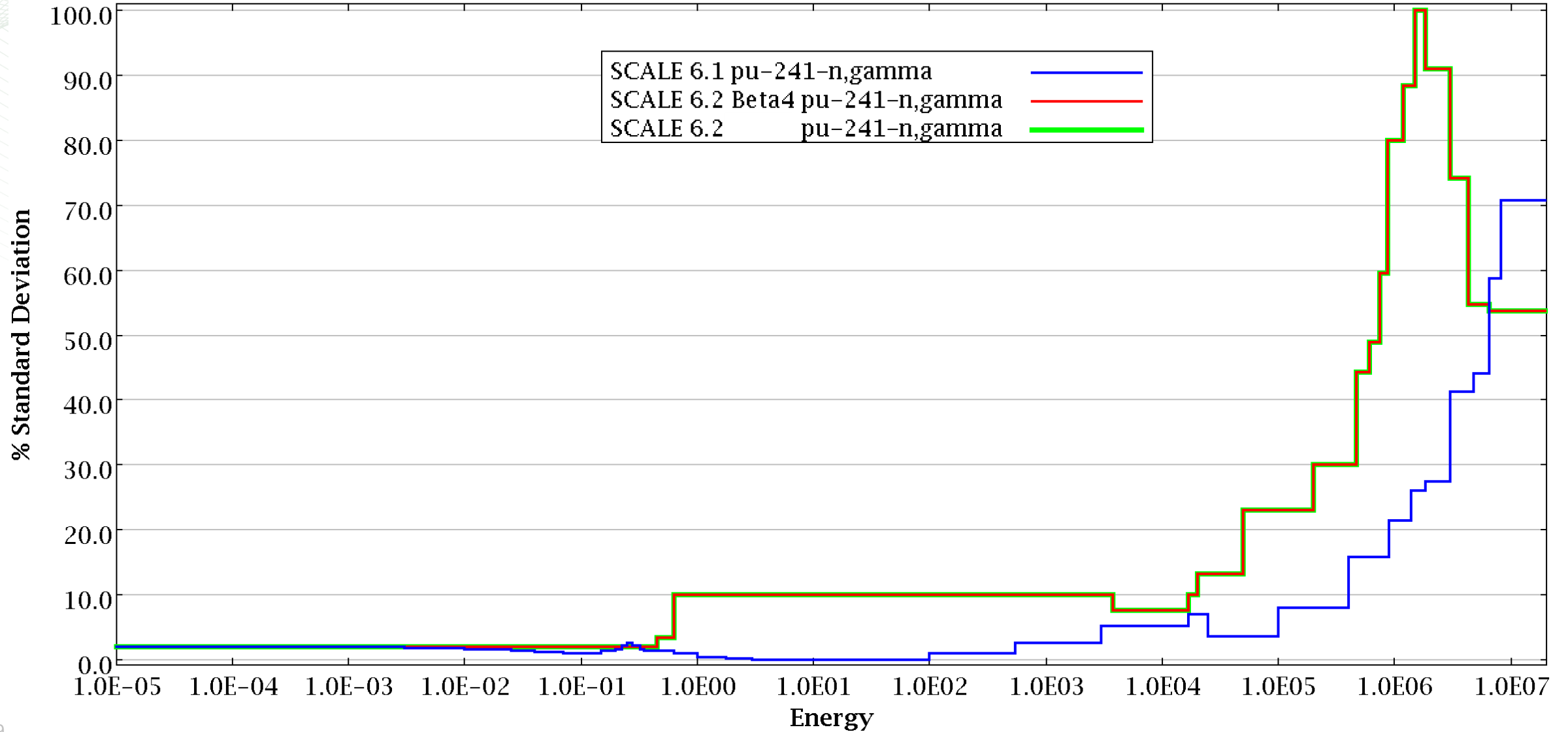
c_k summary

- Increased ^{235}U nubar uncertainty results in higher similarity for LCT systems with SNF storage/transportation models
 - This exacerbates a change resulting from ENDF/B-VII.1 covariance changes to ^{235}U (bigger) and ^{239}Pu (smaller)
- Without reliable covariance data, S/U methods cannot be used to select appropriate experiments for validation
 - Reliability of covariance data is also a significant problem for data adjustment methods (e.g., TSURFER)

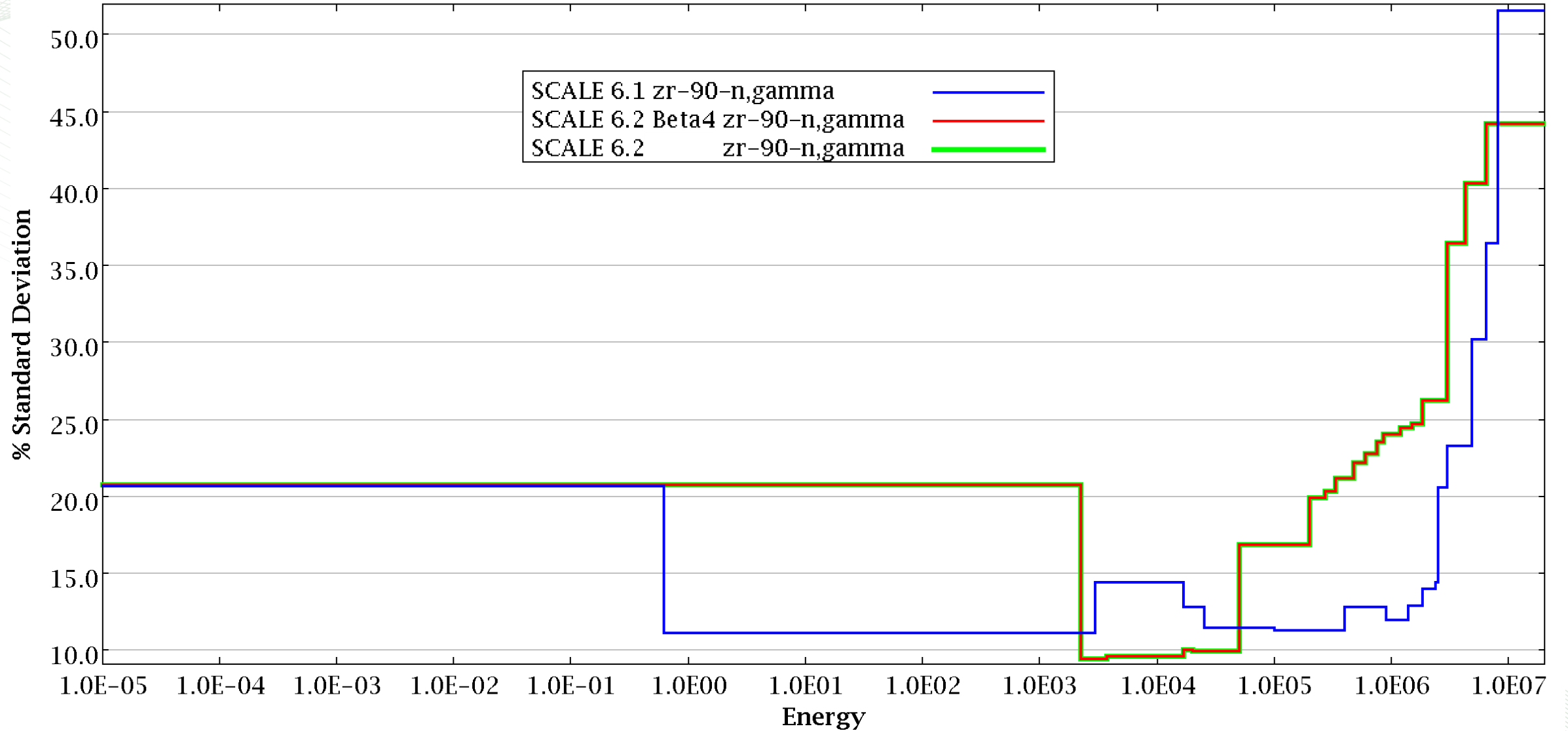
More Contributors to Uncertainty for GBC-32



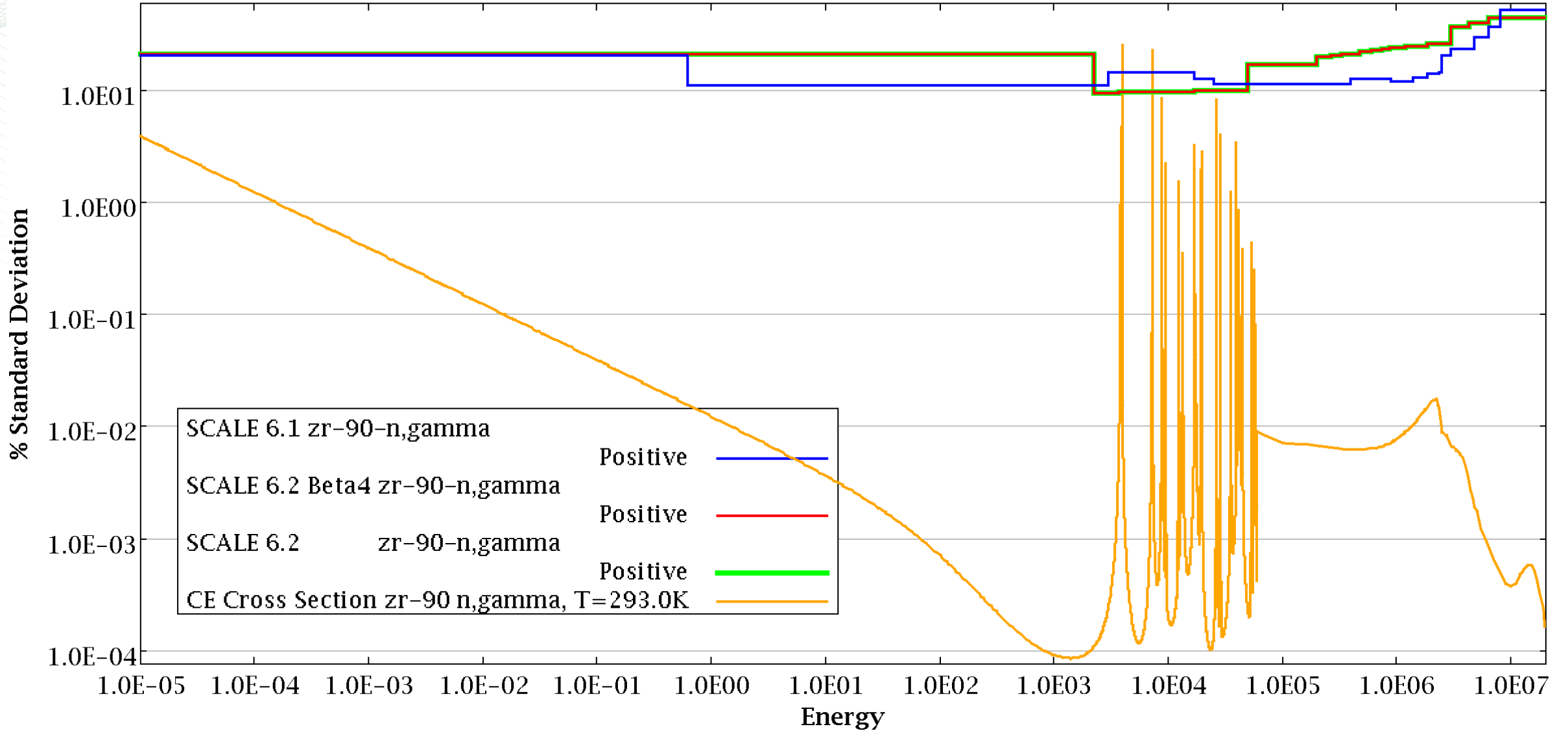
Pu-241 n,gamma uncertainty



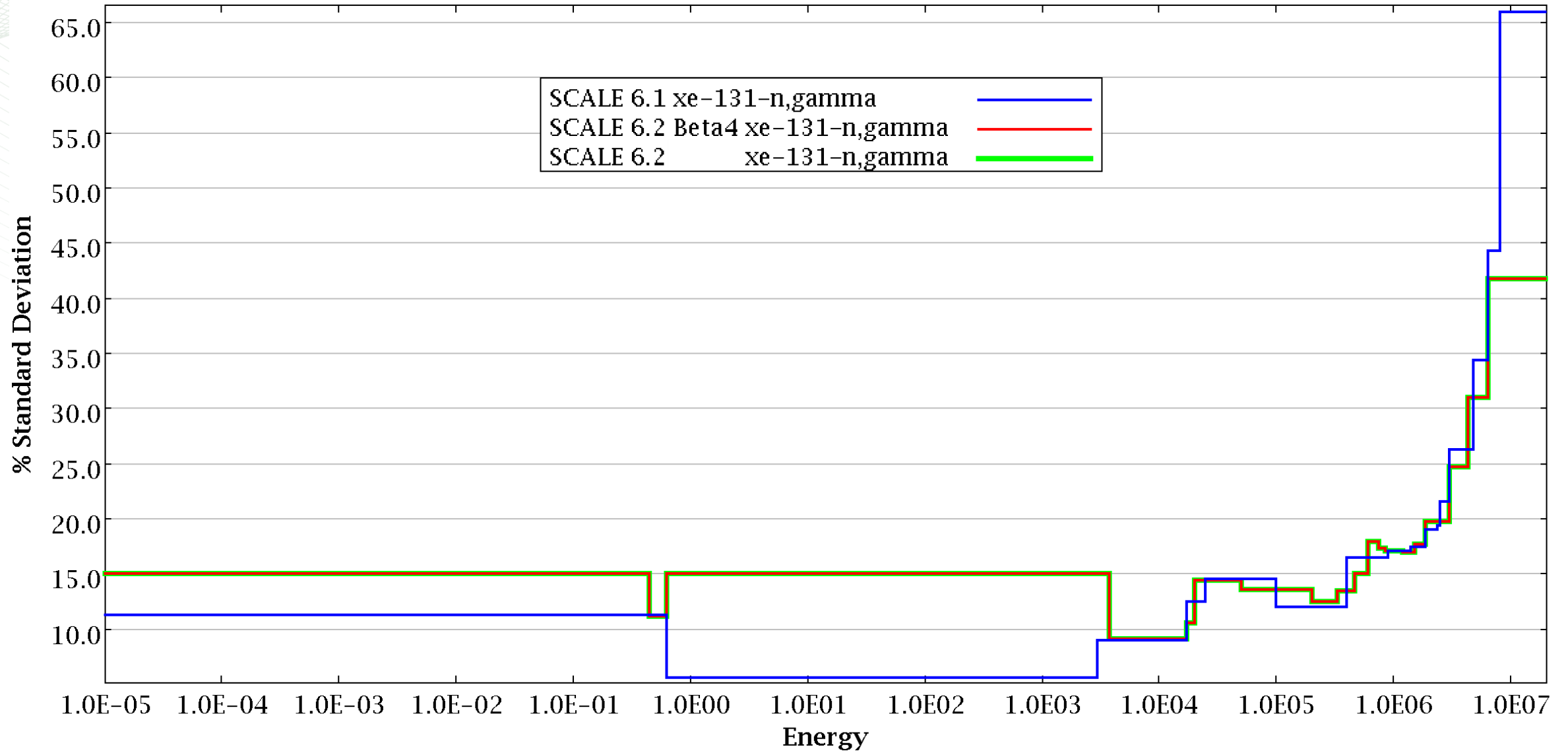
Zr-90 n,gamma uncertainty



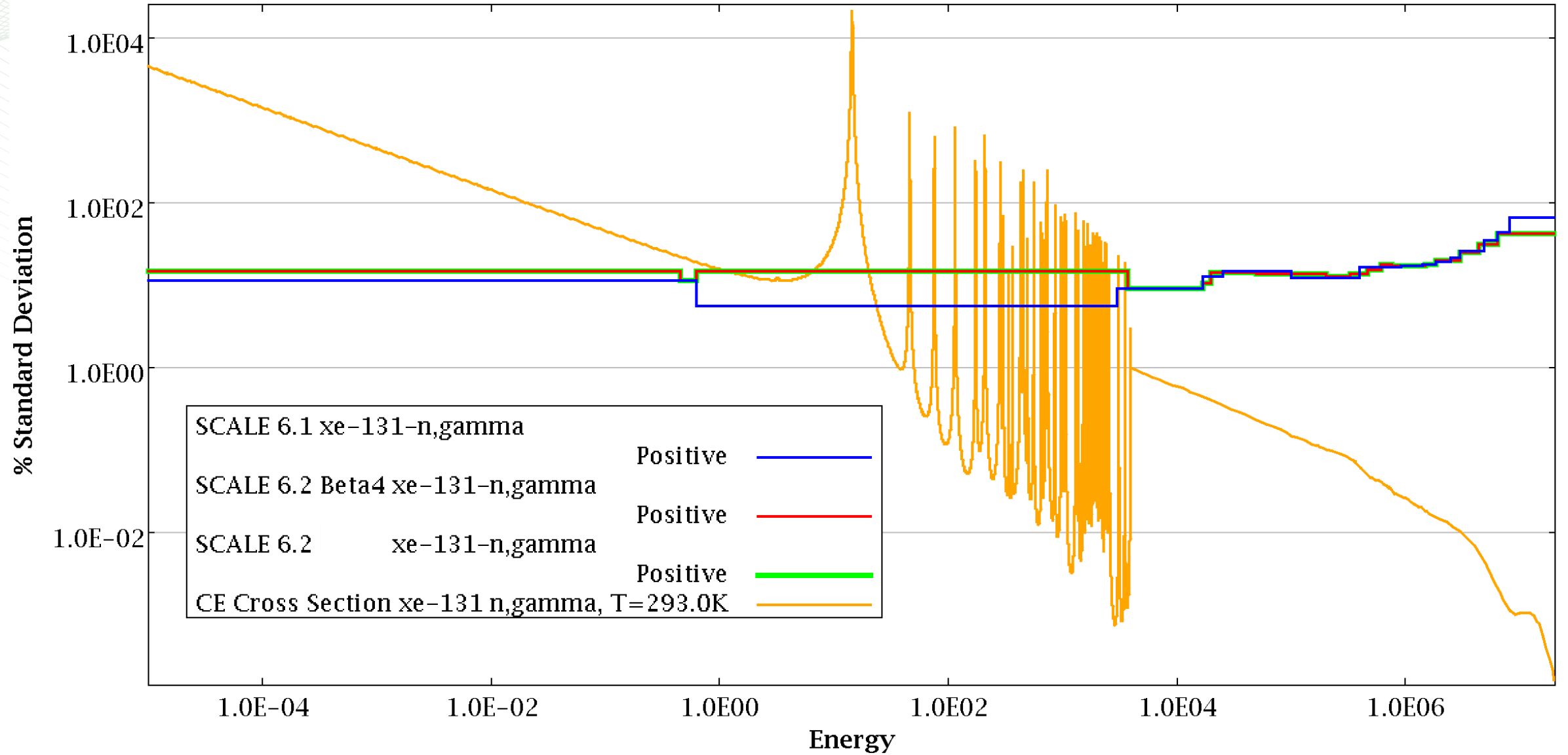
Zr-90



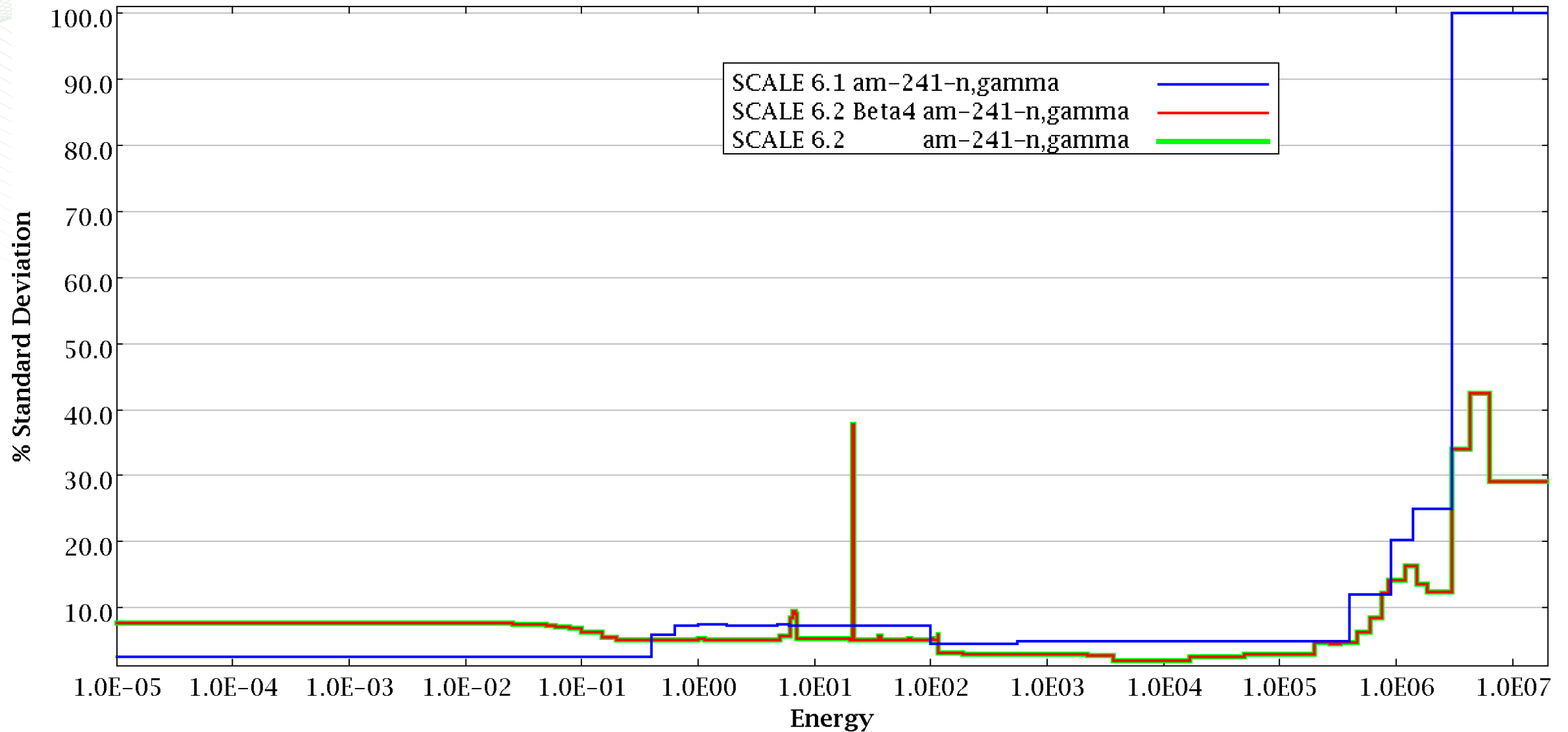
Xe-131 n,gamma uncertainty



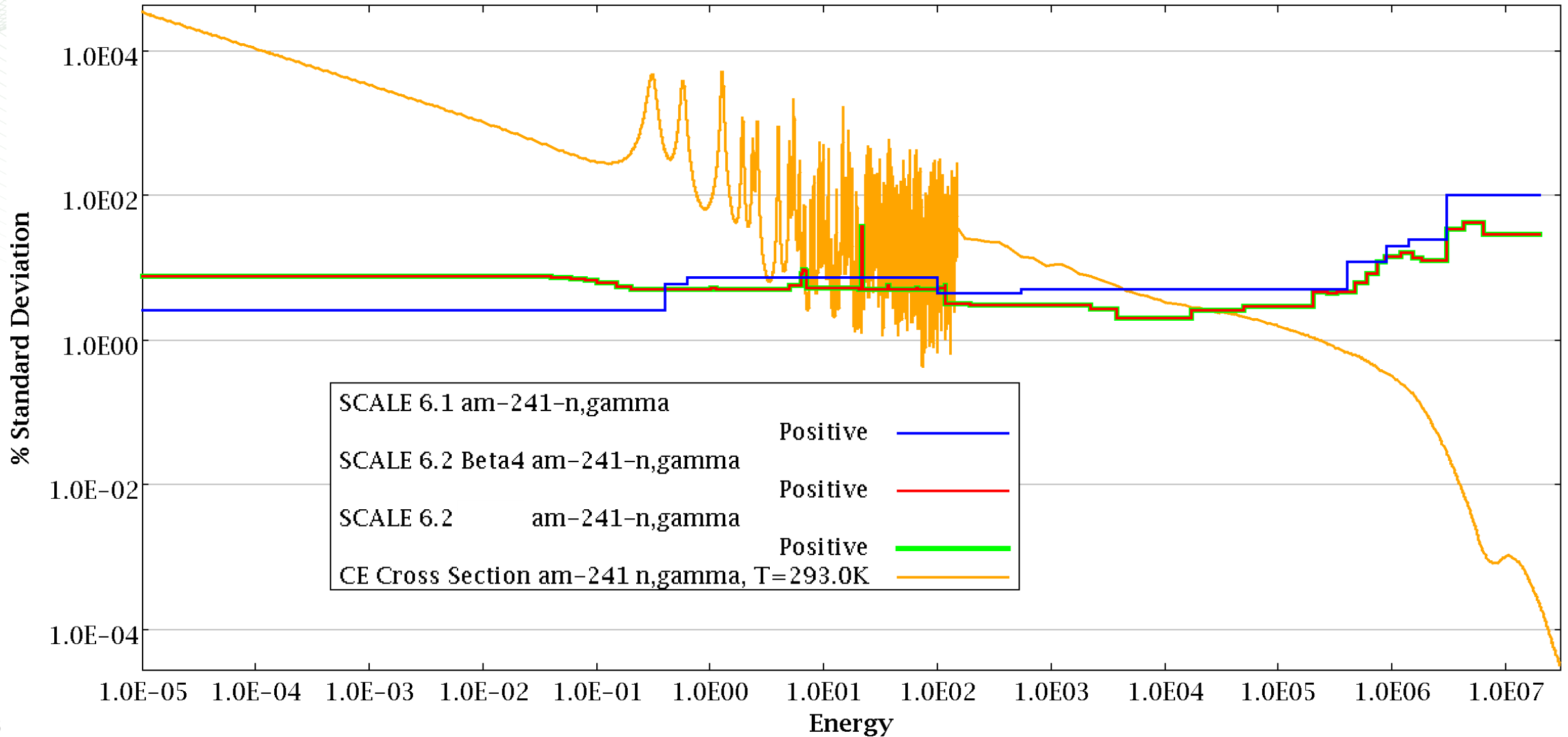
Xe-131



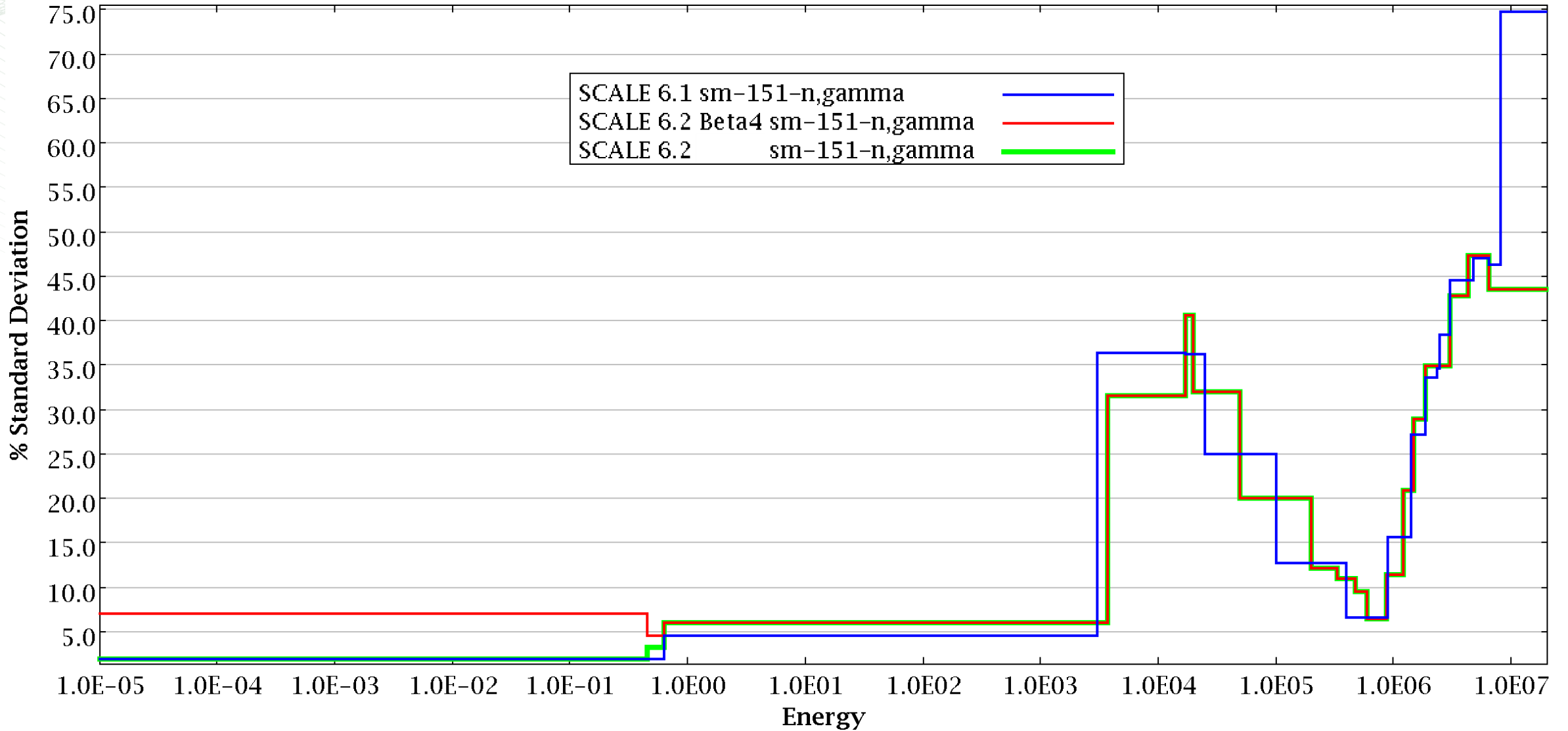
Am-241 n,gamma uncertainty



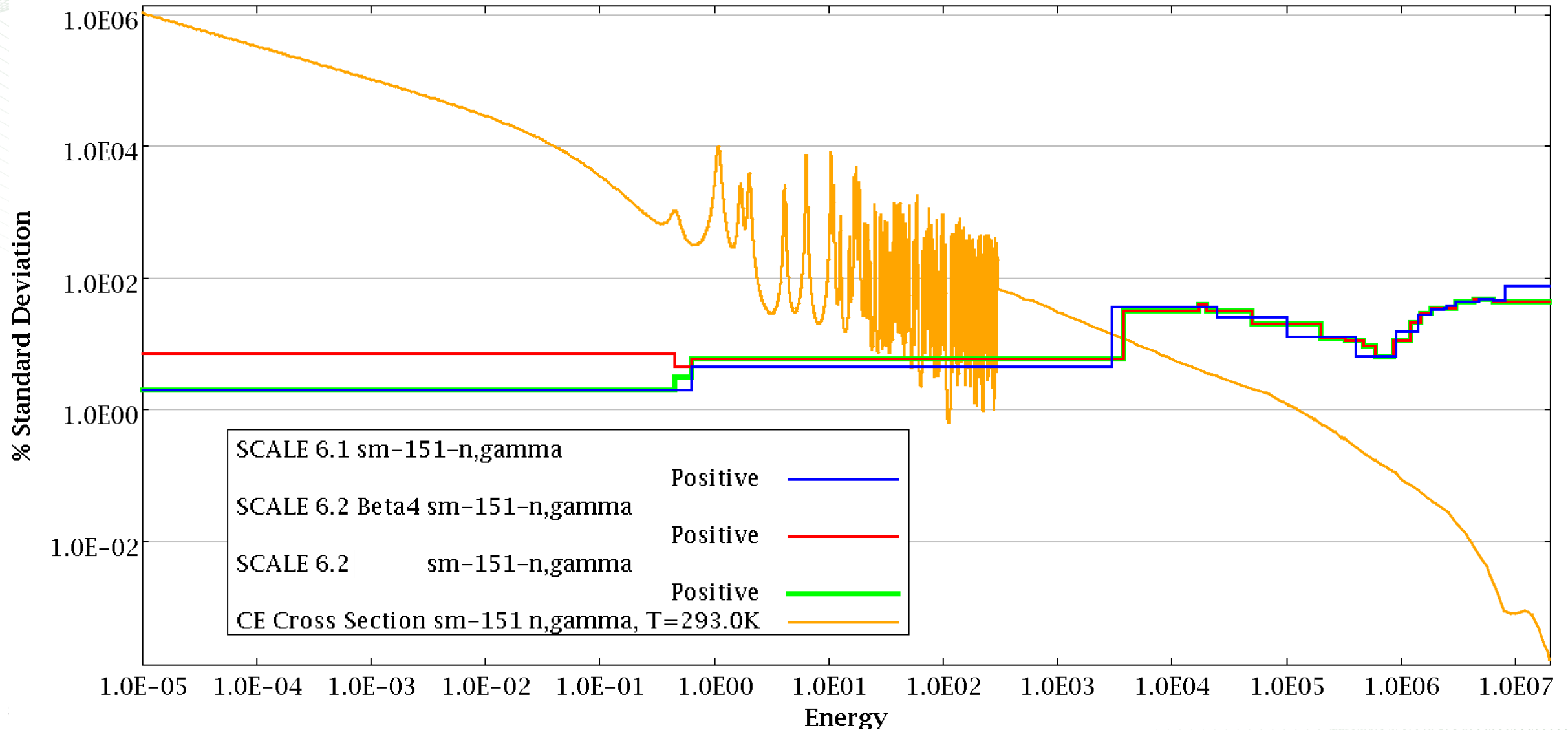
Am-241



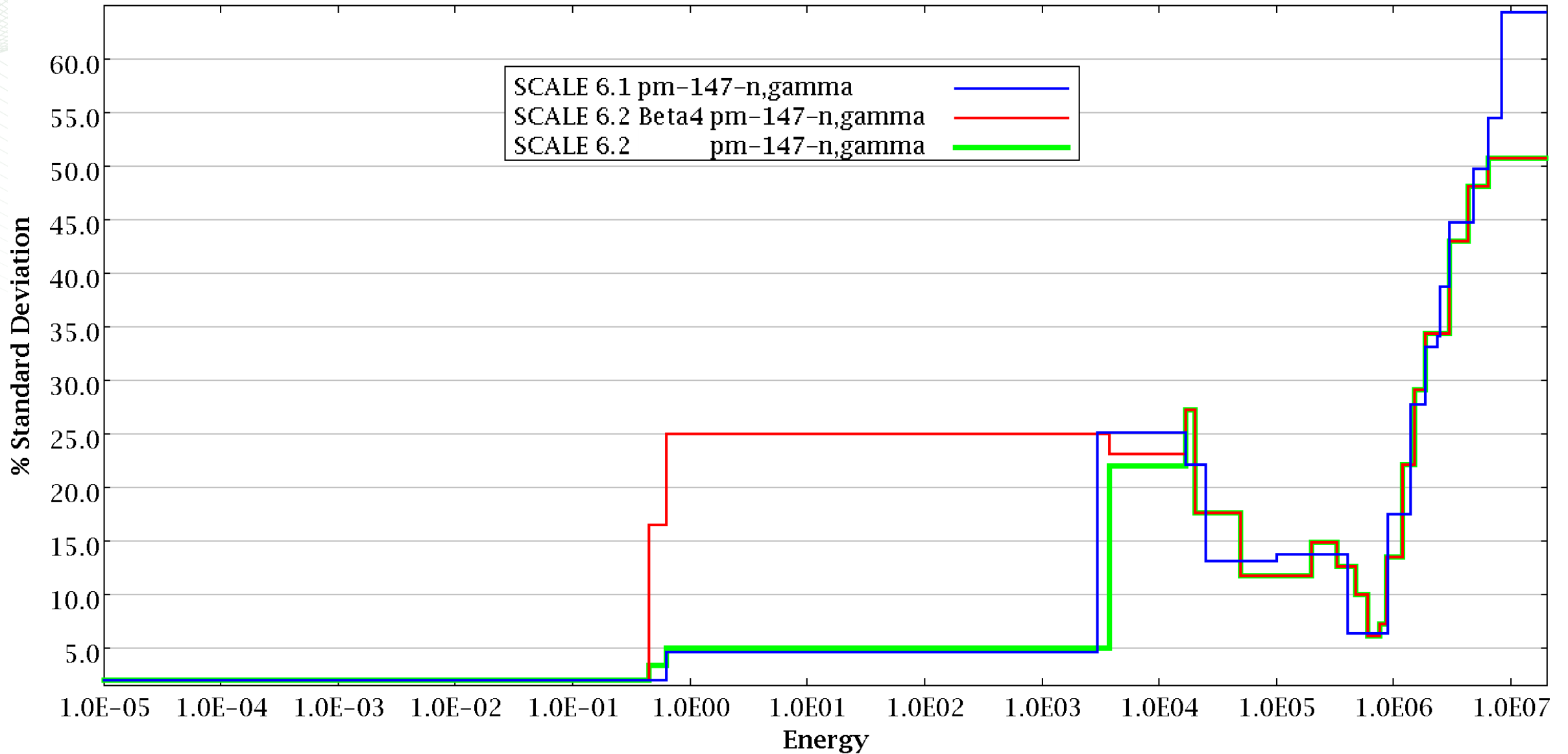
Sm-151 n,gamma uncertainty



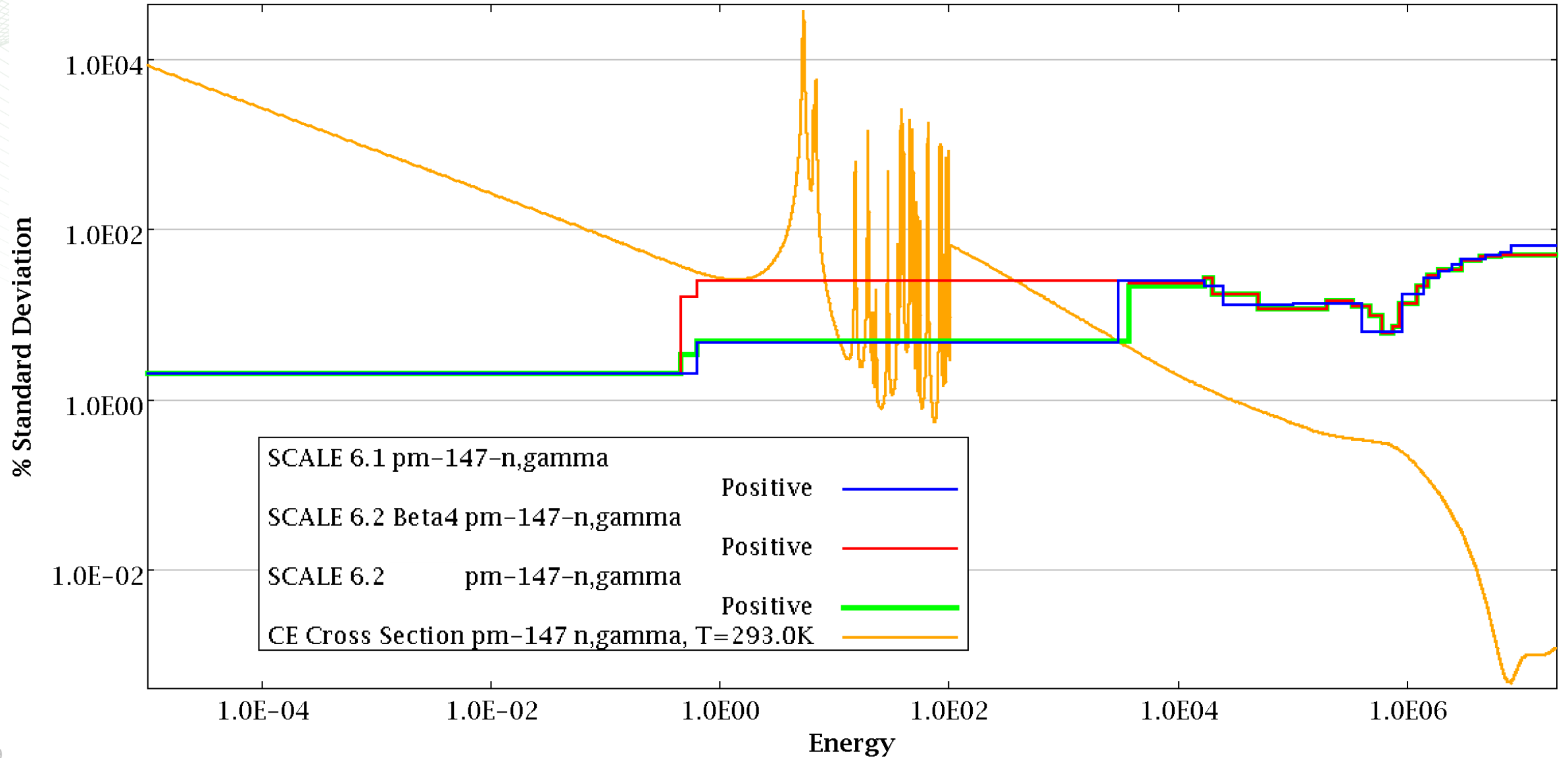
Sm-151



Pm-147 n,gamma uncertainty



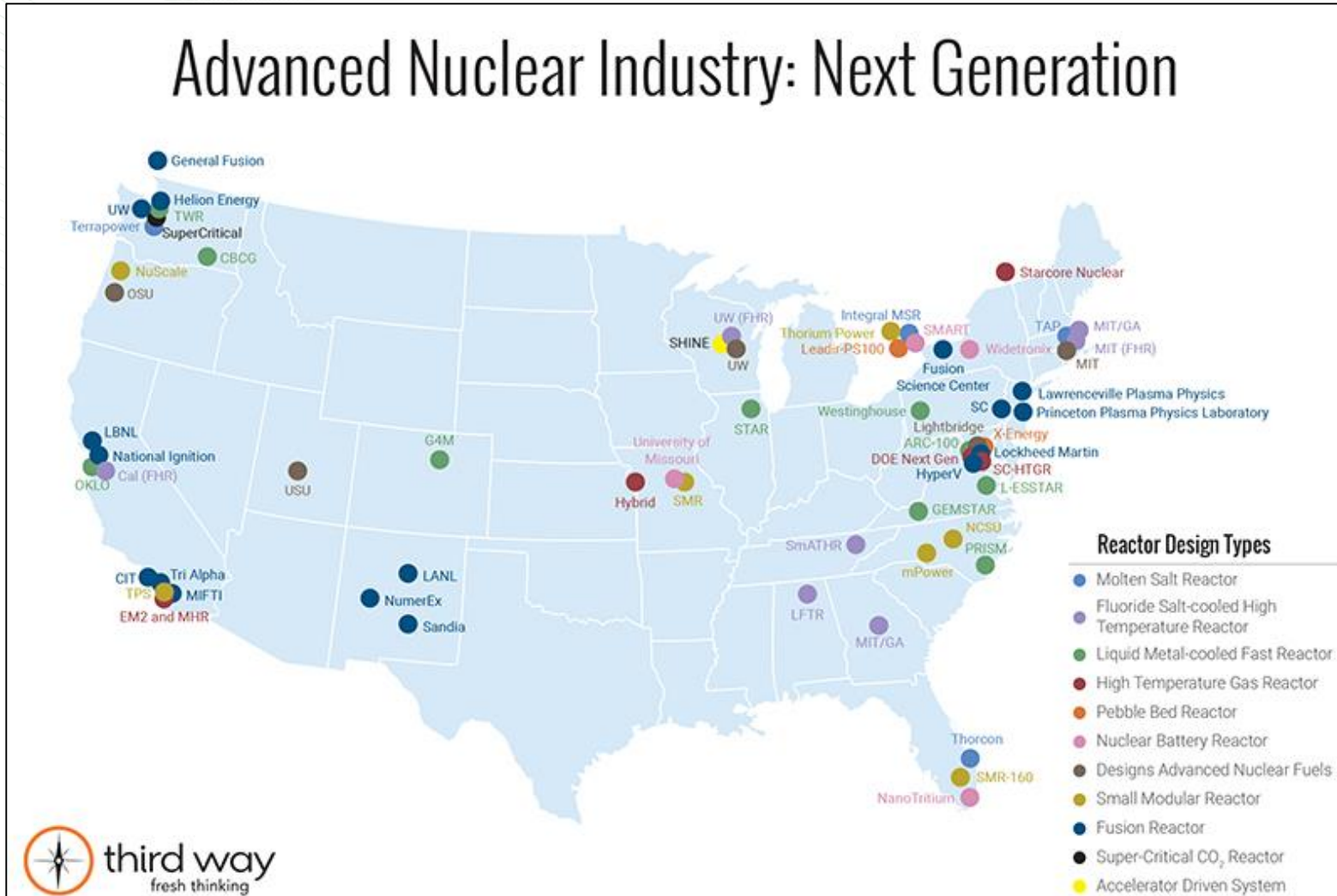
Pm-147



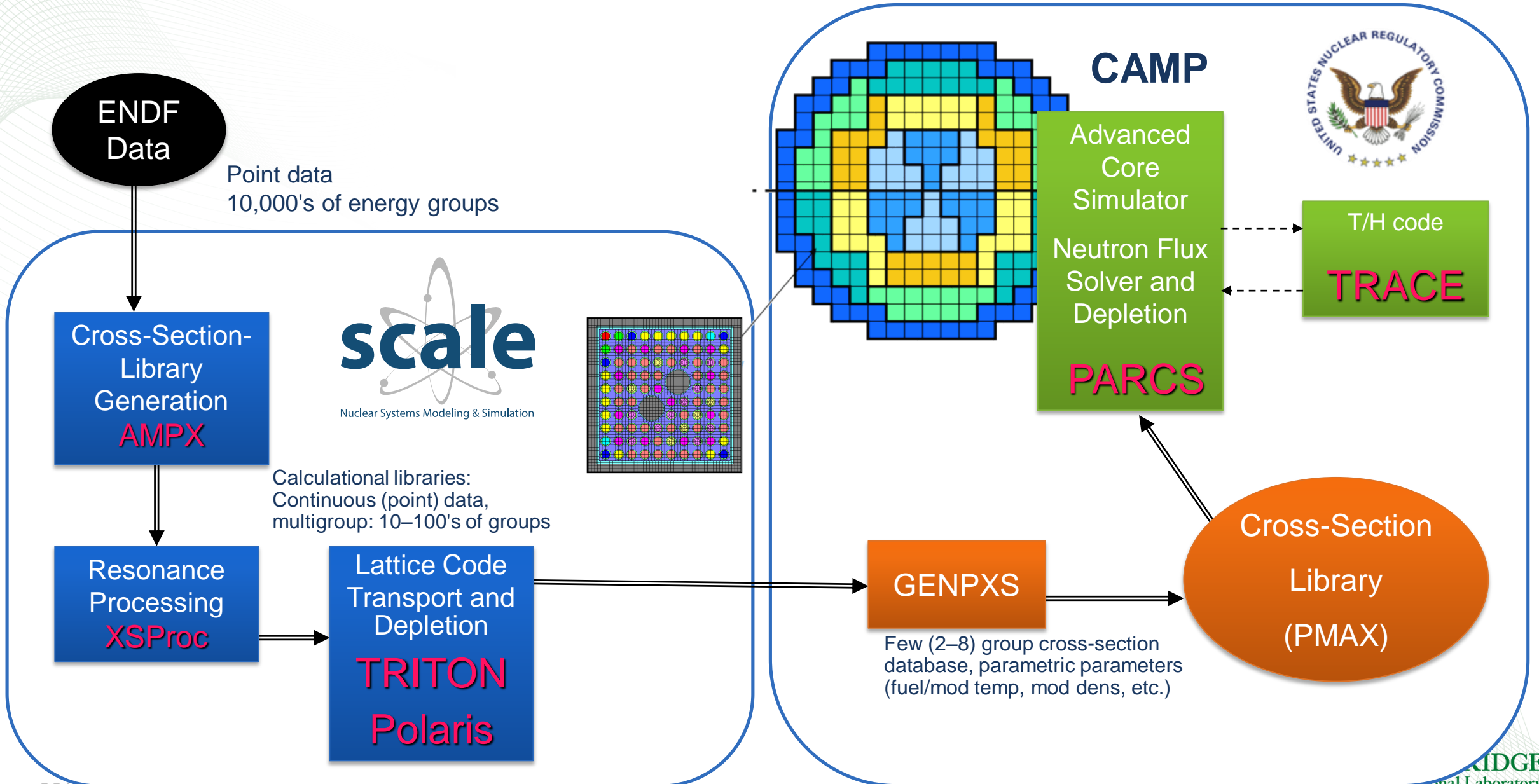
Uncertainties for Spent Fuel Systems (Same cases & models as NUREG/CR-7109 Table 6.10)

| | SFP | | | | GBC32 | | | | BWR | |
|------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| | 10 GWd/MTU | | 40 GWd/MTU | | 10 GWd/MTU | | 40 GWd/MTU | | 11 GWd/MTU | |
| Category | SCALE 6.1 | SCALE 6.2 | SCALE 6.1 | SCALE 6.2 | SCALE 6.1 | SCALE 6.2 | SCALE 6.1 | SCALE 6.2 | SCALE 6.1 | SCALE 6.2 |
| Major Actinides | 0.00463 | 0.00469 | 0.00476 | 0.00416 | 0.00455 | 0.00449 | 0.00466 | 0.00406 | 0.00393 | 0.00447 |
| Minor Actinides | 0.00007 | 0.00007 | 0.00027 | 0.00022 | 0.00007 | 0.00007 | 0.00025 | 0.00022 | 0.00013 | 0.00011 |
| Major Fission Products | 0.00022 | 0.00022 | 0.00052 | 0.00054 | 0.00024 | 0.00024 | 0.00052 | 0.00055 | 0.00023 | 0.00024 |
| Other Actinides | 0.00003 | 0.00006 | 0.00003 | 0.00006 | 0.00000 | 0.00000 | 0.00001 | 0.00001 | 0.00000 | 0.00000 |
| Other Fission Products | 0.00015 | 0.00021 | 0.00034 | 0.00062 | 0.00008 | 0.00015 | 0.00024 | 0.00047 | 0.00014 | 0.00025 |
| Other (structural) | 0.00081 | 0.00123 | 0.00073 | 0.00102 | 0.00106 | 0.00145 | 0.00104 | 0.00127 | 0.00080 | 0.00099 |
| ALL | 0.00471 | 0.00486 | 0.00486 | 0.00437 | 0.00468 | 0.00472 | 0.00481 | 0.00432 | 0.00402 | 0.00459 |

A number of private U.S. companies are pursuing conceptual and technological development of advanced reactors



SCALE is a part of NRC's reactor licensing path





NEAMS (Nuclear Energy Advanced Modeling and Simulation) Program

Aim: Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

Fuels Product Line

MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability

MARMOT
Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

MOOSE
Multiphysics Object-Oriented Simulation Environment

Simulation framework enabling rapid development of FEM-based applications

BISON
Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

Reactor Product Line

Nek5000 – Thermal-Hydraulics
Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics

PROTEUS – Neutronics
Can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling

DIABLO – Structural Dynamics
3-D thermal-structural and thermal mechanics analysis using a time implicit Finite Element Method (FEM)

Integration Product Line

Text Input Preferred by Expert Users with Highlighting and Error Detection

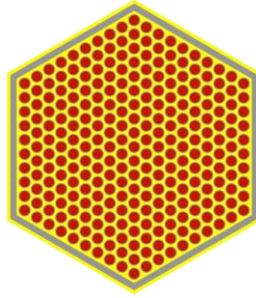
Optional Component Input Preferred by Novice Users

Geometry Visualization

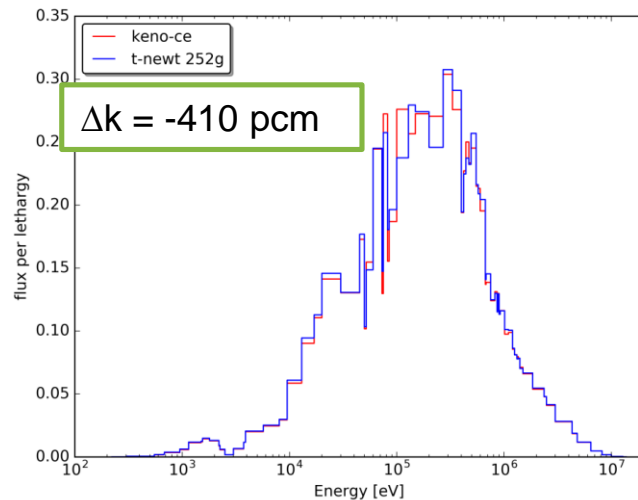
Data Visualization

Mesh Results Overlay

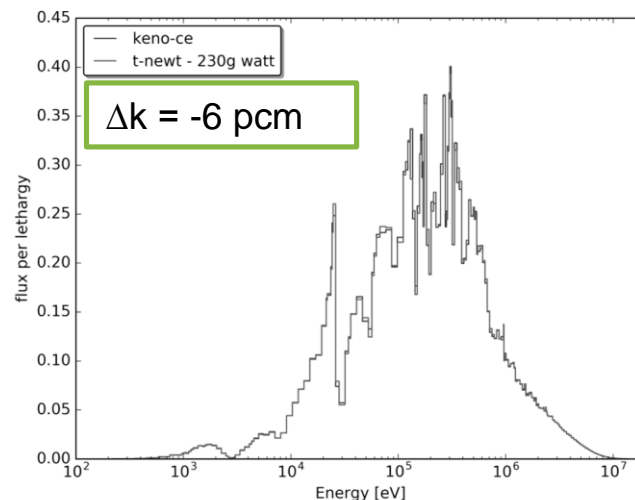
Generation of multigroup libraries and covariance data for advanced reactors – in collaboration with GRS



- Continuous-energy data serve as reference solution to confirm multigroup approximations
- SCALE 6.2 includes multigroup neutronics libraries that are optimized for LWRs
- Multigroup cross sections can be generated for any type of system
 - LWR, HTGR, MSR, FHR, SFR, etc. with appropriate energy group structure and weighting spectrum
- Uncertainties in cross sections (covariance data) quantify confidence in deployed data libraries
- Example for SFR:



Incorrect group structure/weighting



Correct group structure/weighting

Uncertainty in k_{eff} Due to Nuclear Data
Uncertainties: 1,435 pcm!

| nuclide-reaction | covariance matrix with nuclide-reaction | | % $\Delta k/k$ due to this matrix |
|------------------|---|---------|-----------------------------------|
| u-238 n,n' | u-238 | n,n' | 1.2053(9) |
| na-23 elastic | na-23 | elastic | 0.3242(2) |
| fe-56 elastic | fe-56 | elastic | 0.2590(3) |
| u-238 n,gamma | u-238 | n,gamma | 0.2435(1) |
| fe-56 n,n' | fe-56 | n,n' | 0.2388(1) |

Summary and conclusions

- Spent fuel, advanced reactors, and other challenging application areas require advanced methods for design optimization, validation, and licensing
- High quality and consistent covariance data is needed for setting safety limits and optimizing design
- Overall uncertainties in ENDF appear to be too large
- Drastic changes and/or errors in covariance data erode confidence in S/U methods
- The community needs SG-44 to stimulate coordination and provide the highest quality covariance data