Sensitivity and Uncertainty Enhancements in SCALE 6.2

Presented to:

WPEC SG39

May 11, 2016

Bradley T. Rearden, PhD
Manager, SCALE Code System
Reactor and Nuclear Systems Division

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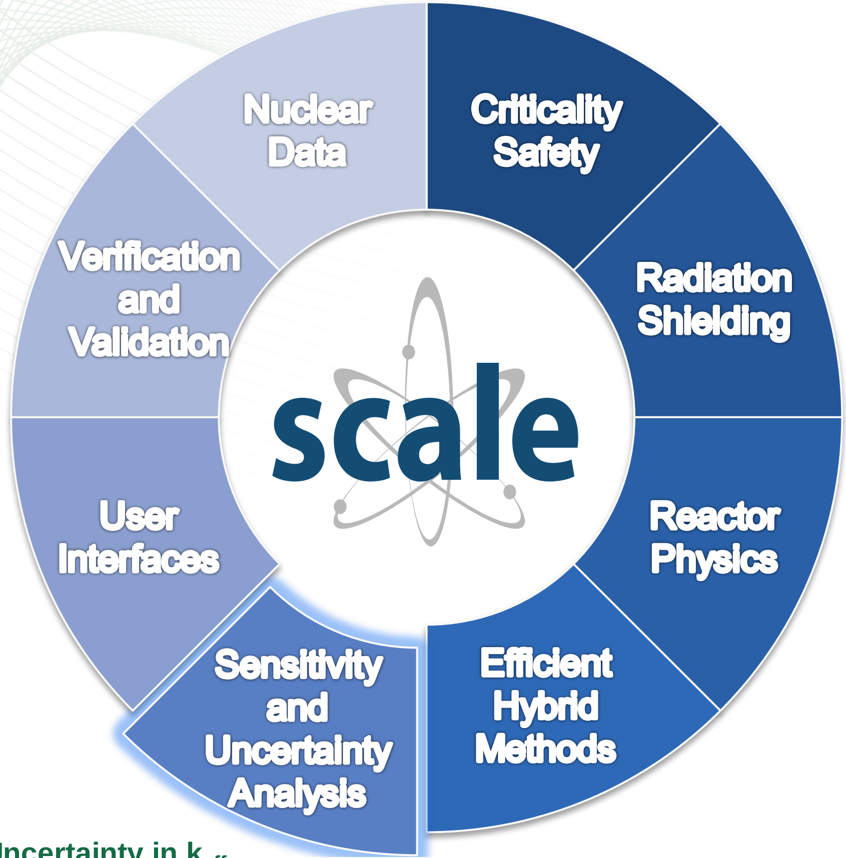
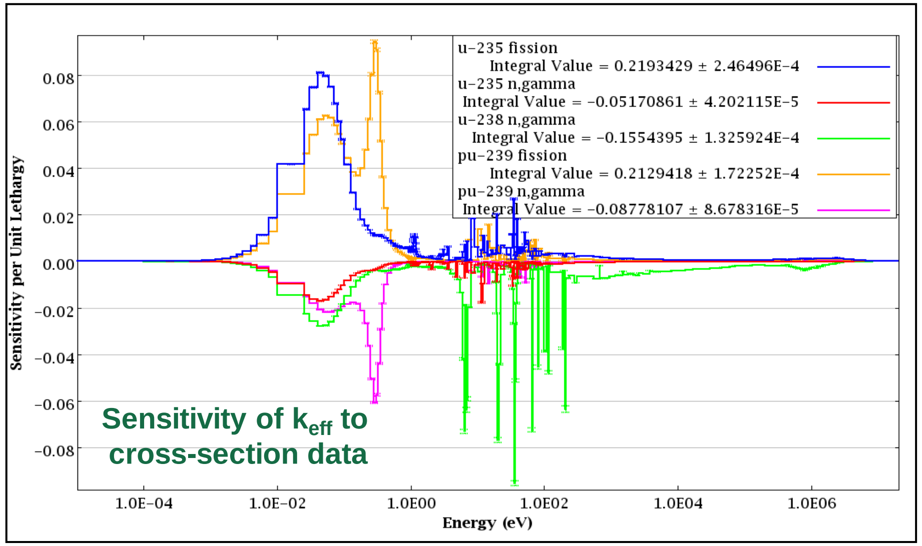
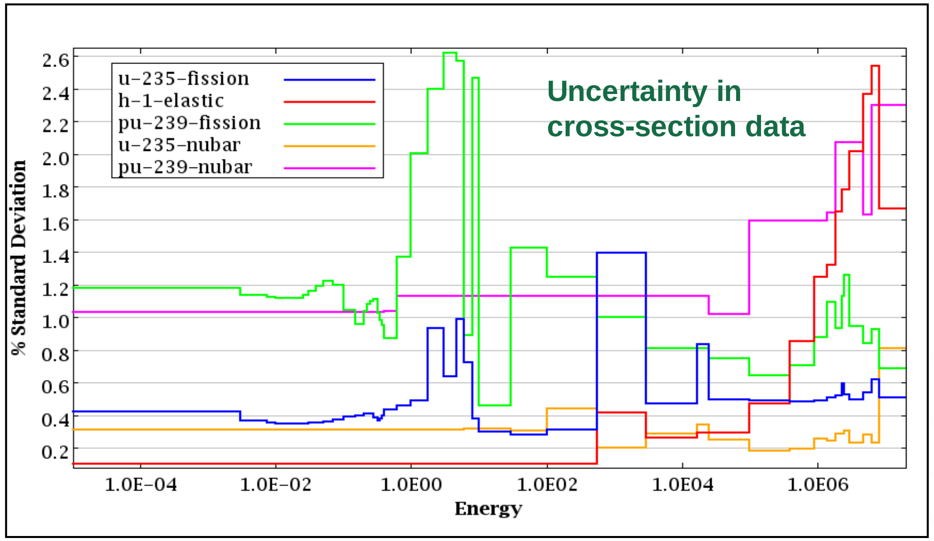
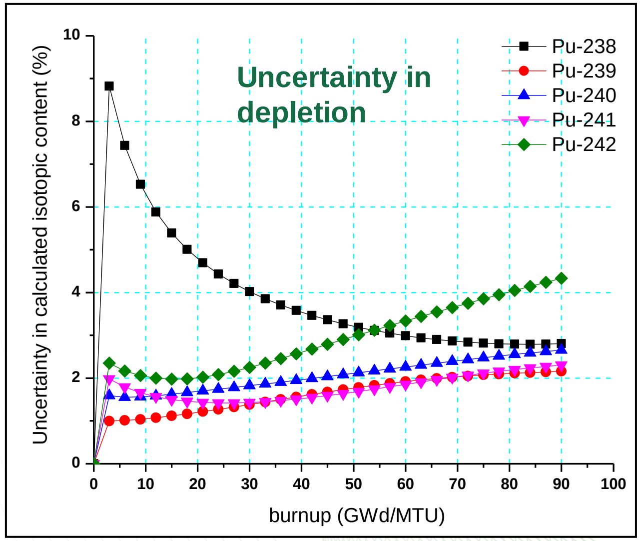
Sensitivity and Uncertainty Analysis









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 ± 2.5625E-06
^{238}U n,gamma	^{238}U n,gamma	1.9457E-01 ± 1.2387E-05
^{239}Pu fission	^{239}Pu fission	1.5501E-01 ± 1.0838E-05
^{235}U nubar	^{235}U nubar	1.3981E-01 ± 5.0038E-07
^{239}Pu fission	^{239}Pu n,gamma	1.2261E-01 ± 4.3564E-06

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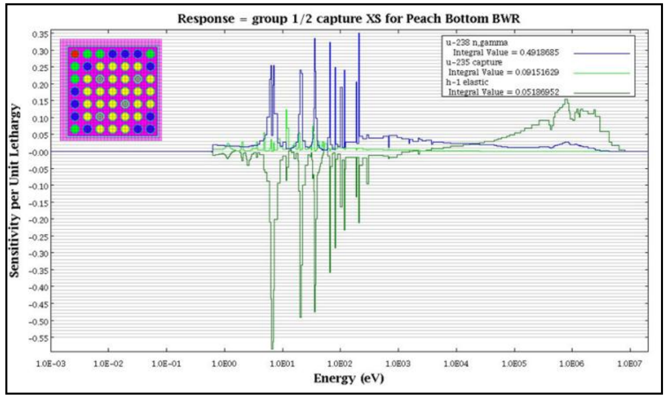
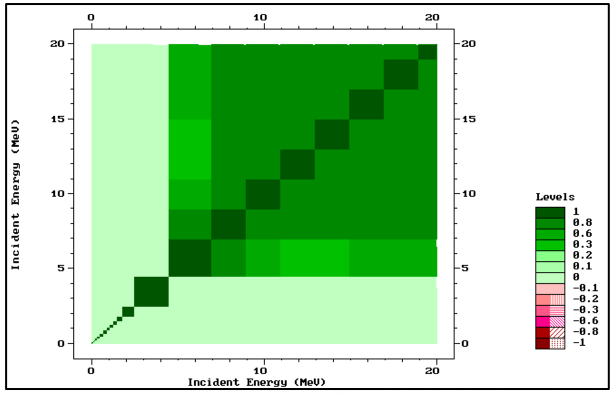
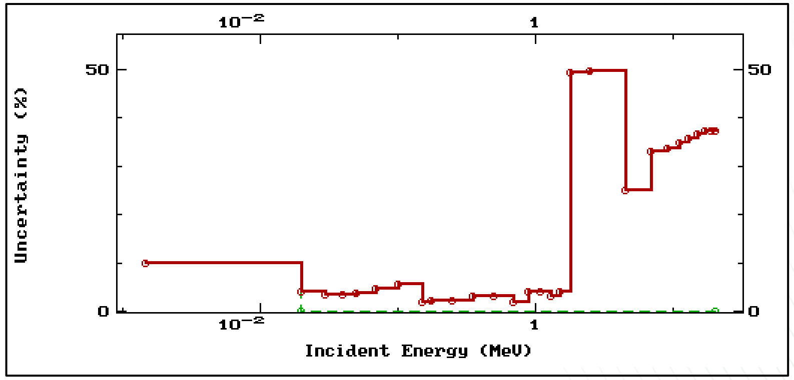
Sensitivity and Uncertainty Enhancements

- Sensitivity computations with continuous-energy Monte Carlo for eigenvalue and GPT responses
- New statistical sampling code "Sampler" for general UQ of Scale MG Sequences
- New 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







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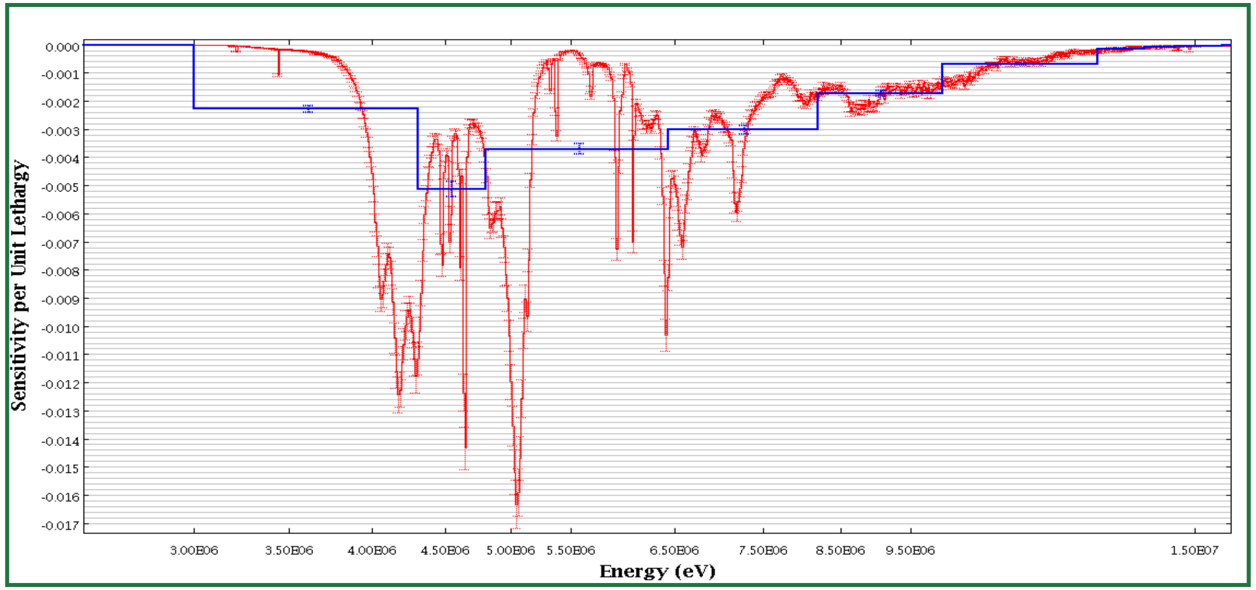
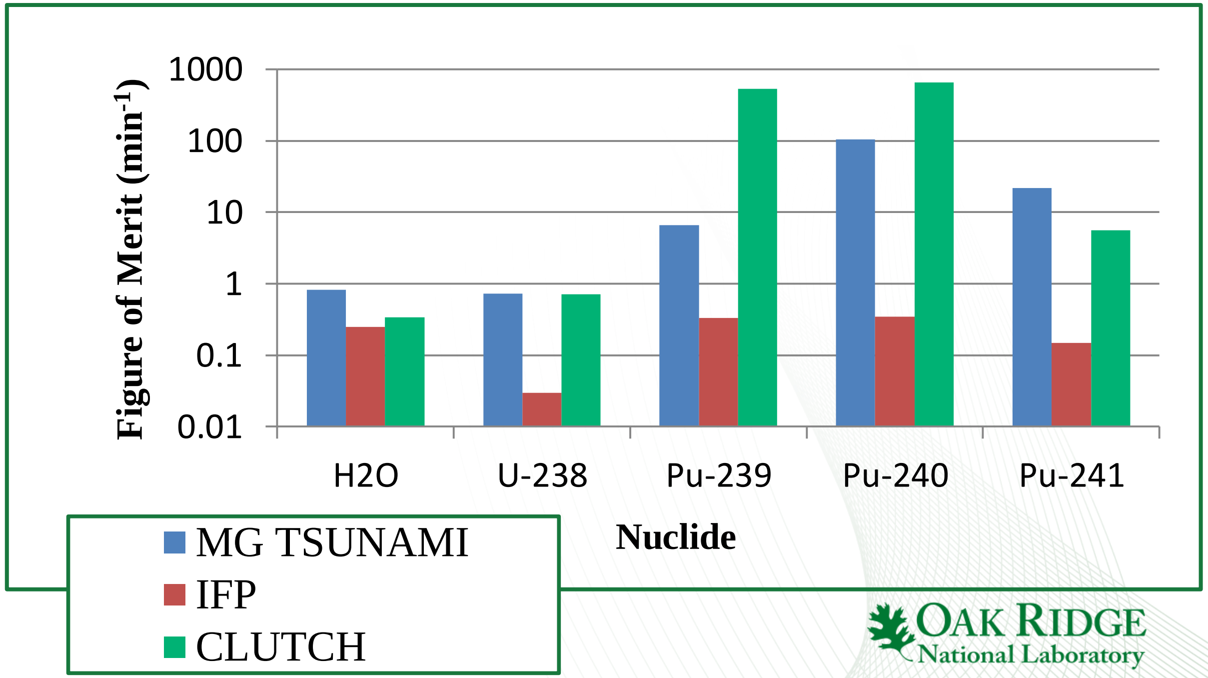
Continuous-energy TSUNAMI-3D

- 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



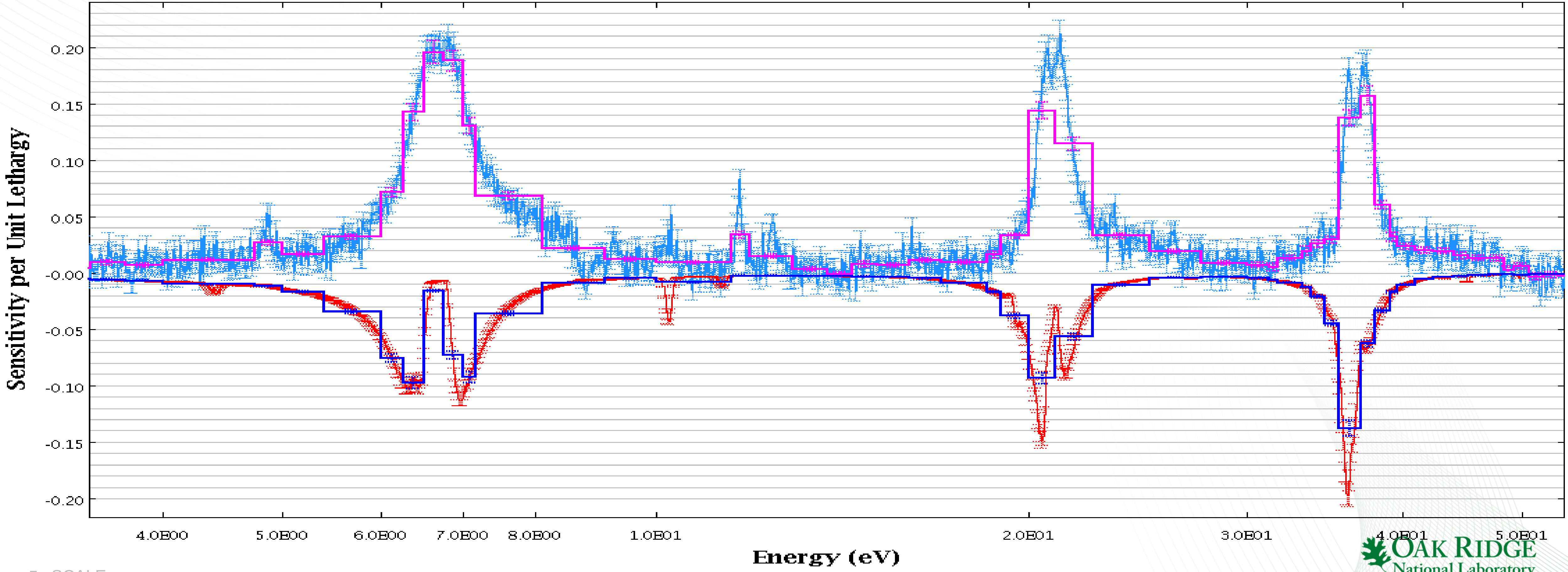
MIX-COMP-THERM-004-001
FoM Comparison



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



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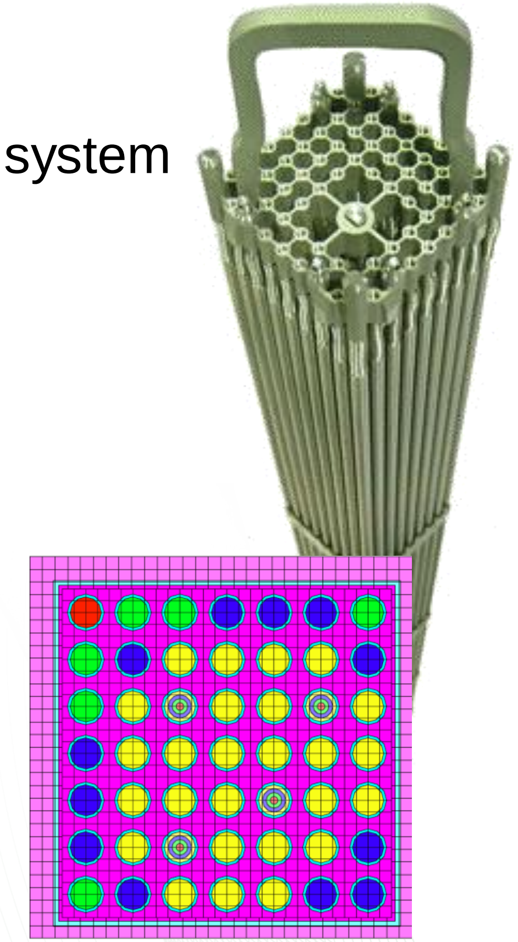
Generalized Perturbation Theory

- 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

OECD UAM GPT Benchmark Phase 1-2 Results

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.

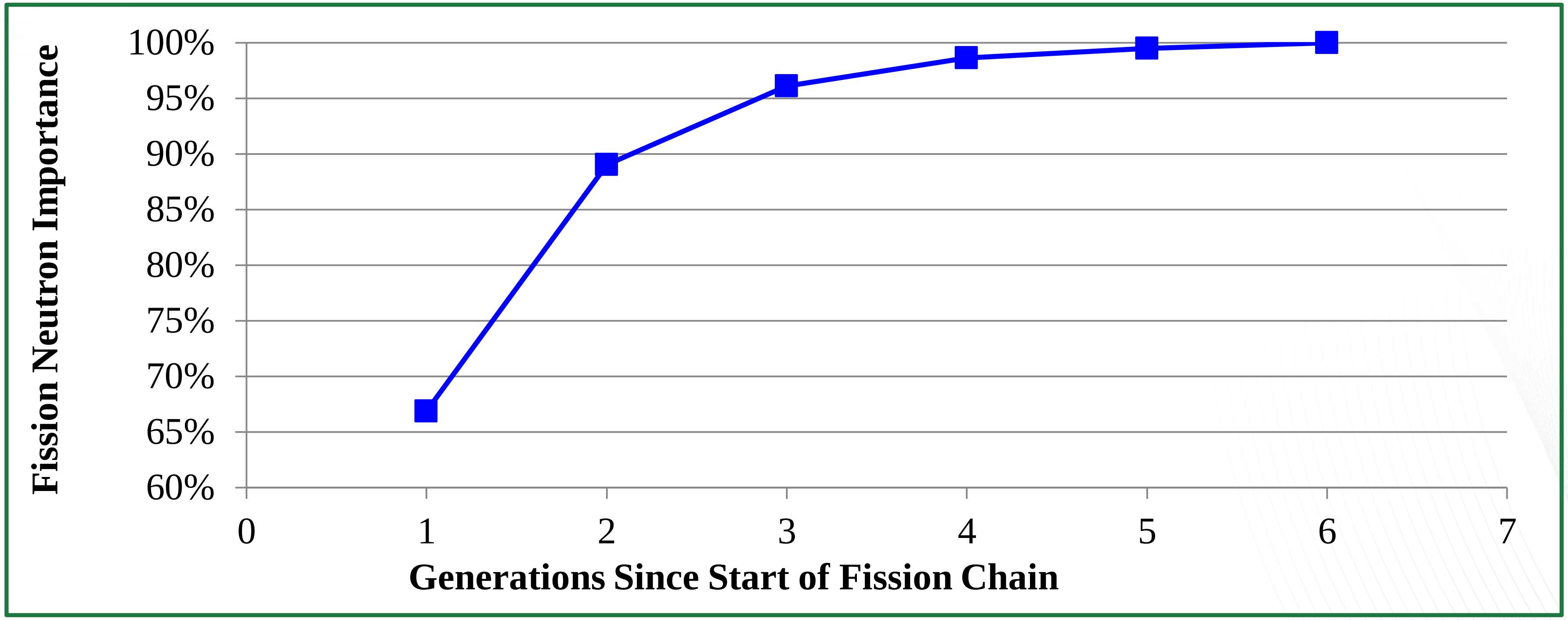
$$\Gamma^{\dagger}(\tau_s) = \boxed{\frac{1}{Q_s}\langle\frac{1}{R}\frac{\partial R}{\partial\phi}(r)\phi(\tau_s \rightarrow r)\rangle} + \boxed{\frac{\lambda}{Q_s}\langle\Gamma^{\dagger}(r)P(r)\phi(\tau_s \rightarrow r)\rangle}$$

- 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.
- For more background on this methodology, see:

C. M. Perfetti, B. T. Rearden, "Continuous-Energy Monte Carlo Methods for calculating Generalized Response Sensitivities using TSUNAMI-3D," in *Proc. of the 2014 International Conference on the Physics of Reactors (PHYSOR 2014),* Kyoto, Japan, September 28 – October 3, 2014.

Inter-generational Importance

- The inter-generational term is calculated by tallying the intra-generational importance generated by neutrons in a fission chain as that importance approaches zero.



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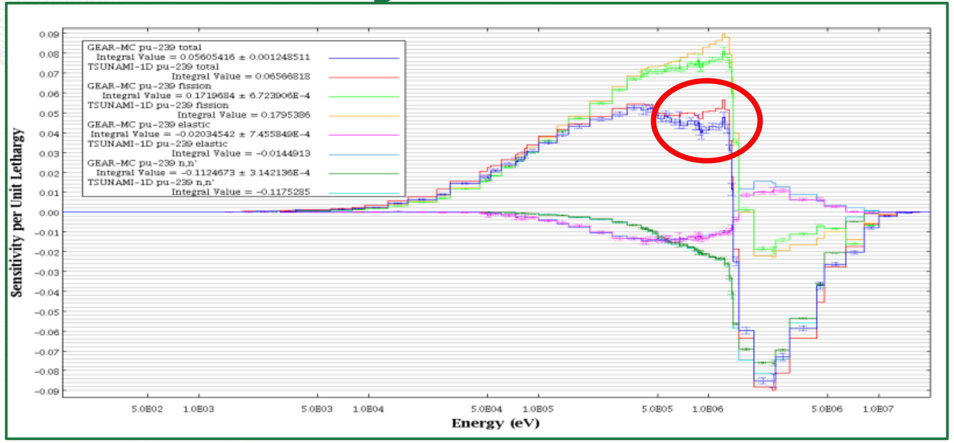
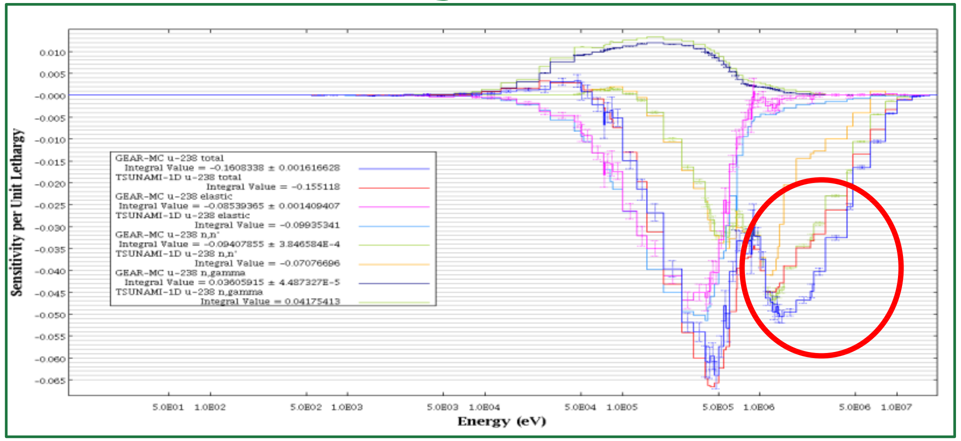
GPT Flattop Foil Response Sensitivity Coefficients

F28/F25 Pu-239 Sensitivity Coefficients



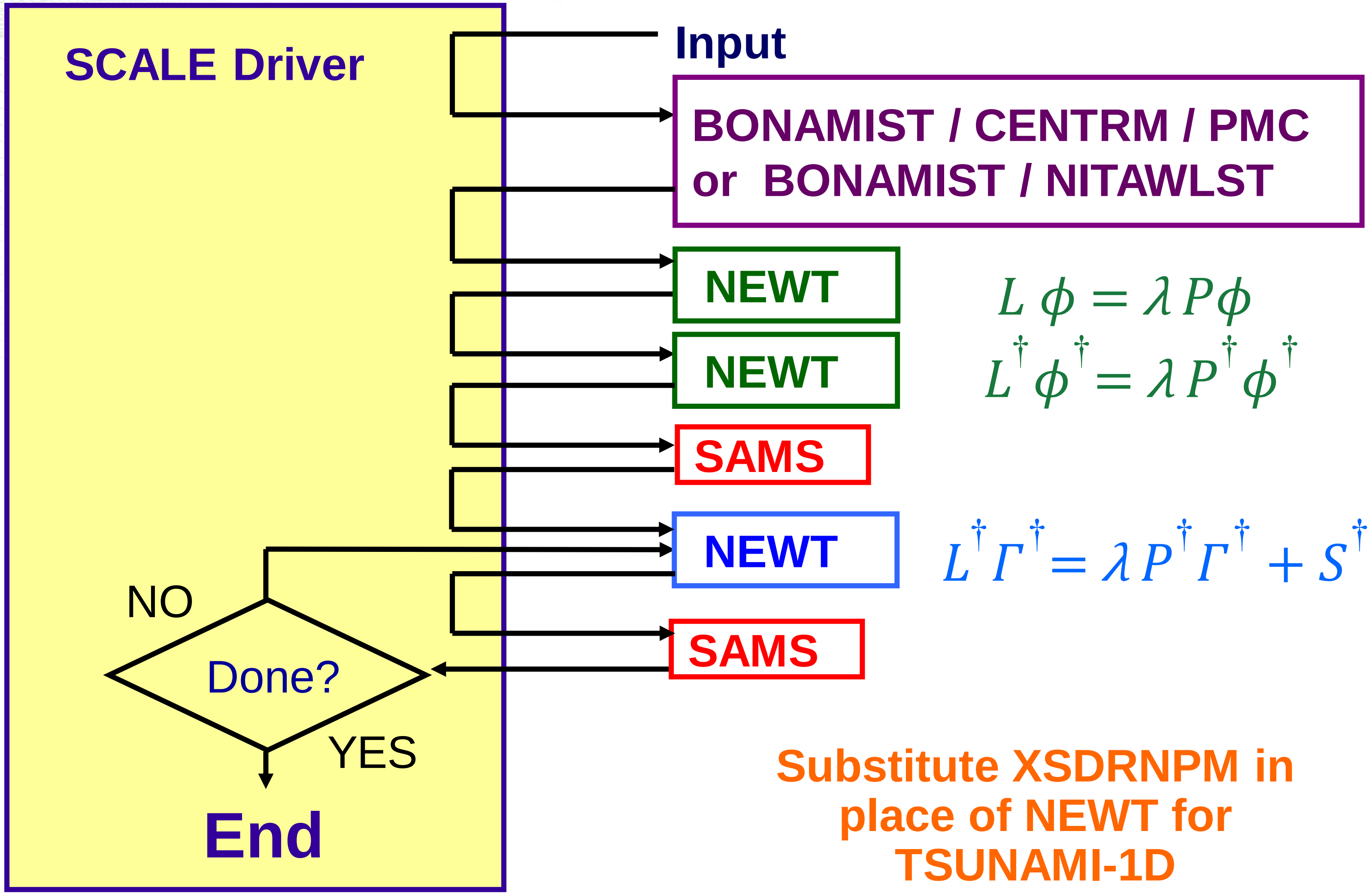
F37/F25 U-238 Sensitivity Coefficients



Flattop Total Nuclide Foil Response Sensitivities

Experiment	Response	Isotope	Direct Pert.	TSUNAMI-1D	TSUNAMI-3D
Flattop	F28 / F25	^{238}U	0.8006 ± 0.0533	0.8024 **(0.03 σ)**	0.7954 ± 0.0018 **(-0.10 σ)**
		^{239}Pu	0.0528 ± 0.0043	0.0657 **(2.99 σ)**	0.0561 ± 0.0012 **(0.73 σ)**
	F37 / F25	^{238}U	-0.1540 ± 0.0102	-0.1551 **(-0.11 σ)**	-0.1608 ± 0.0016 **(-0.66 σ)**
		^{239}Pu	0.0543 ± 0.0048	0.0736 **(3.99 σ)**	0.0489 ± 0.0010 **(-1.10 σ)**

TSUNAMI-1D/2D GPT Sequences



Resonance cross-section processing (repeated for all cells)

2D discrete ordinates

2D discrete ordinates adjoint calculation

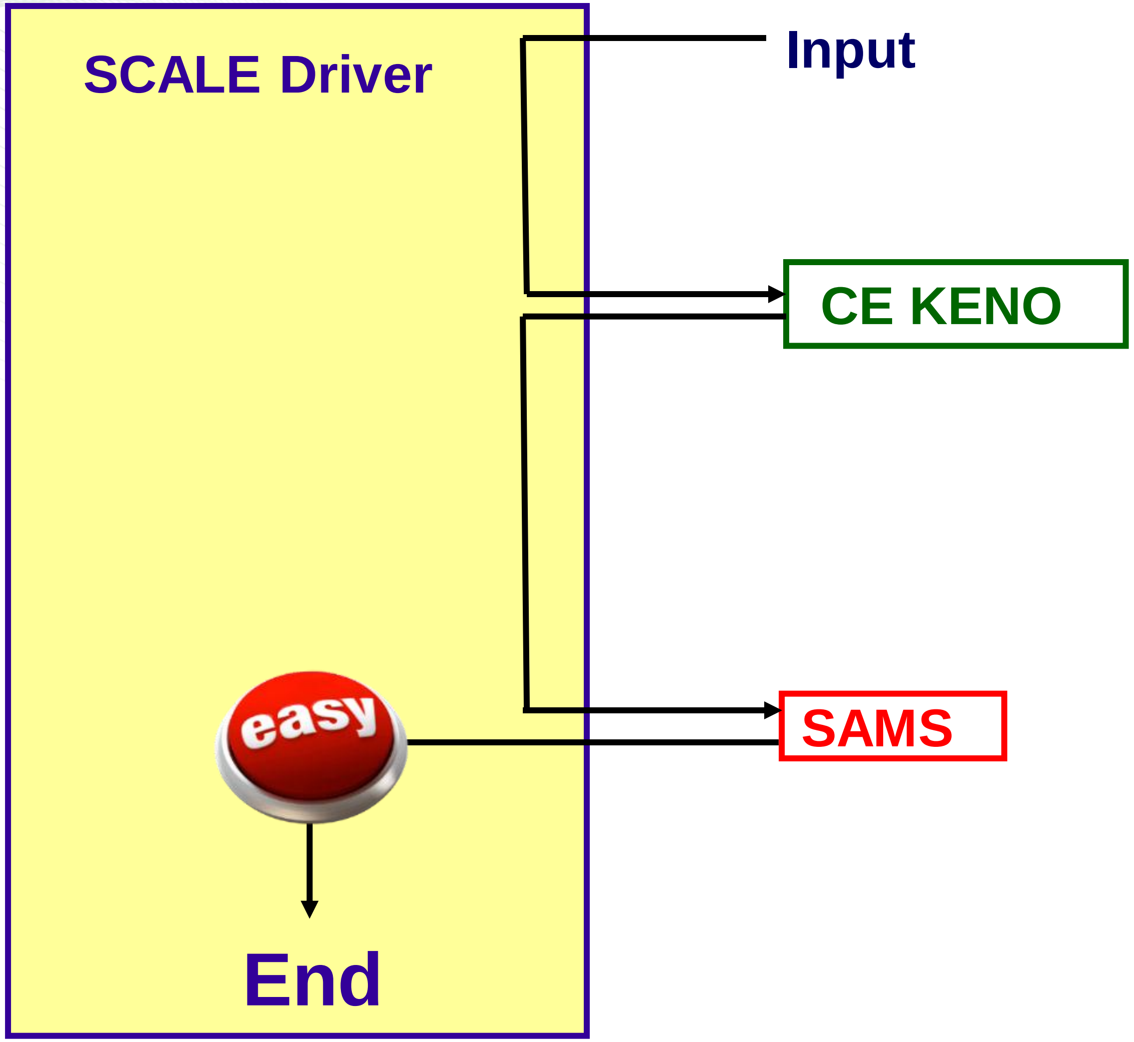
S/U calculation for k_{eff}

2D discrete ordinates inhomogeneous adjoint calculation for each response

S/U calculation for a user-defined response

Substitute XSDRNPM in place of NEWT for TSUNAMI-1D

CE TSUNAMI-3D GPT Sequence: Improved Efficiency and Scalability



3D Monte Carlo

$$L\phi = \lambda P\phi$$
$$L^{\dagger}\phi^{\dagger} = \lambda P^{\dagger}\phi^{\dagger}$$
$$L^{\dagger}\Gamma^{\dagger} = \lambda P^{\dagger}\Gamma^{\dagger} + S^{\dagger}$$

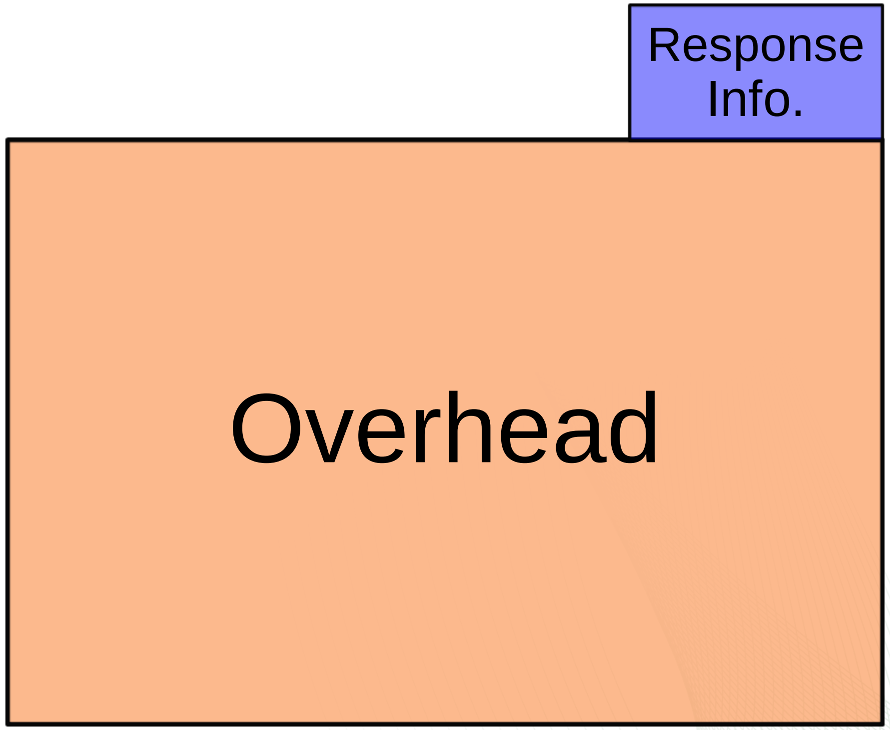
S/U calculation for k_{eff} and user-defined responses

Multi-response CE TSUNAMI-3D GPT Calculations

- The CE TSUNAMI-3D GPT capability has been improved to allow for multiple GPT response sensitivity calculations within a single simulation.
- Performing sensitivity calculations for additional GPT responses generally requires a modest increase in the problem’s runtime and memory footprint.
- The input for entering GPT responses in CE TSUNAMI-3D is consistent with the format for GPT TSUNAMI-1D/2D.

IFP Sensitivity Methods:

Large Initial Overhead,
Low Additional Memory per Response



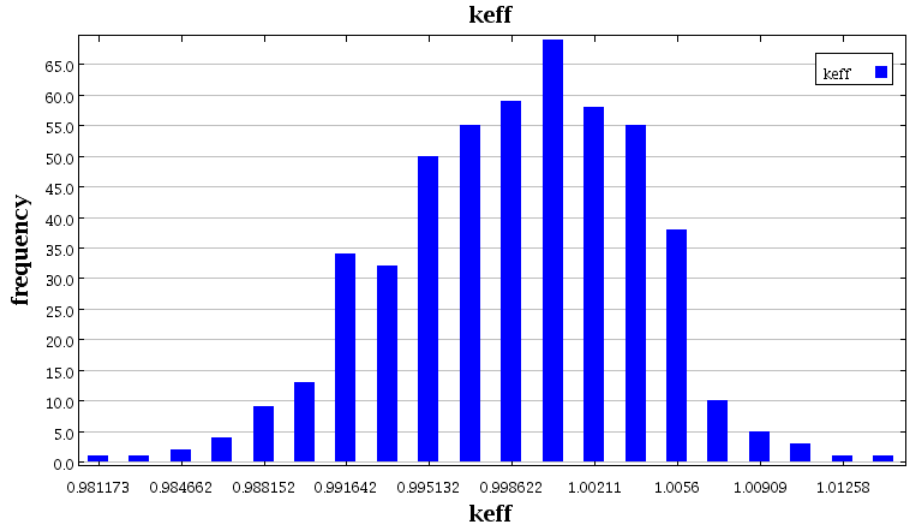
CE TSUNAMI-3D GPT Algorithms Scale Well for Multi-response Problems

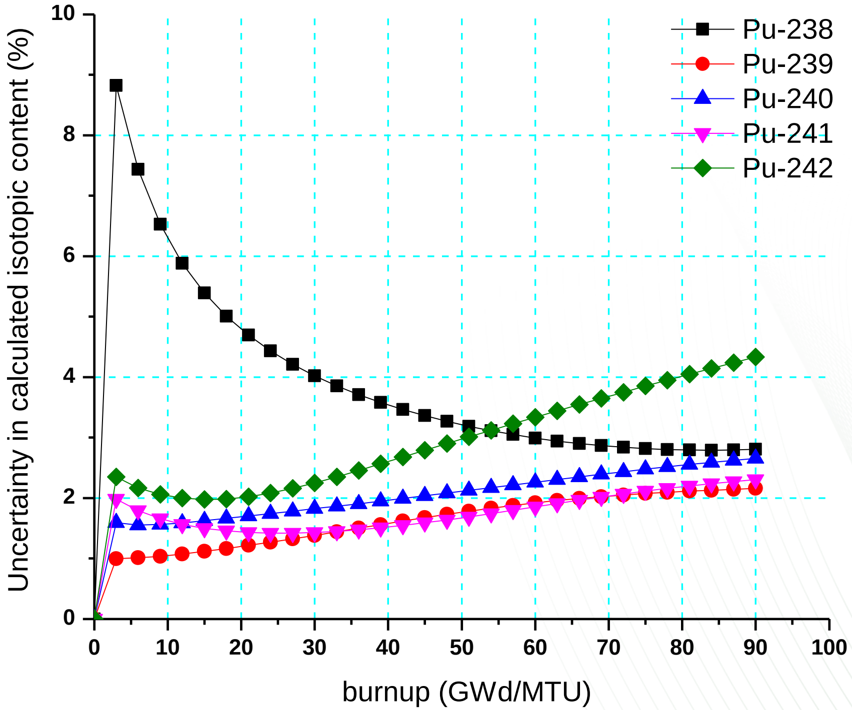
HFIR Isotope Production Sample Application		
CE TSUNAMI GPT Calculation	**Computational Performance**	
	Memory Footprint*	**Time per Gen.**
2 Responses	28.22 GB	4.52 min
4 Responses	28.73 GB	4.61 min
6 Responses	29.24 GB	4.65 min
24 Responses	33.83 GB (+0.9% per response)	5.40 min (+0.9% per response)

***This memory footprint is very parallelizable.**

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 depletion calculations
- Correlations between systems are also computed





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SCALE 6.0–6.1 Covariance Library (401 materials)

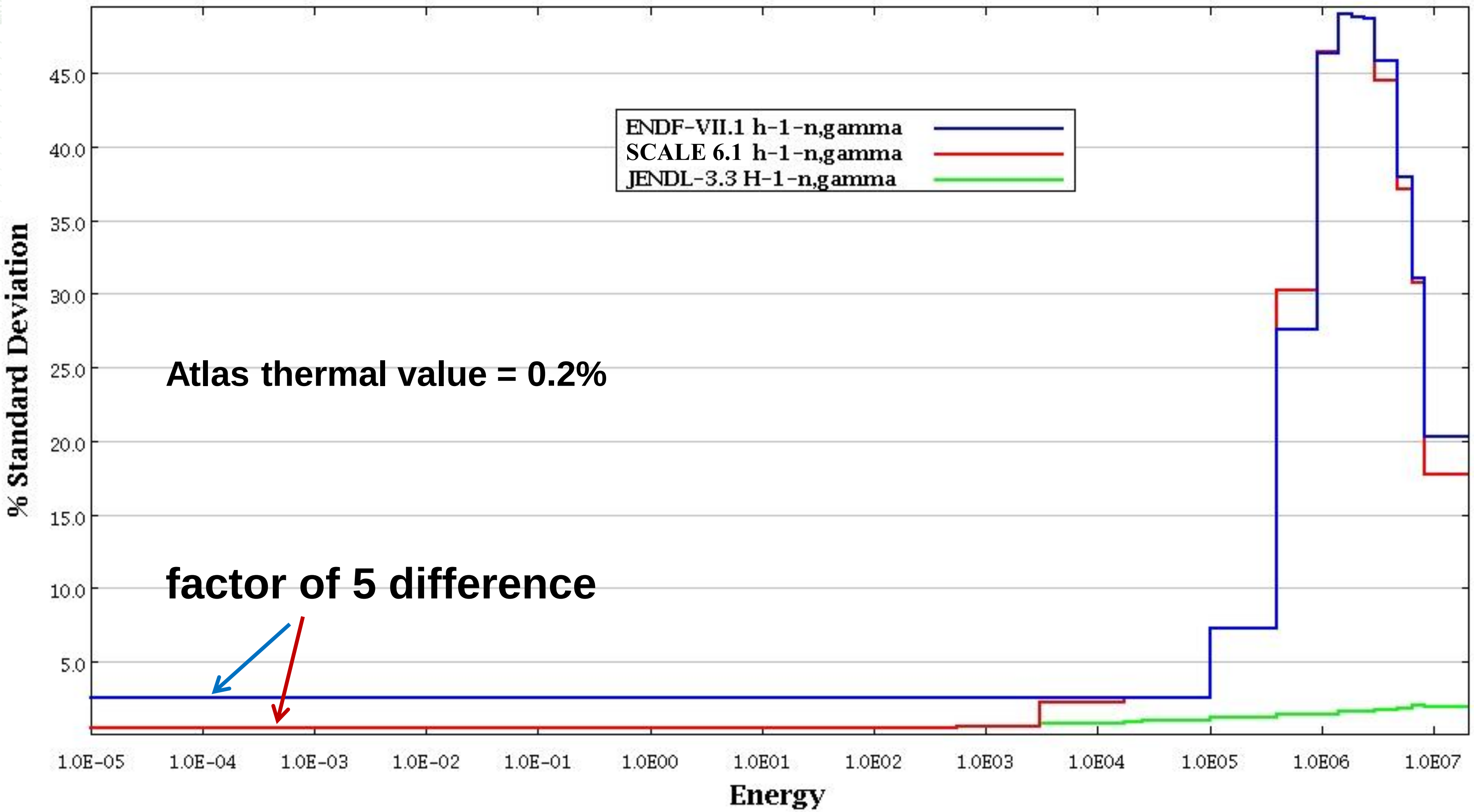
Data Source	Materials
ENDF/B-VII.0	$^{152,154-158,160}$Gd, ^{191,193}Ir, ^{7}Li, ^{99}Tc, ^{232}Th
ENDF/B-VII-p	^{197}Au, ^{209}Bi, ^{59}Co, ^{23}Na, ^{93}Nb, ^{58}Ni, ^{239}Pu, ^{48}Ti, ^{233,235,238}U*, V
ENDF/B-VI	^{27}Al, ^{241}Am, C, C-graphite, $^{50,52-54}$Cr, ^{65}Cu, ^{156}Dy, $^{54,56-58}$Fe, 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 (**B**rookhaven, **L**os Alamos, **O**RNL)
ENDF/B-VI: evaluated covariance data released with ENDF/B-VI	**BLO LANL evaluation**: LANL R-matrix evaluation from BLO project
* ^{235}U thermal nubar 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-d20	
ti49	mo100	sm149	tl205	np234	cm250	h-poly	

H Capture Uncertainty



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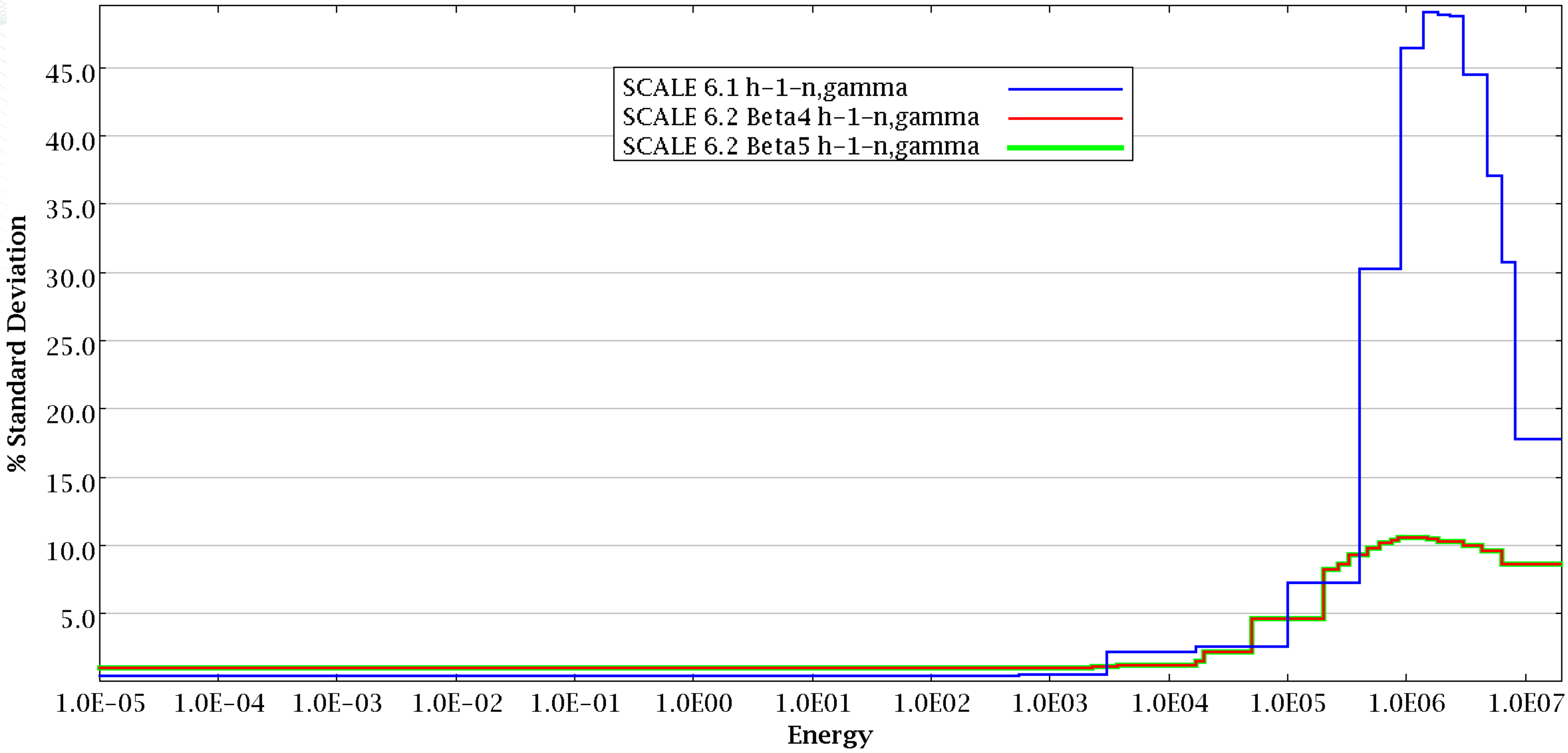
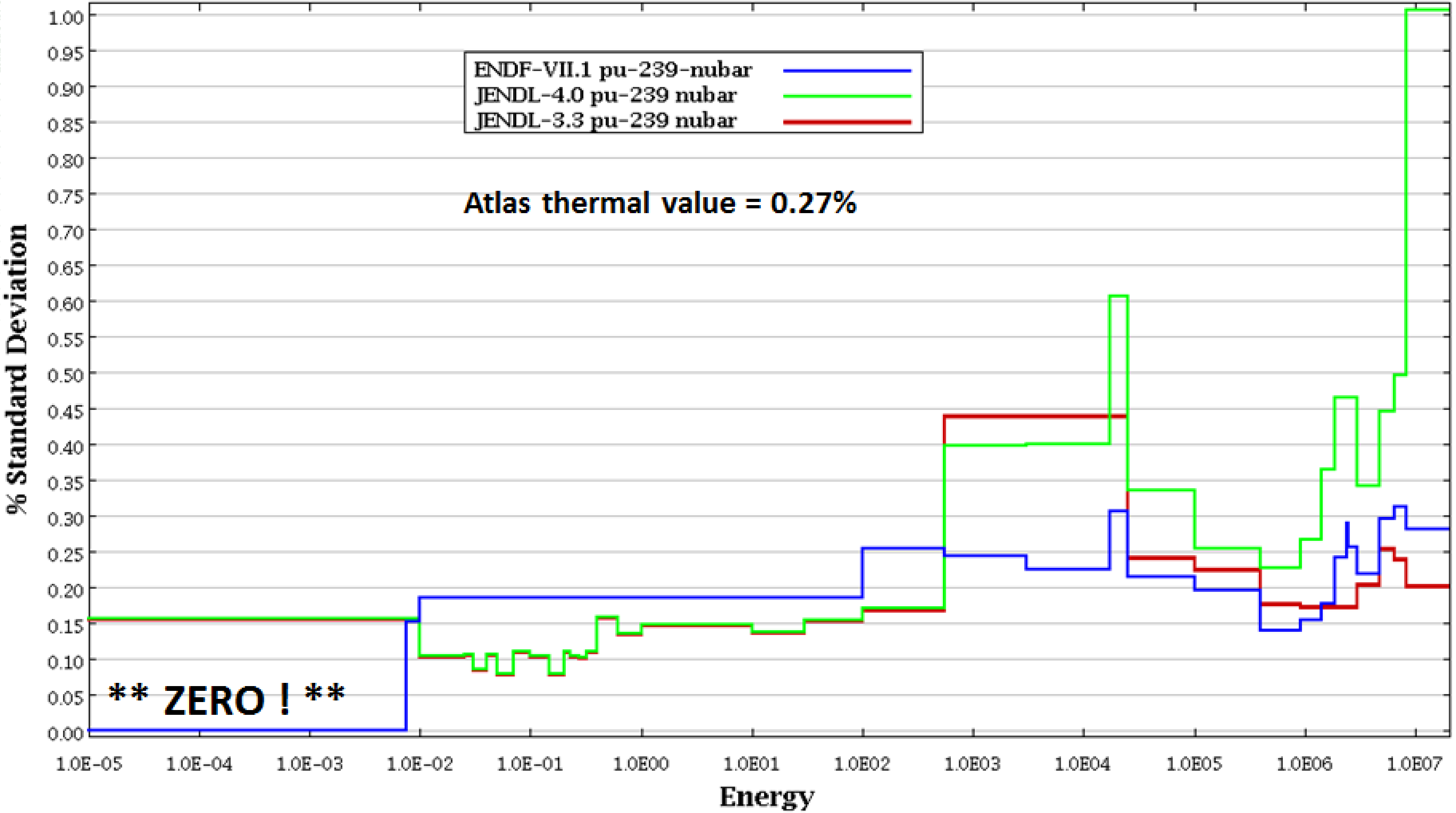
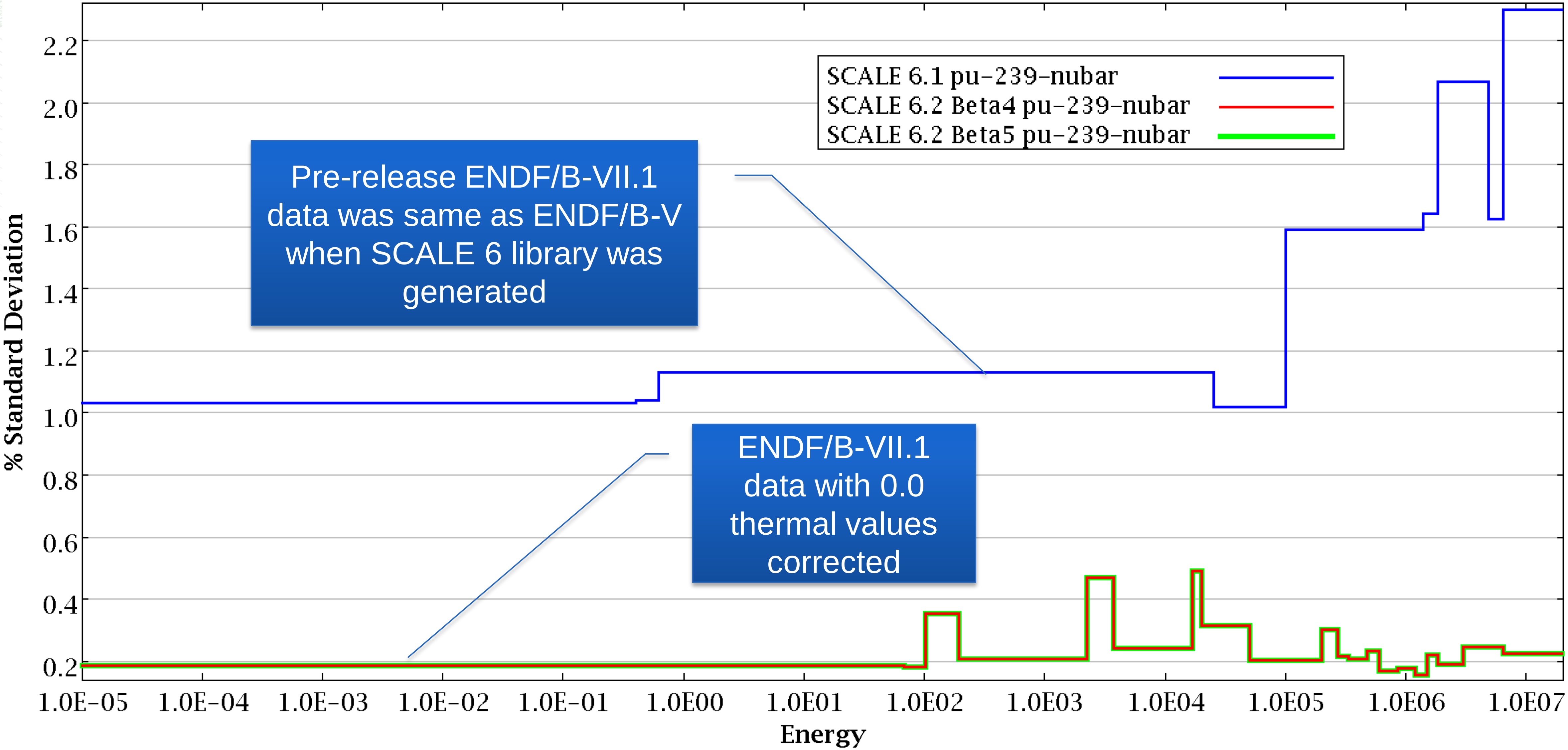
H Capture Uncertainty



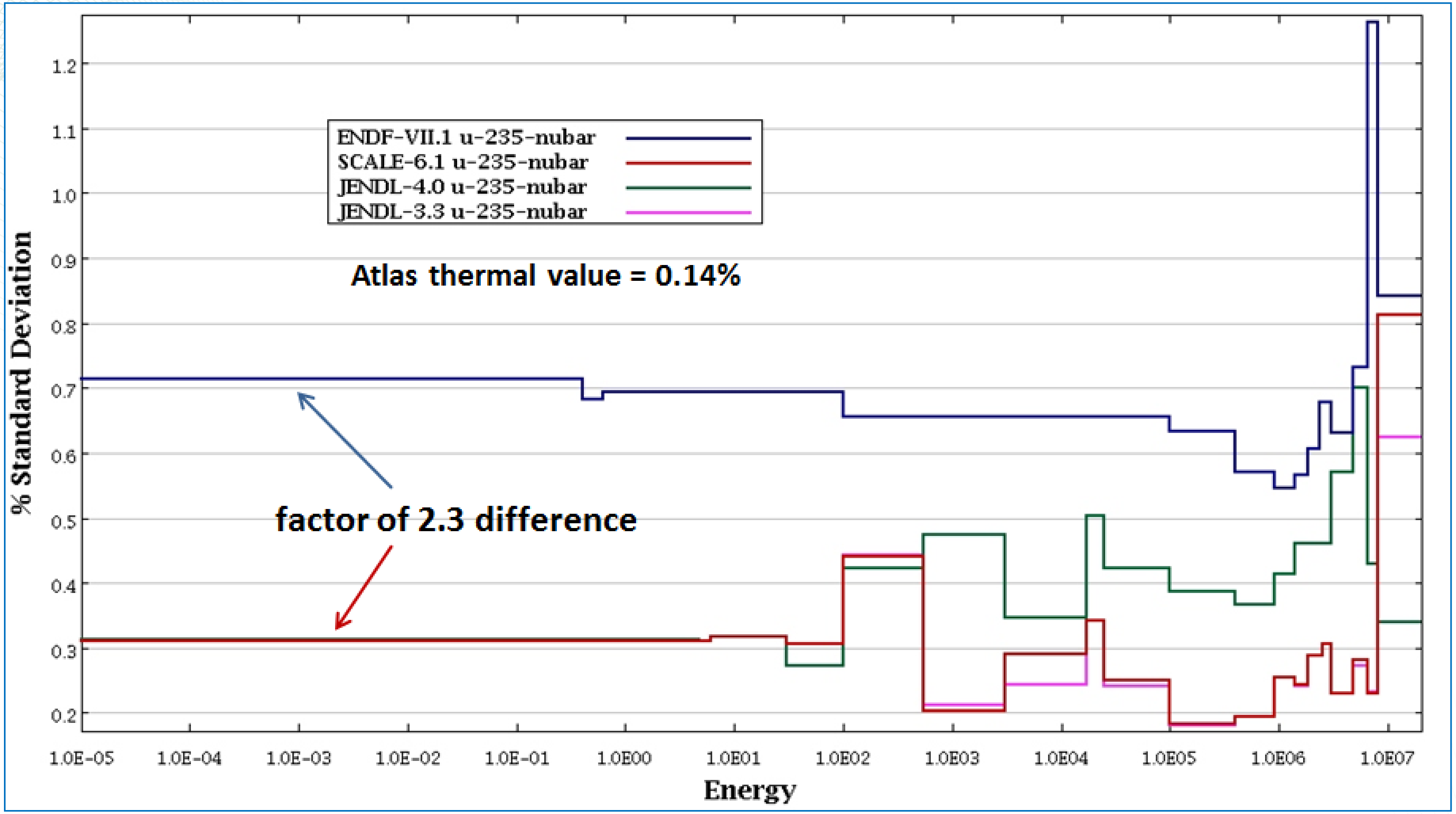
Pu-239 nubar uncertainty



Pu-239 nubar uncertainty



U-235 nubar uncertainty



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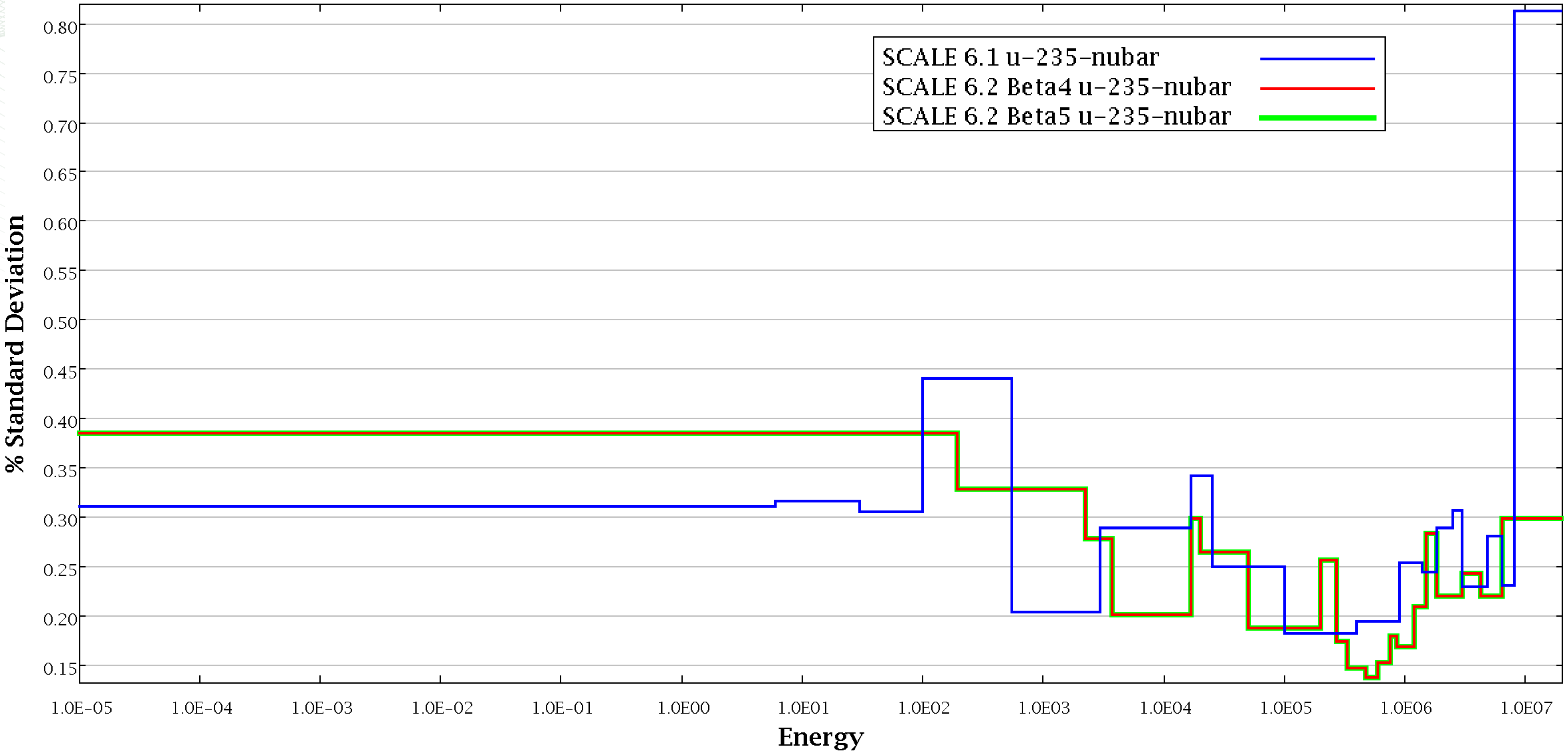
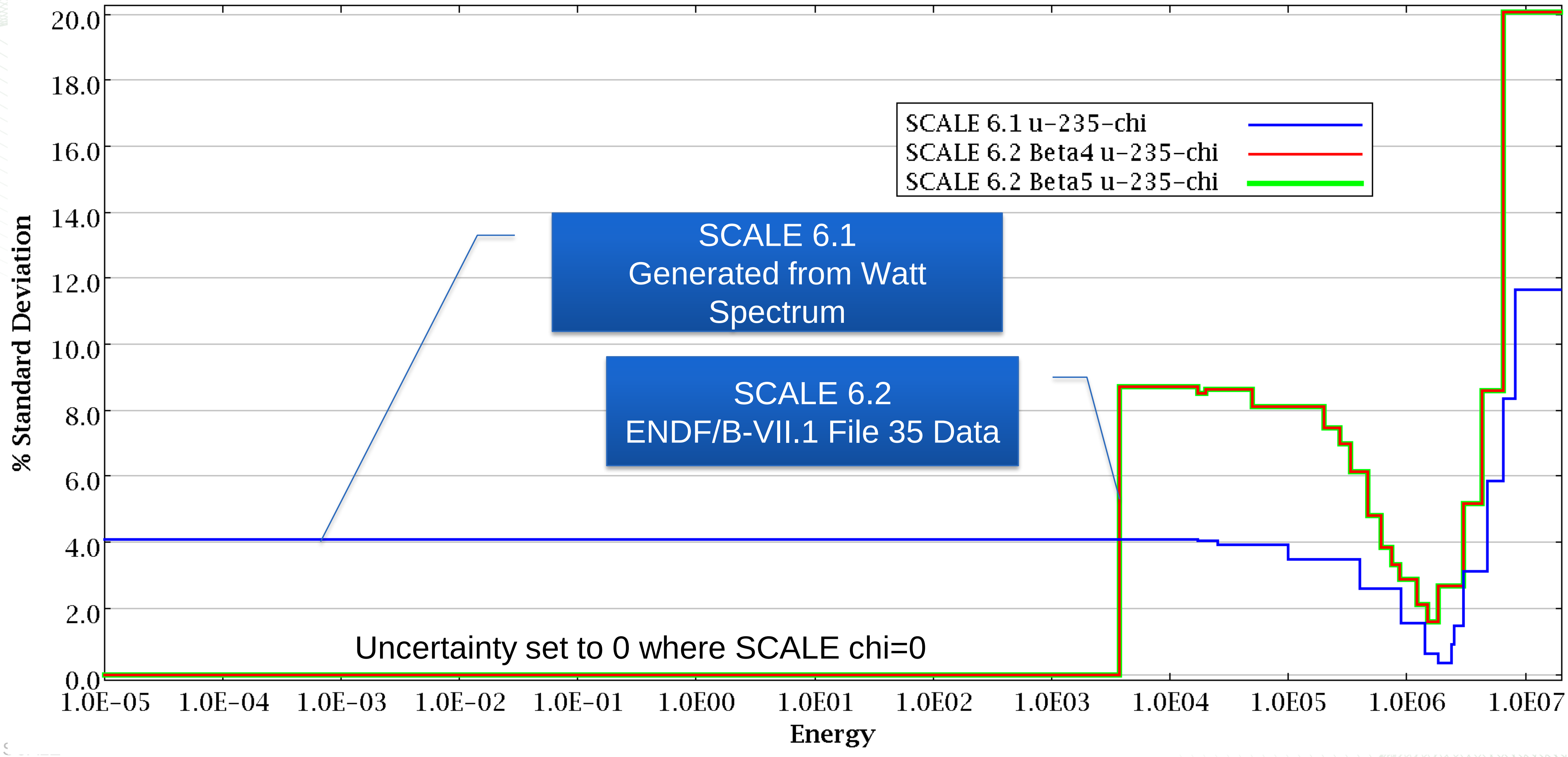
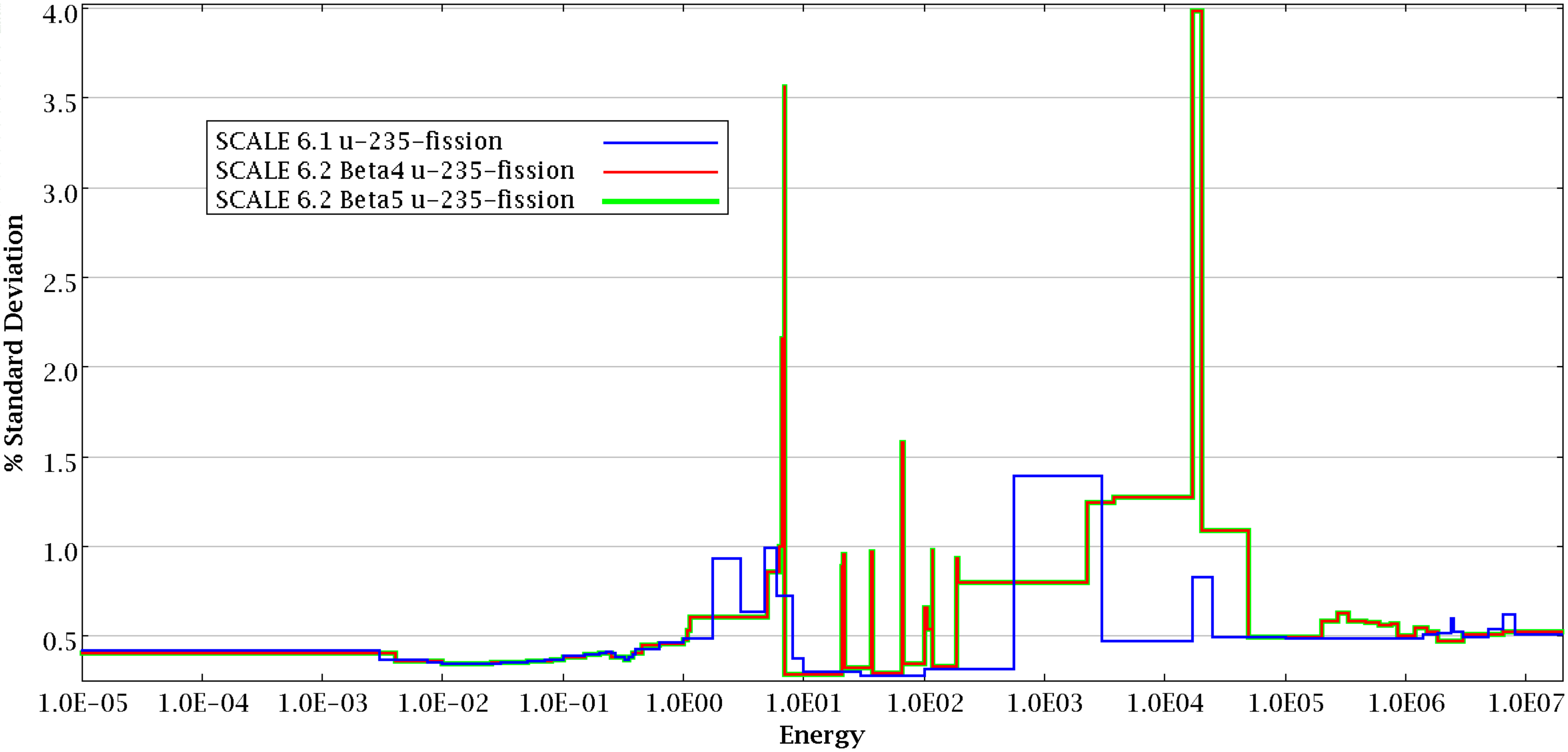
U-235 nubar uncertainty



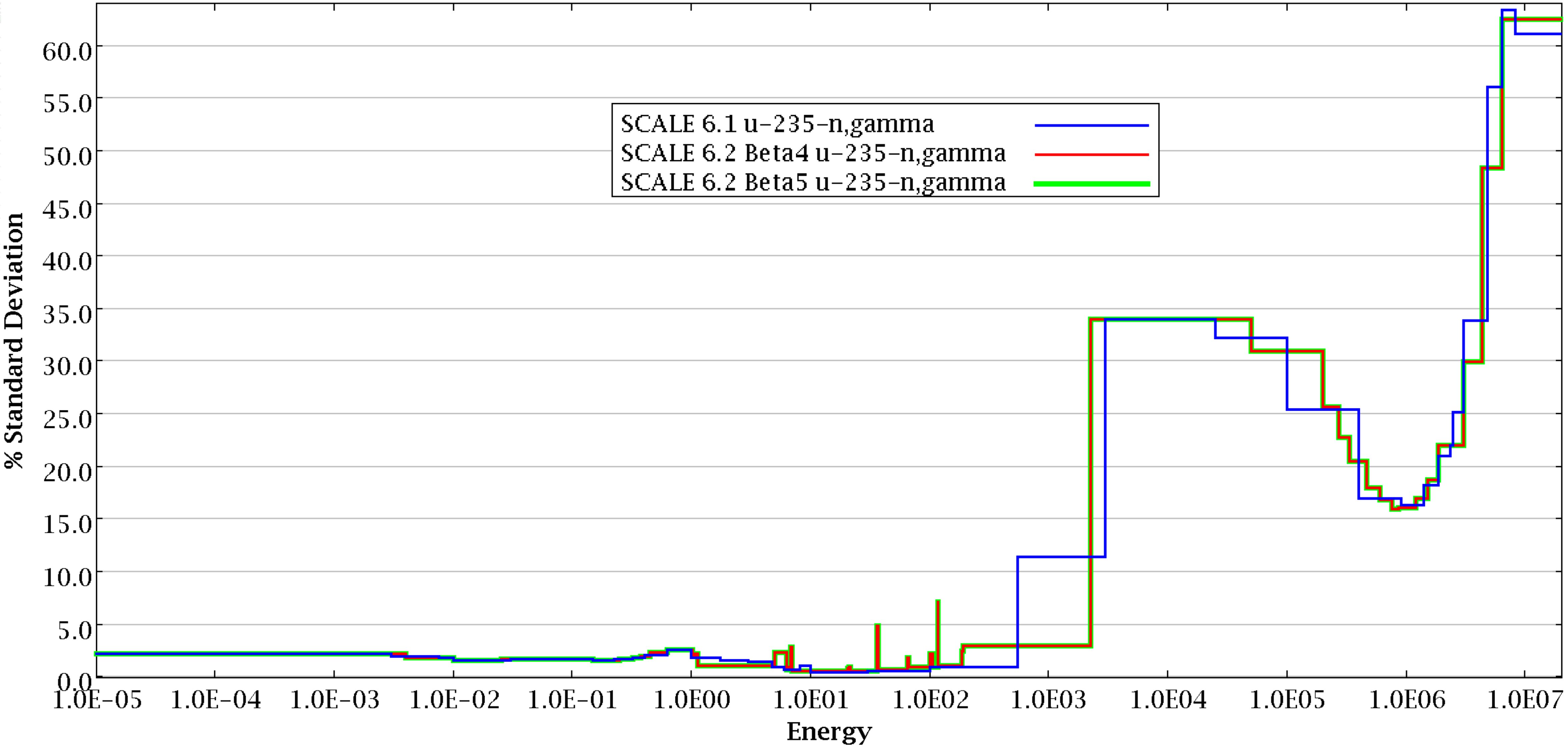
U-235 chi uncertainty



U-235 fission uncertainty

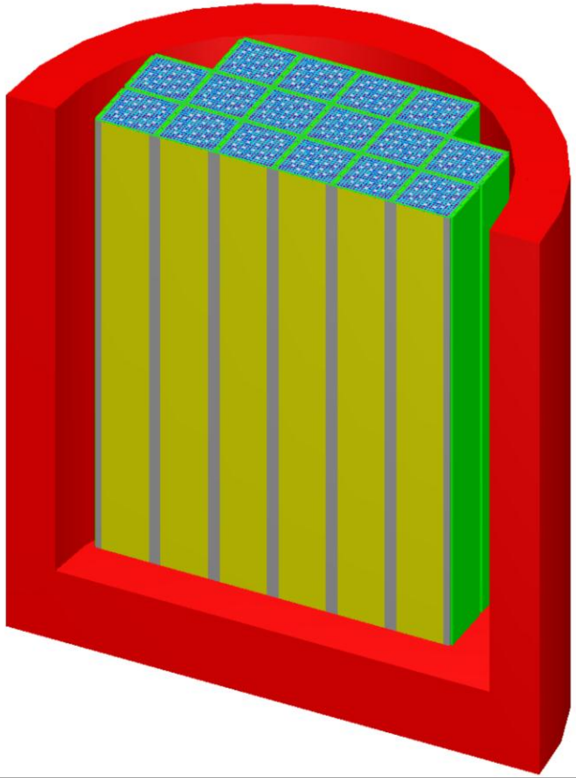


U-235 n,gamma uncertainty

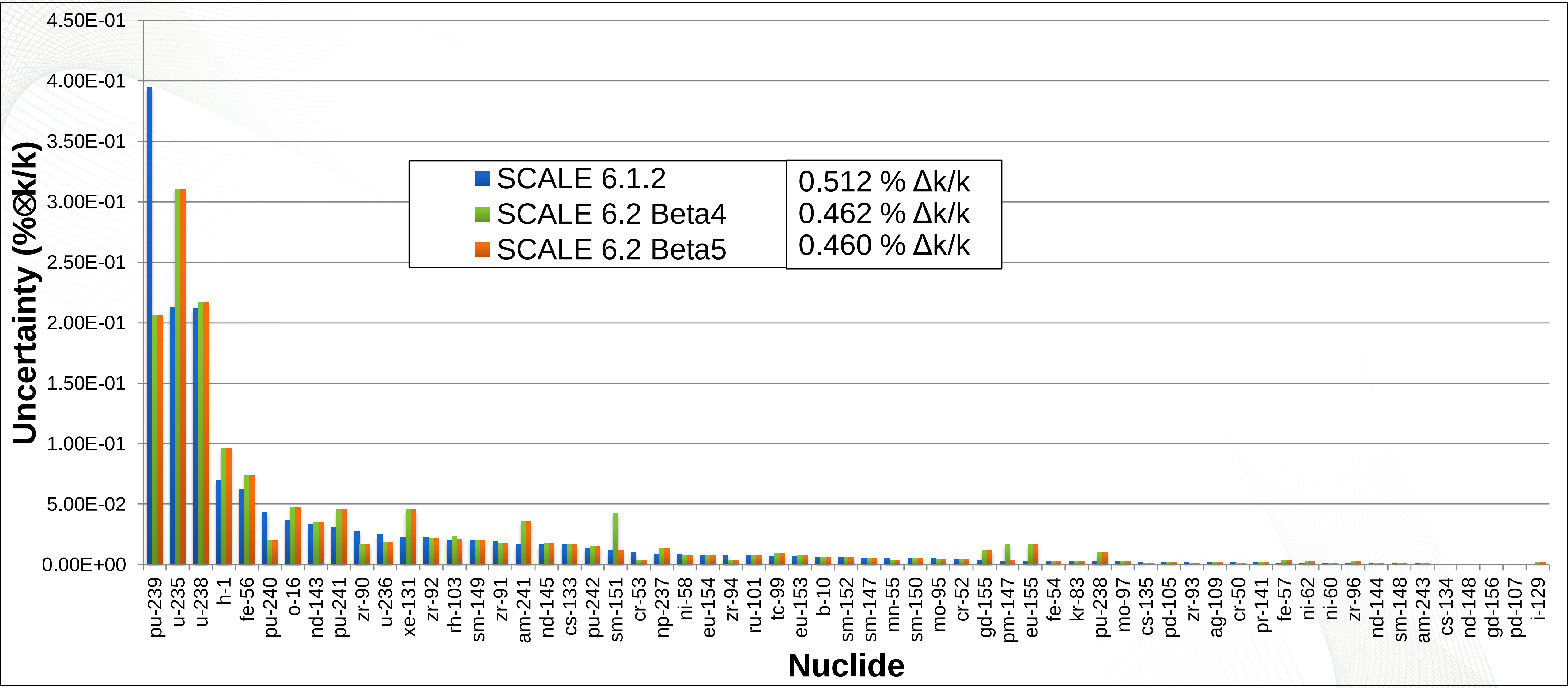


Criticality Analysis for Used Nuclear Fuel (UNF)

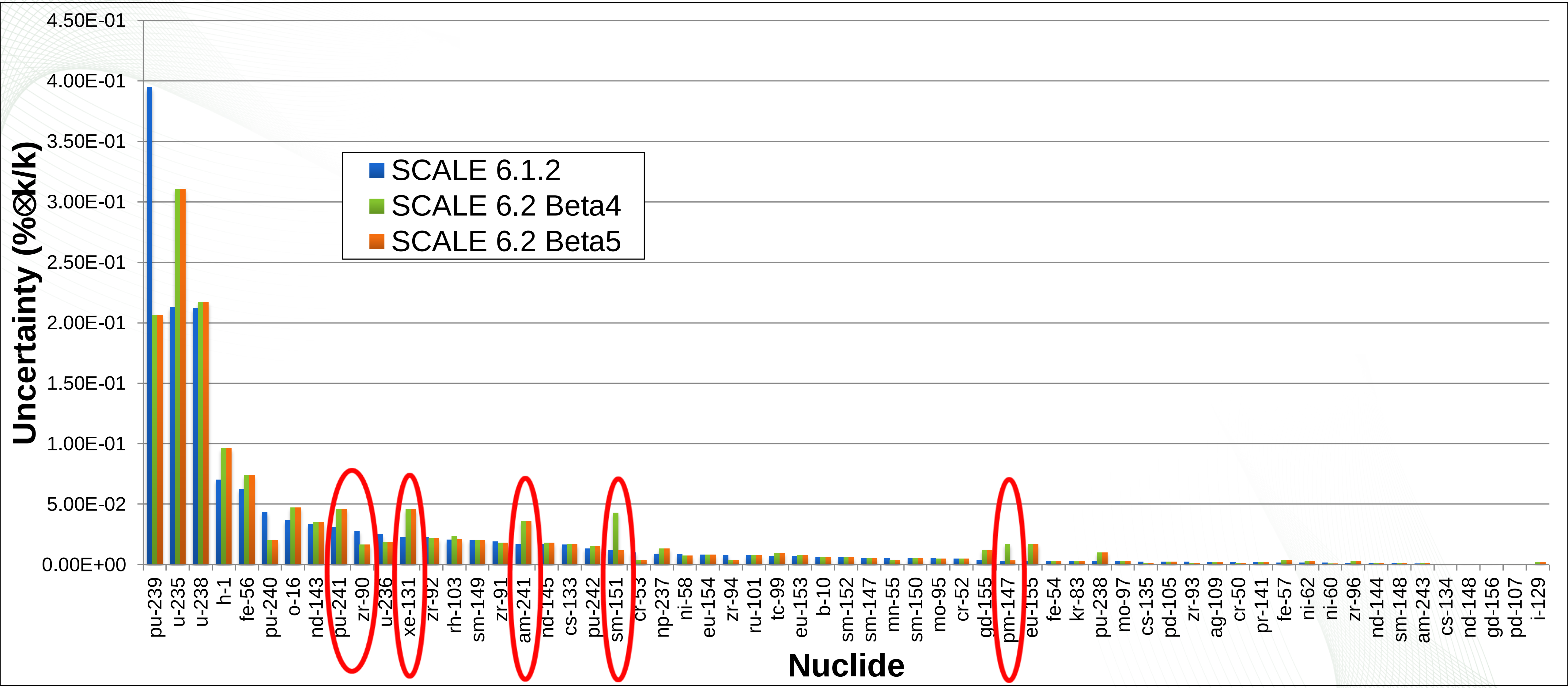
- UNF contains many actinides and fission products
- A limiting condition on UNF cask storage is sub-criticality margin
- NRC allows “burnup credit” for burned fuel and certain FP nuclides
- Uncertainties are important consideration
  - SCALE 6.1 used in S/U for U.S. NRC



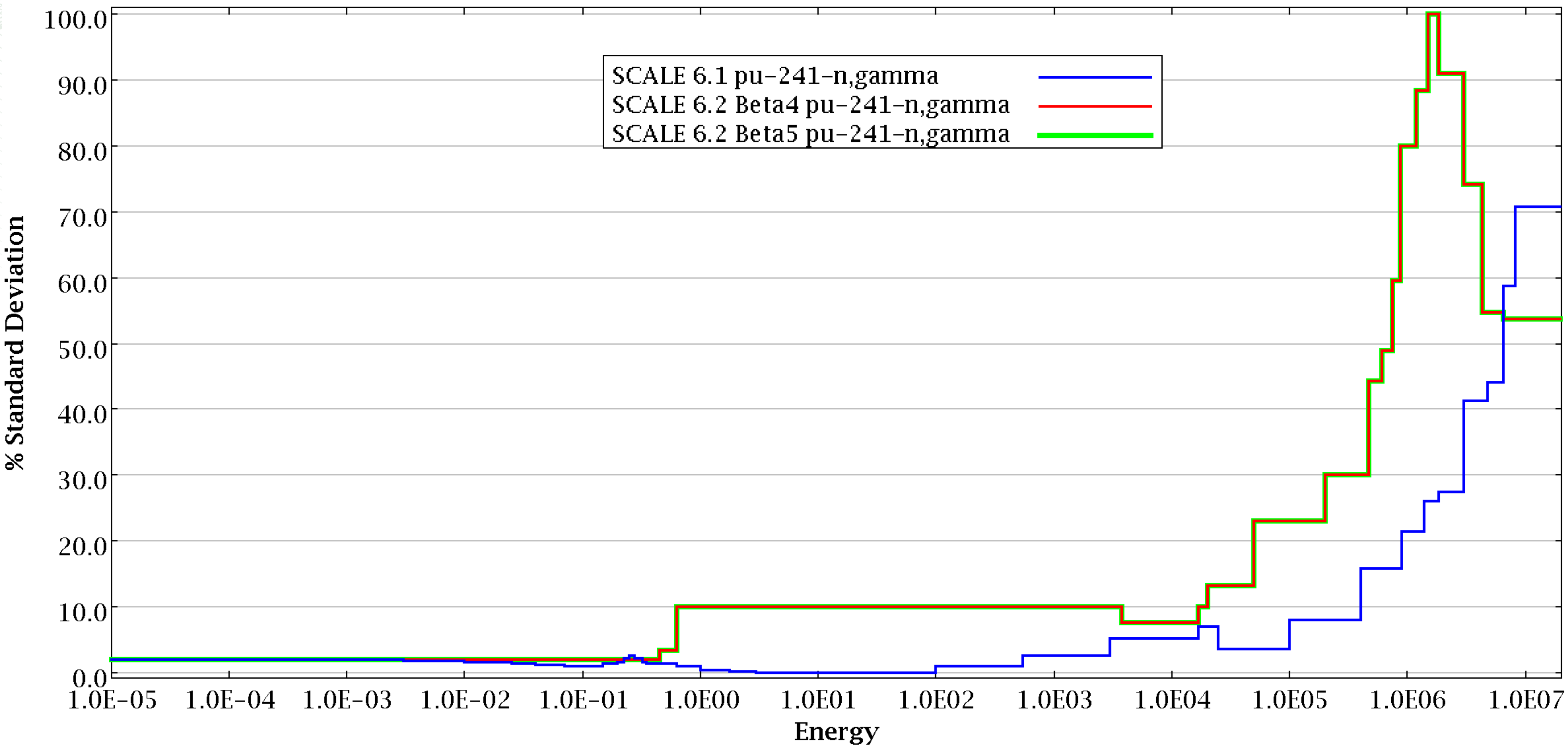
Top Contributors to Uncertainty for GBC-32



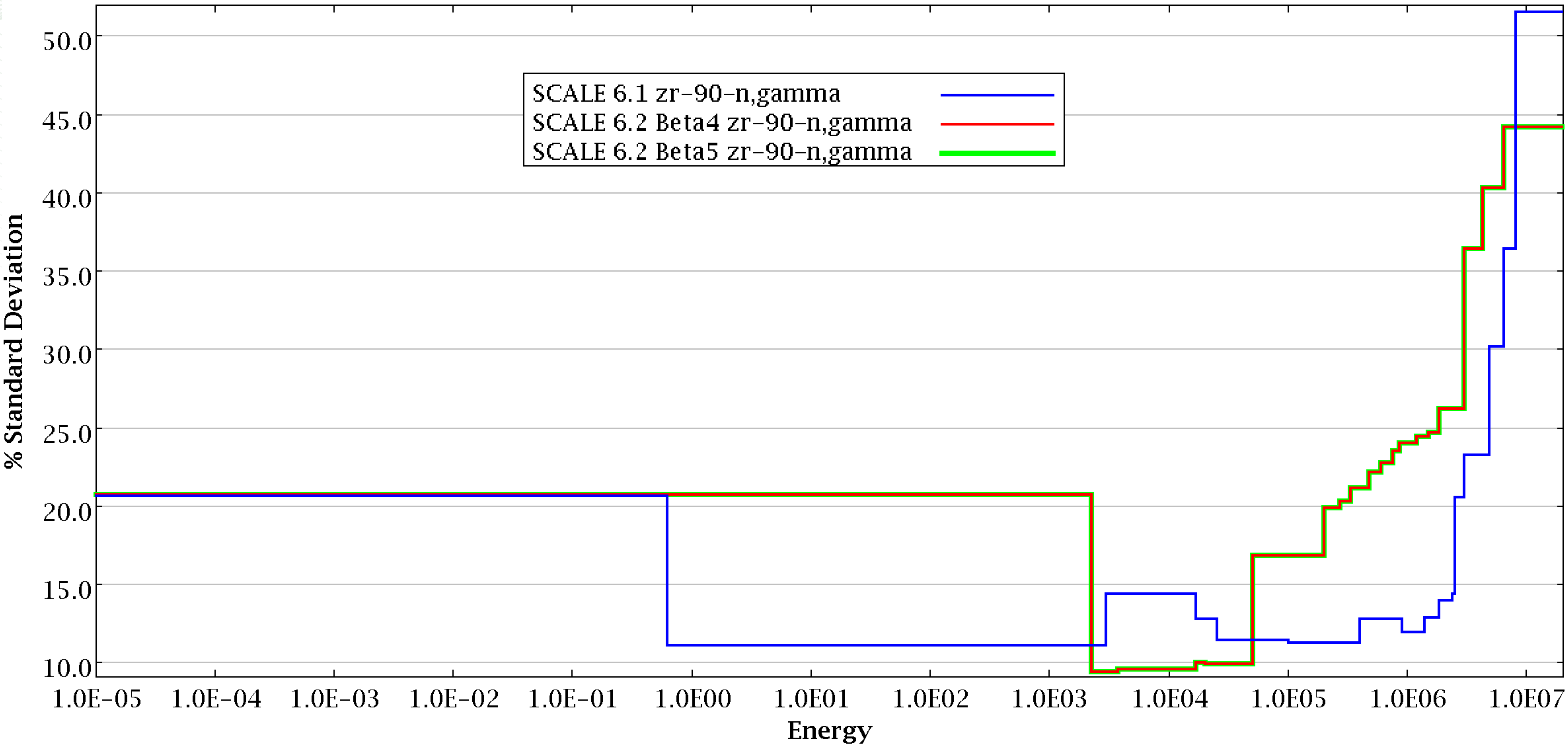
Top Contributors to Uncertainty for GBC-32



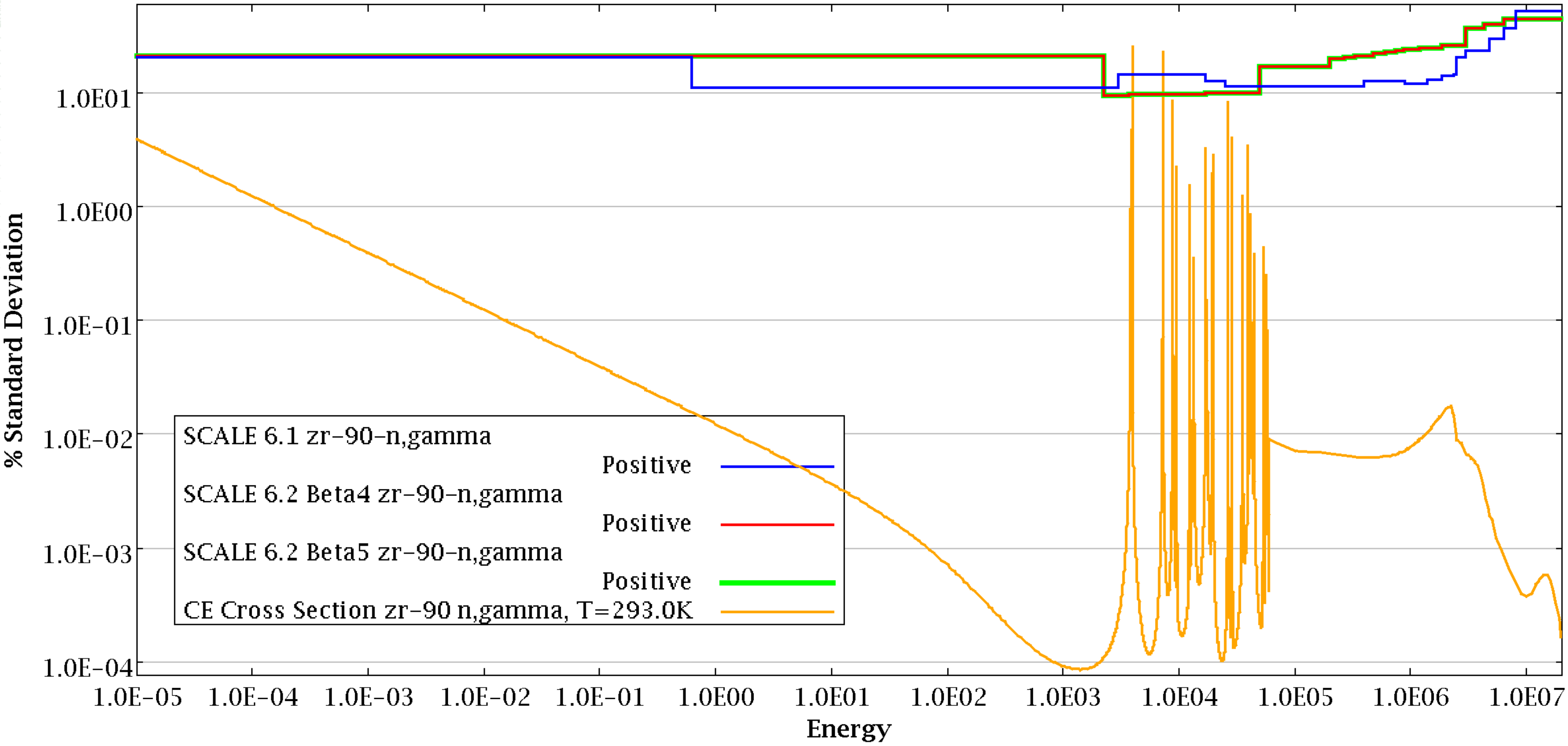
Pu-241 n,gamma uncertainty



Zr-90 n,gamma uncertainty

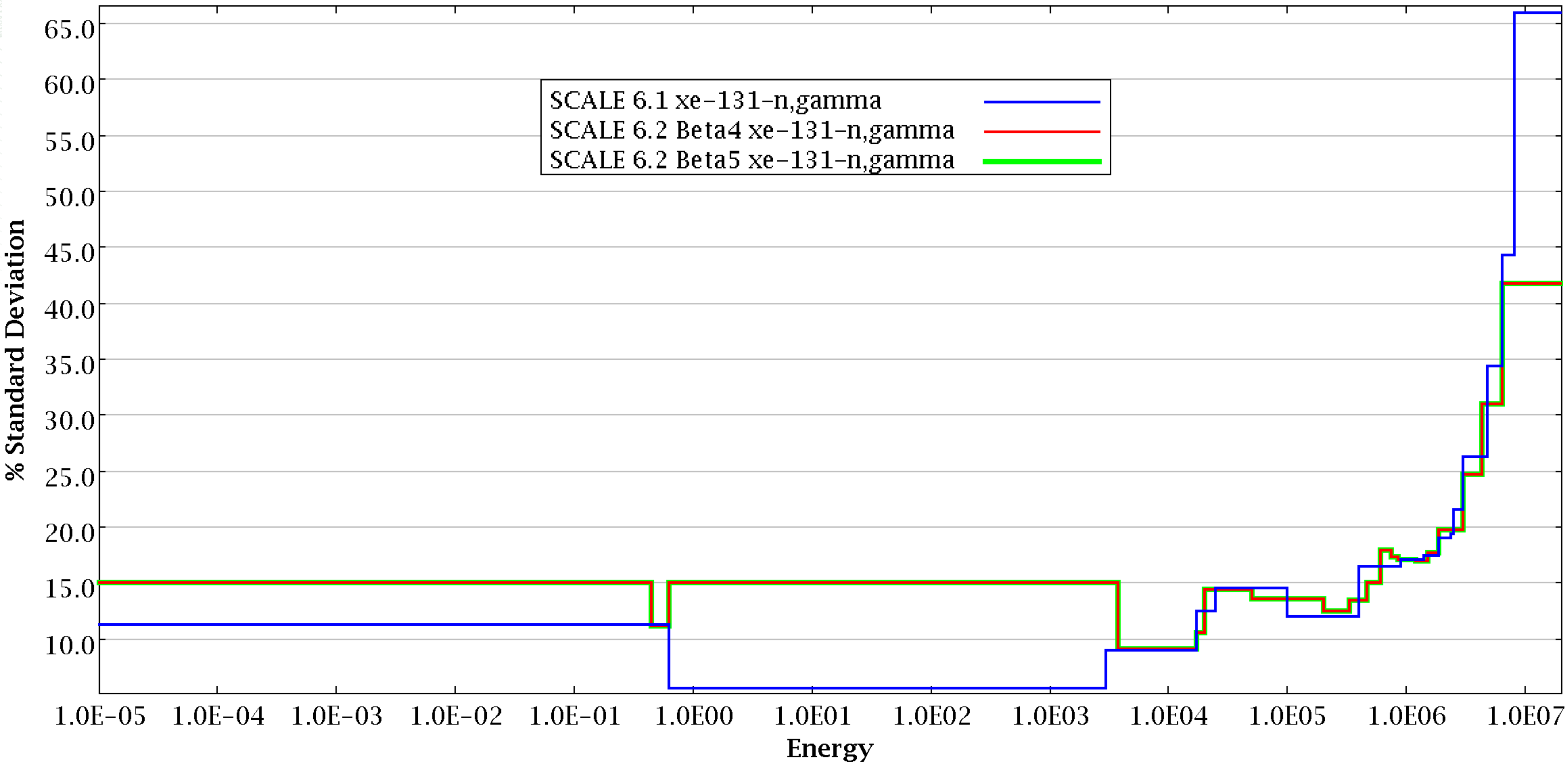


Zr-90

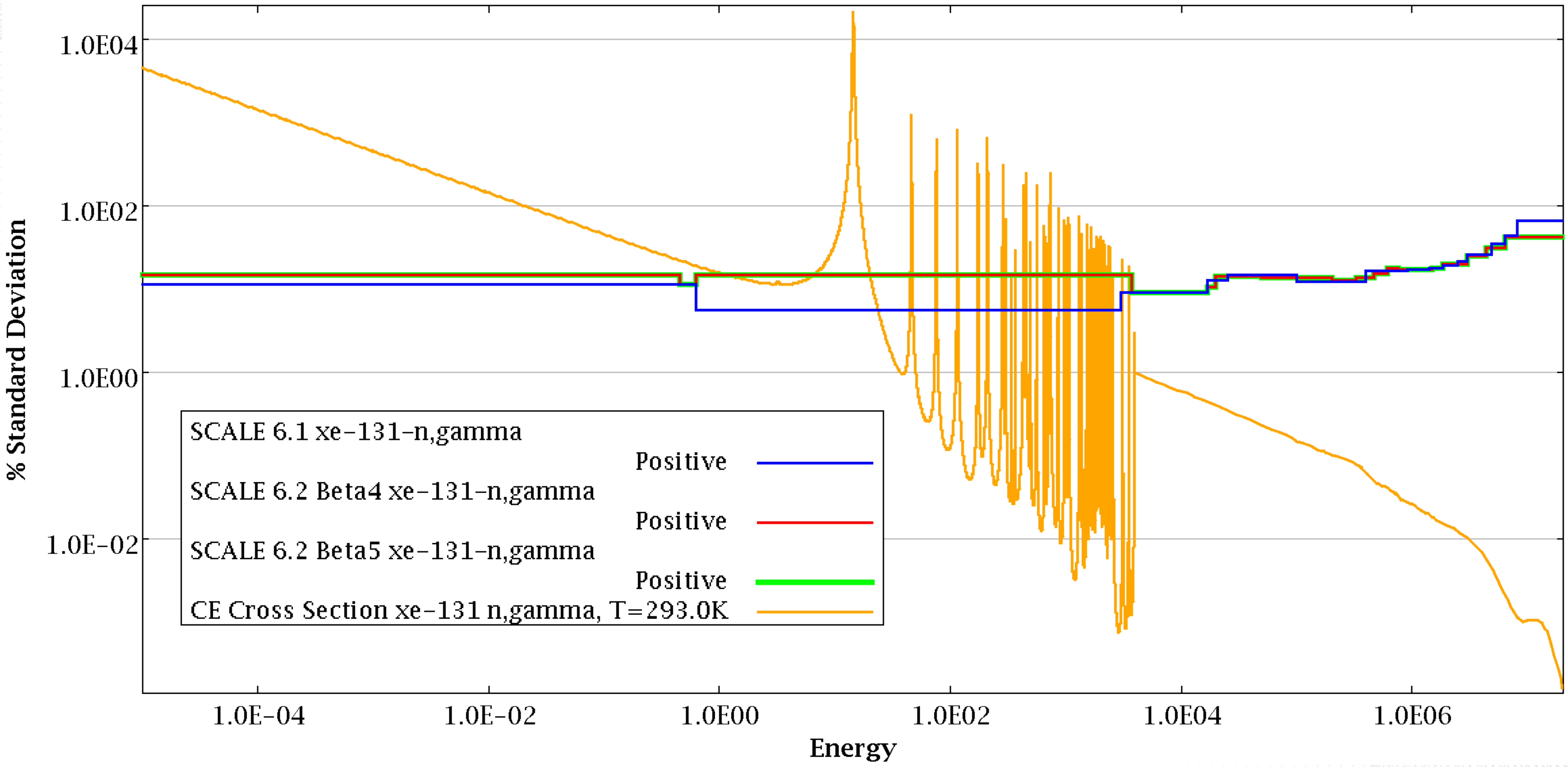


% Standard Deviation
1.0E01
1.0E00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-04
1.0E-03
1.0E-02
1.0E-01
1.0E00
1.0E01
1.0E02
1.0E03
1.0E04
1.0E05
1.0E06
1.0E07
Energy
SCALE 6.1 zr-90-n,gamma
Positive
SCALE 6.2 Beta4 zr-90-n,gamma
Positive
SCALE 6.2 Beta5 zr-90-n,gamma
Positive
CE Cross Section zr-90 n,gamma, T=293.0K

Xe-131 n,gamma uncertainty

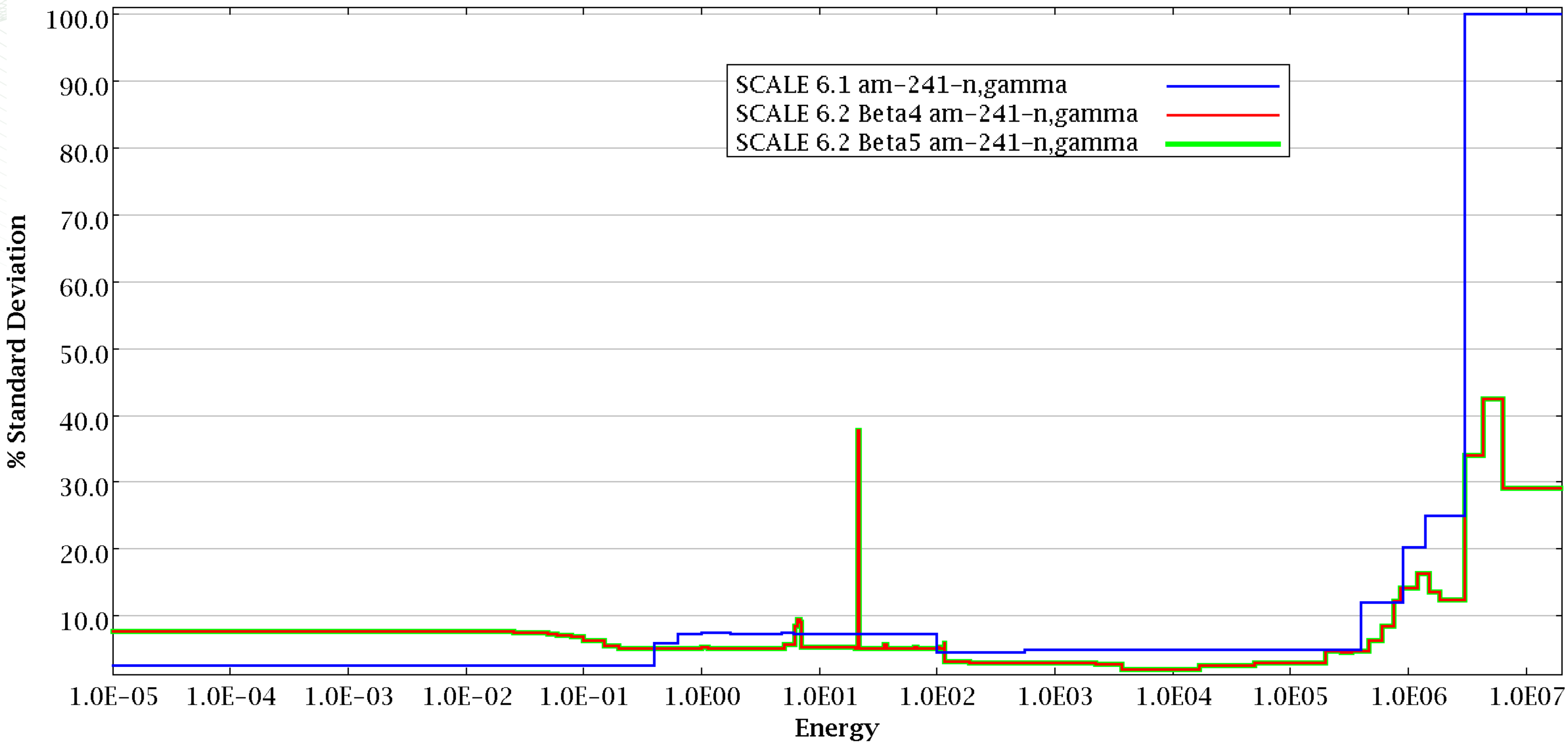


Xe-131

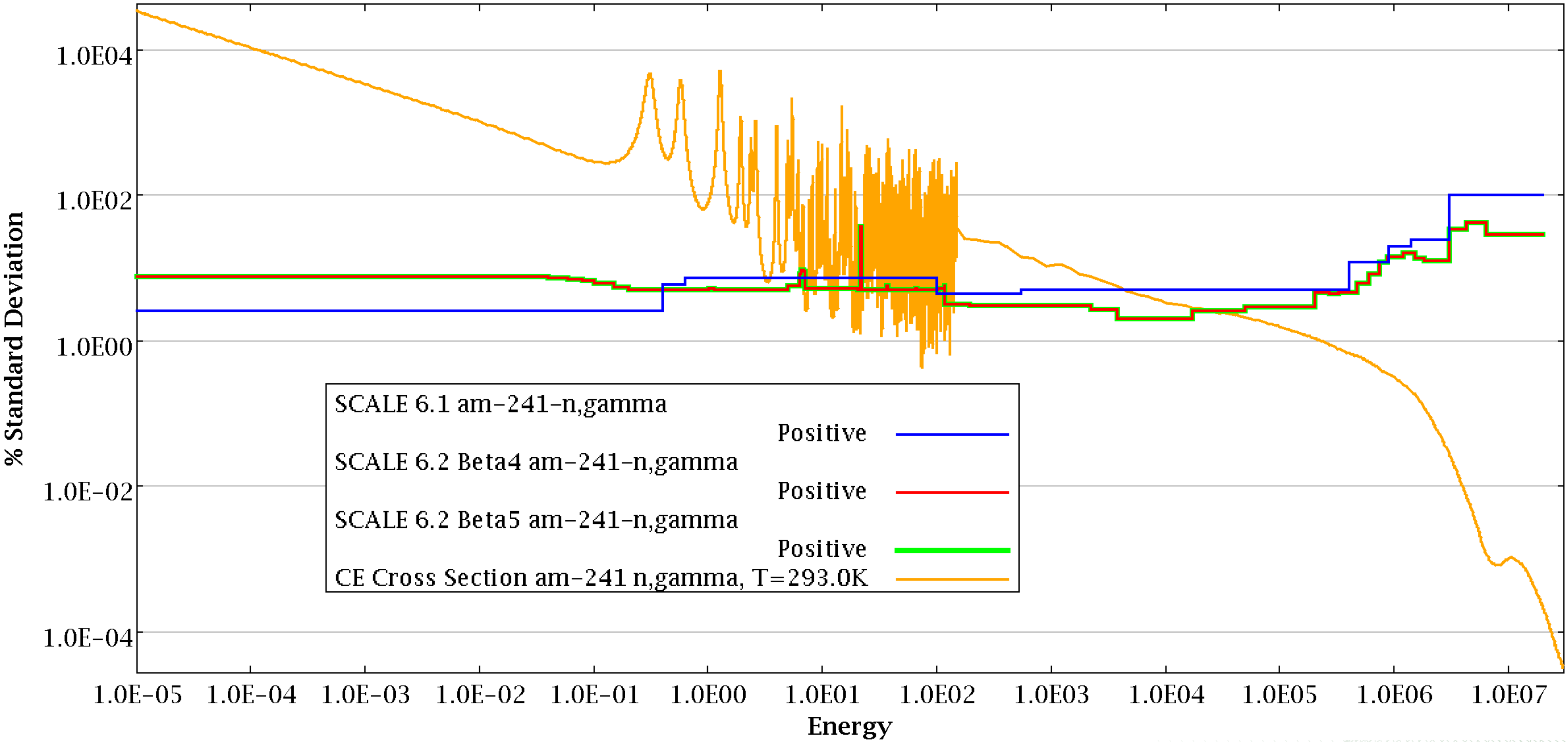


1.0E04
1.0E02
1.0E00
1.0E-02
% Standard Deviation
1.0E-04
1.0E-02
1.0E00
1.0E02
1.0E04
1.0E06
Energy
SCALE 6.1 xe-131-n,gamma
Positive
SCALE 6.2 Beta4 xe-131-n,gamma
Positive
SCALE 6.2 Beta5 xe-131-n,gamma
Positive
CE Cross Section xe-131 n,gamma, T=293.0K

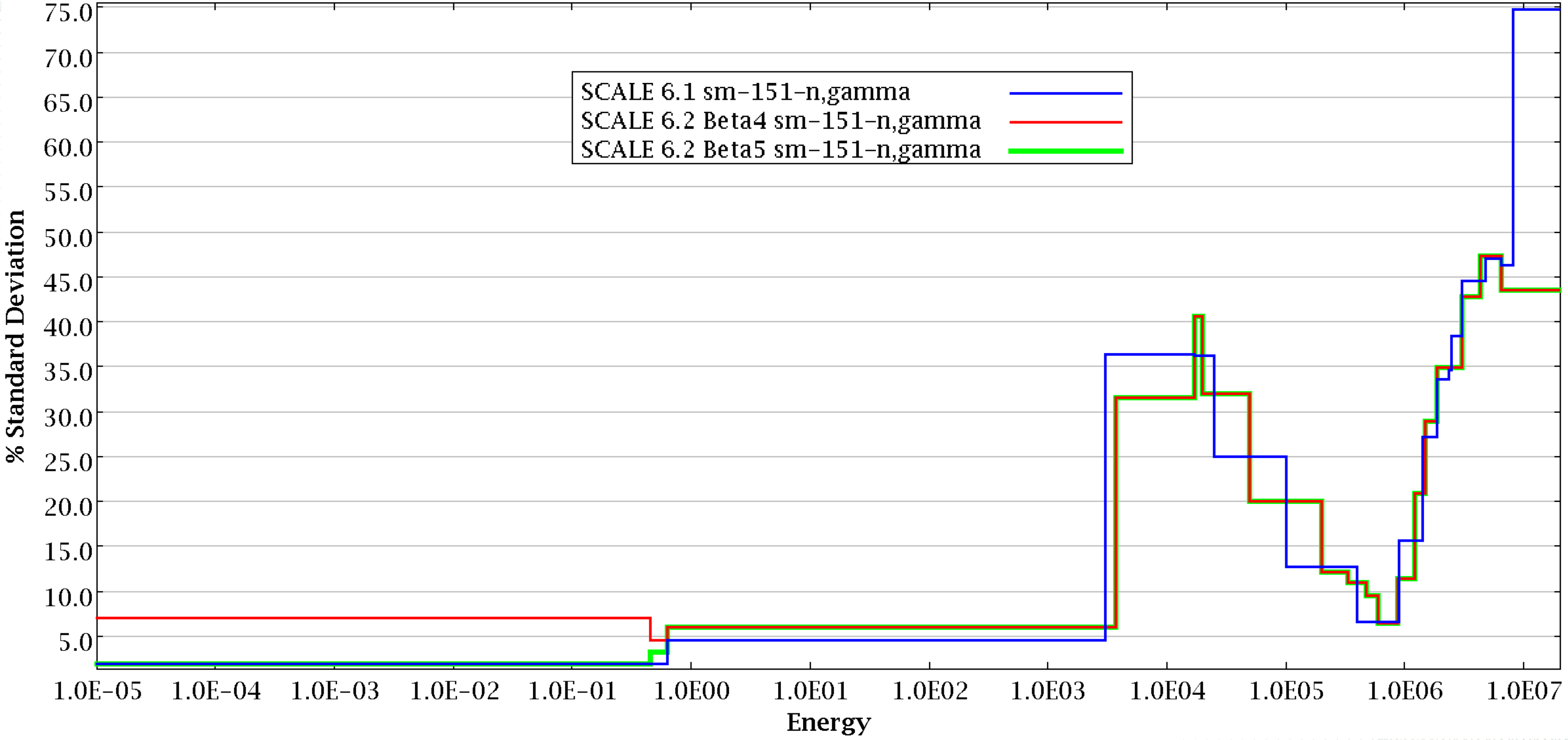
Am-241 n,gamma uncertainty



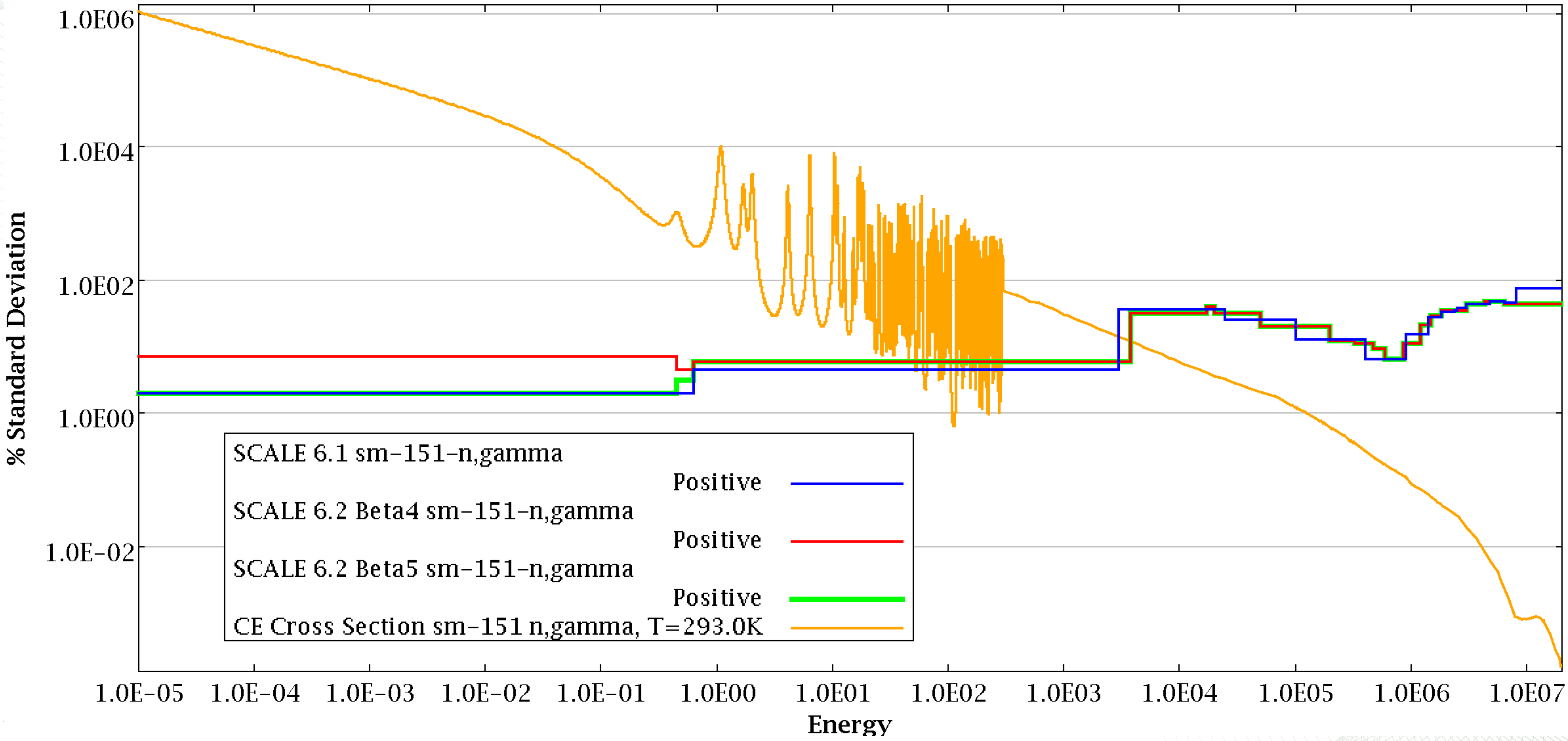
Am-241


1.0E04
1.0E02
1.0E00
1.0E-02
1.0E-04
% Standard Deviation
1.0E-05
1.0E-04
1.0E-03
1.0E-02
1.0E-01
1.0E00
1.0E01
1.0E02
1.0E03
1.0E04
1.0E05
1.0E06
1.0E07
Energy
SCALE 6.1 am-241-n,gamma
Positive
SCALE 6.2 Beta4 am-241-n,gamma
Positive
SCALE 6.2 Beta5 am-241-n,gamma
Positive
CE Cross Section am-241 n,gamma, T=293.0K

Sm-151 n,gamma uncertainty

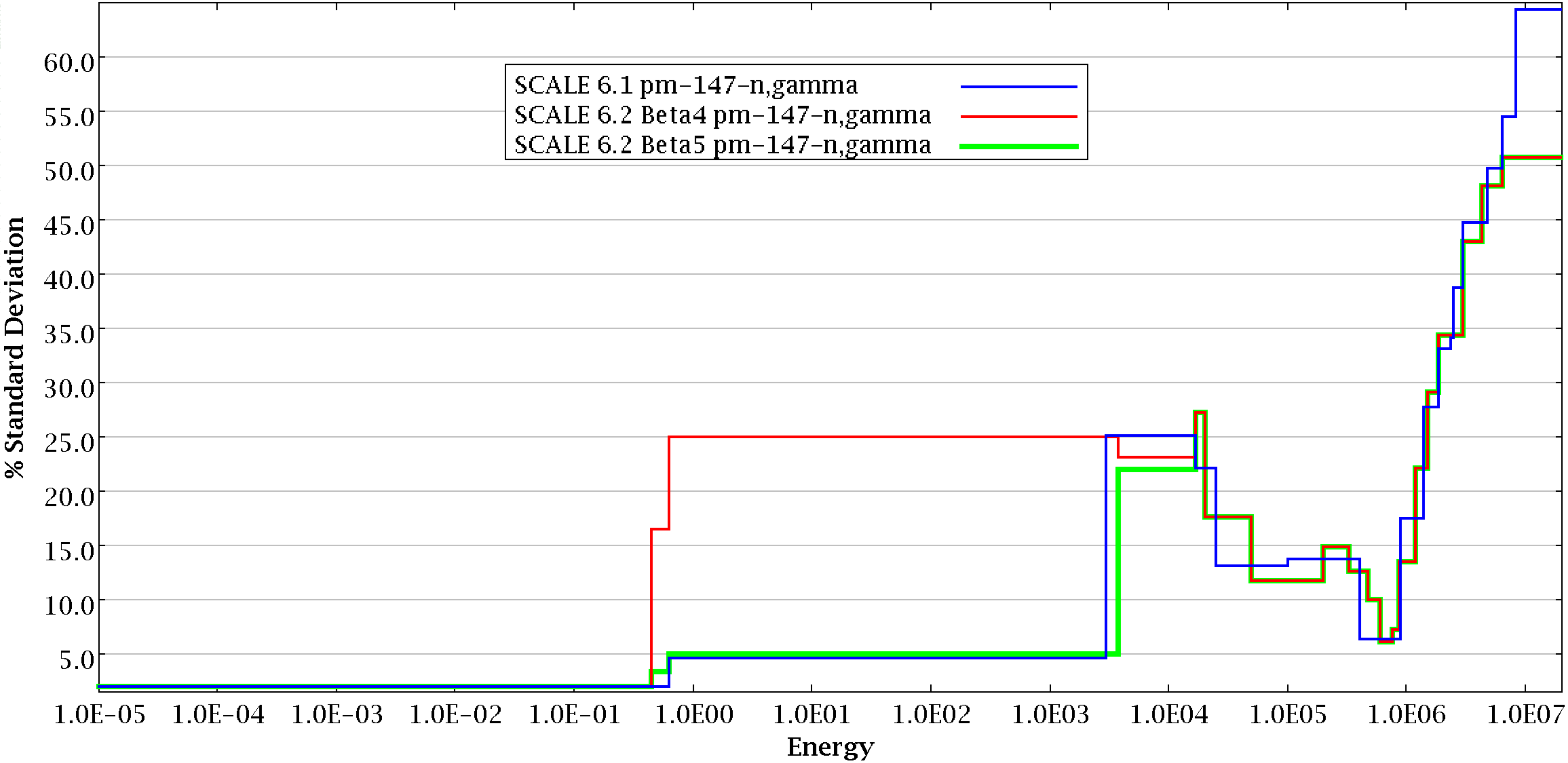


Sm-151

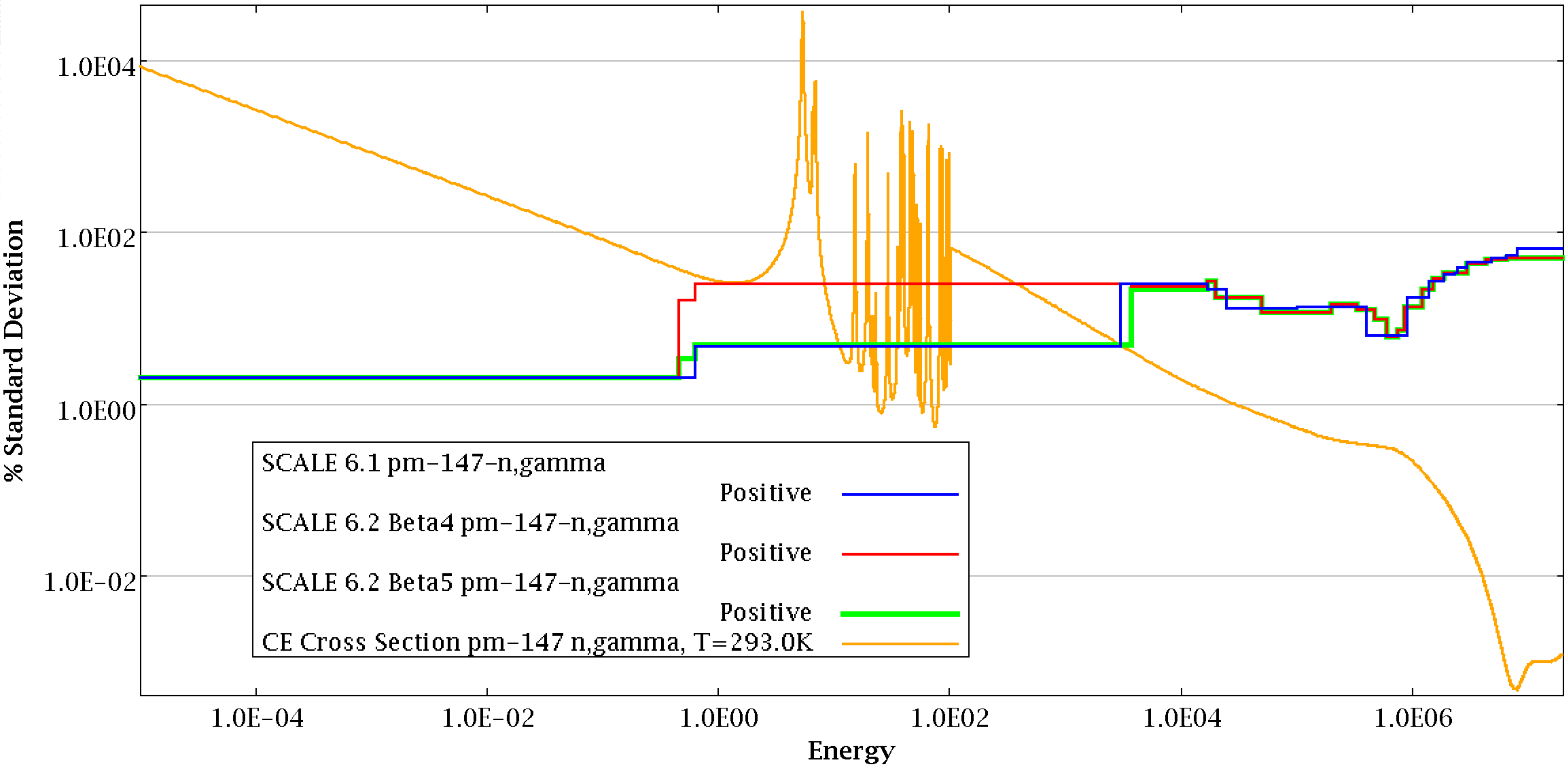


1.0E06
1.0E04
1.0E02
1.0E00
1.0E-02
% Standard Deviation
1.0E-05
1.0E-04
1.0E-03
1.0E-02
1.0E-01
1.0E00
1.0E01
1.0E02
1.0E03
1.0E04
1.0E05
1.0E06
1.0E07
Energy
SCALE 6.1 sm-151-n,gamma
Positive
SCALE 6.2 Beta4 sm-151-n,gamma
Positive
SCALE 6.2 Beta5 sm-151-n,gamma
Positive
CE Cross Section sm-151 n,gamma, T=293.0K

Pm-147 n,gamma uncertainty



Pm-147



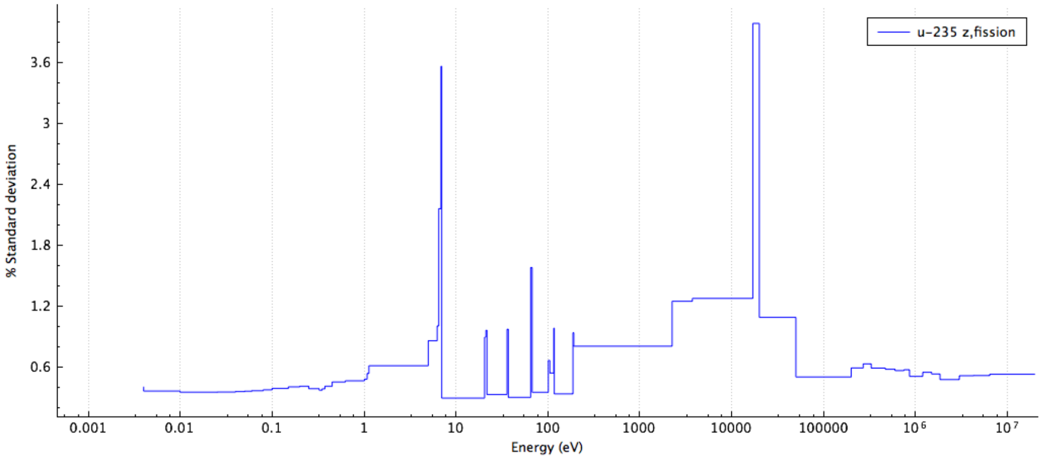
% Standard Deviation
1.0E04
1.0E02
1.0E00
1.0E-02
1.0E-04
1.0E-02
1.0E00
1.0E02
1.0E04
1.0E06
Energy
SCALE 6.1 pm-147-n,gamma
Positive
SCALE 6.2 Beta4 pm-147-n,gamma
Positive
SCALE 6.2 Beta5 pm-147-n,gamma
Positive
CE Cross Section pm-147 n,gamma, T=293.0K

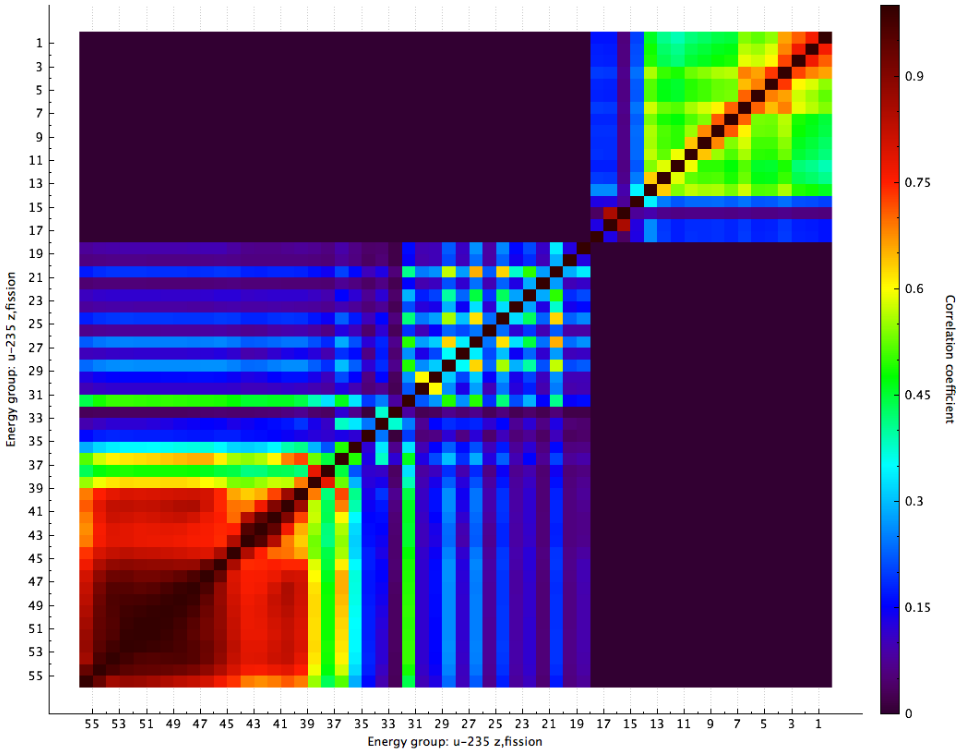
Uncertainties for Spent Fuel Systems (Same cases & models as NUREG/CR-7109 Table 6.10)

	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

SCALE 6.2 Covariance Library

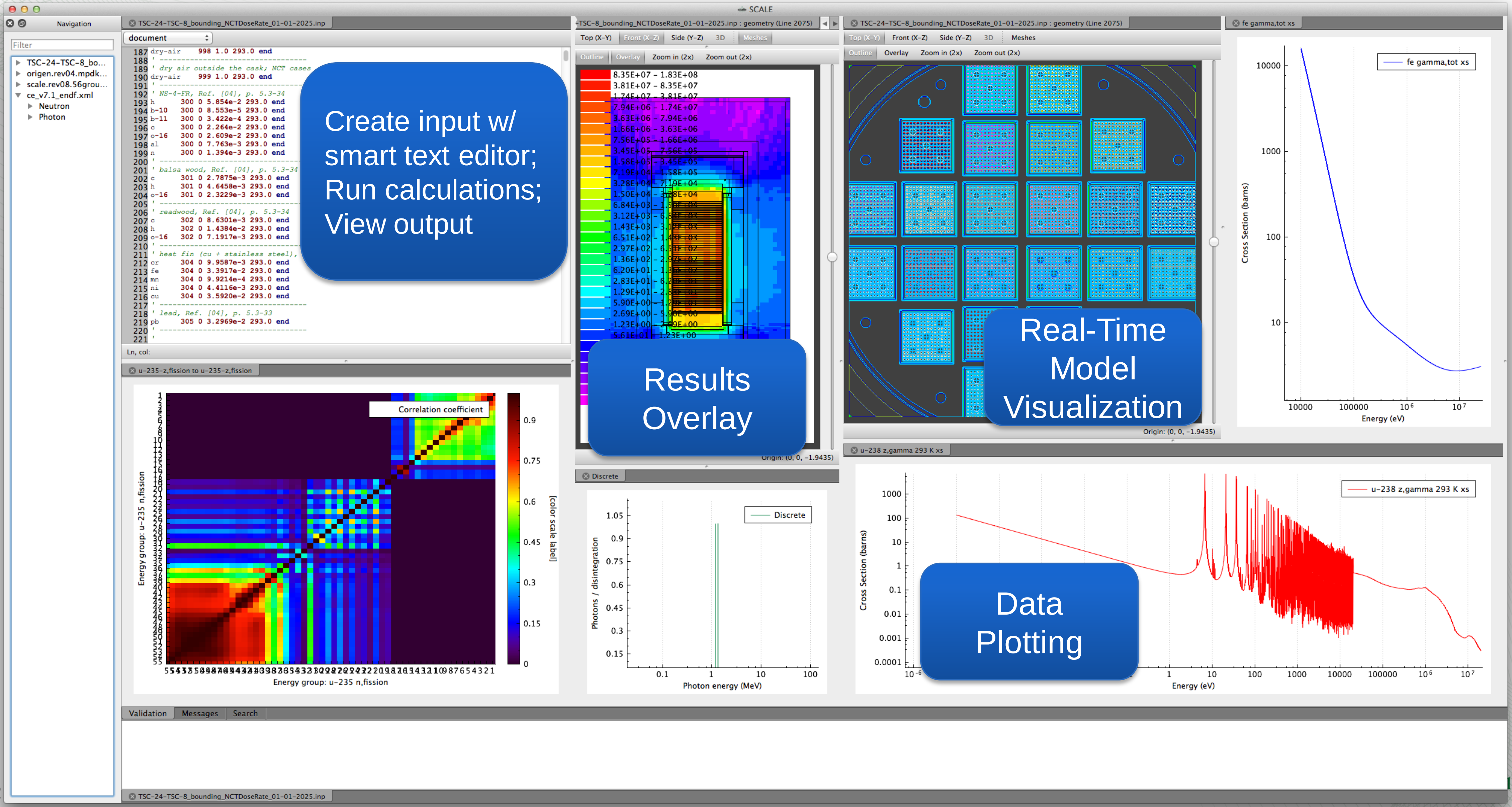
- ENDF/B-VII.1 for 187 isotopes
- SCALE 6.1 data retained for ~215 missing nuclides
- Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF/A repository
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 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





OAK RIDGE National Laboratory

Fulcrum – Integrated User Interface



Path Forward for SCALE

- SCALE 6.2 is done!!
- Continue to enhance test suite, with focus on nuclear data testing, integrated unit testing, and generation of V&V reports
- Review modernization plan and QA plan
- Continue to improve innovation, accuracy, efficiency, and ease-of-use
- Integrate all components into modern parallel framework with shared data resources
- Complete Shift to consolidate Monte Carlo capabilities
- Continue to enhance the Fulcrum user interface