Evaluation of ENDF/B-VIII Covariance Data

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Overview

- Three general categories of testing performed
  - Two focus on uncertainty in k_{eff} due to cross section covariance data
  - Other examines c_k (similarity) of a reference set of experiments with reference applications
- Each test will be presented
  - Purpose: What is this test assessing and why is the test important?
  - Methodology: How is it done and what are the metrics?
  - Results: How do the results look for the ENDF/B-VIII covariance data?
    - Covariance library generated by Doro Wiarda based on data in repository on April 17

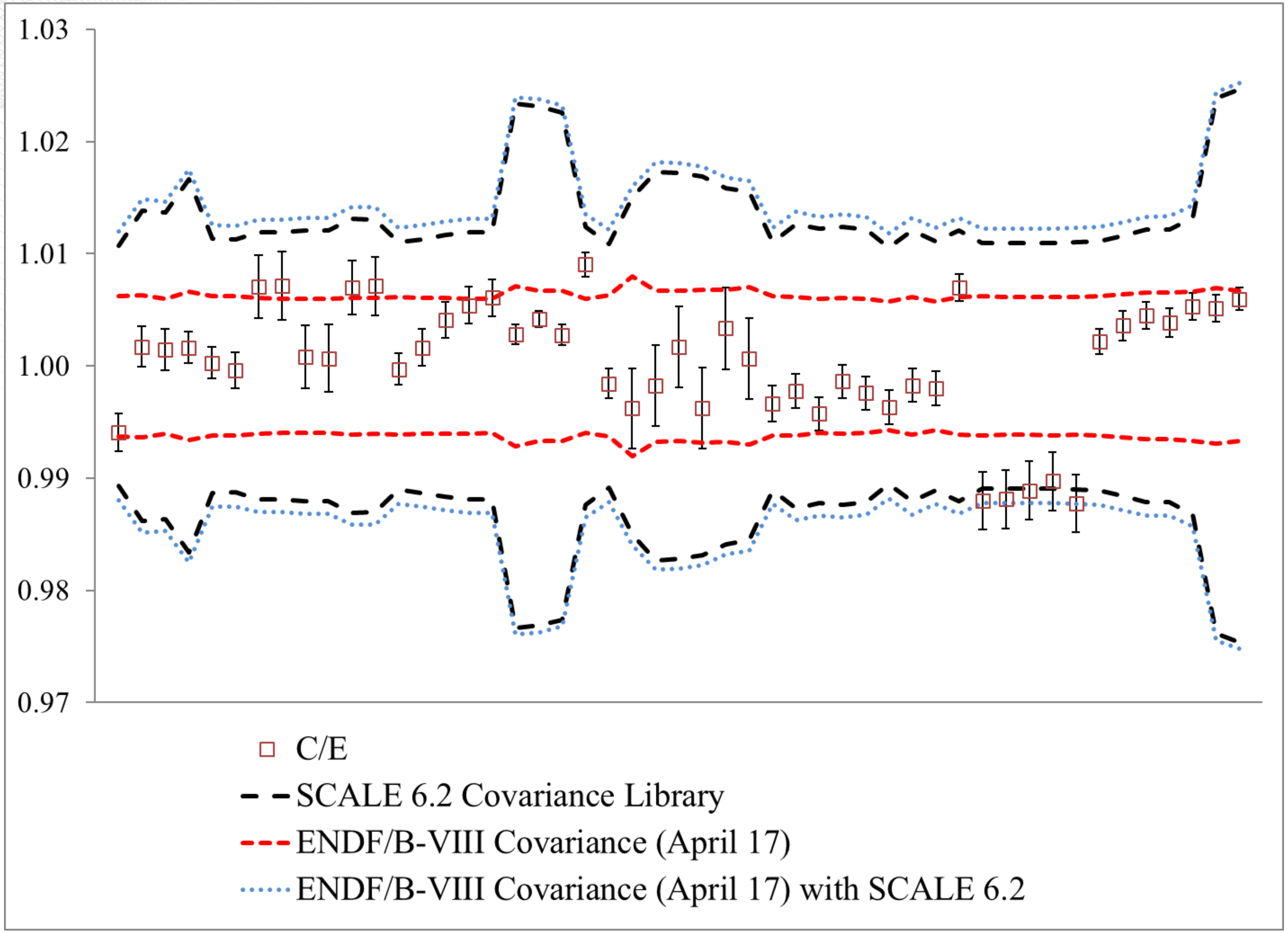
Caveats

- Technical
  - Sensitivity data used in testing was generated in SCALE 6.1 using ENDF/B-VII.0 cross sections
    - Covariance library contains relative uncertainties, so should be applicable regardless
    - 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!
    - Plan to regenerate sensitivity data with SCALE 6.2.2 & ENDF/B-VII.1 this year
- Less technical
  - I am not a nuclear data expert; I'm a criticality safety applications guy
  - As will become clear, I believe the covariances are too large
  - Do not take anything I say as a personal attack on your work

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: 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

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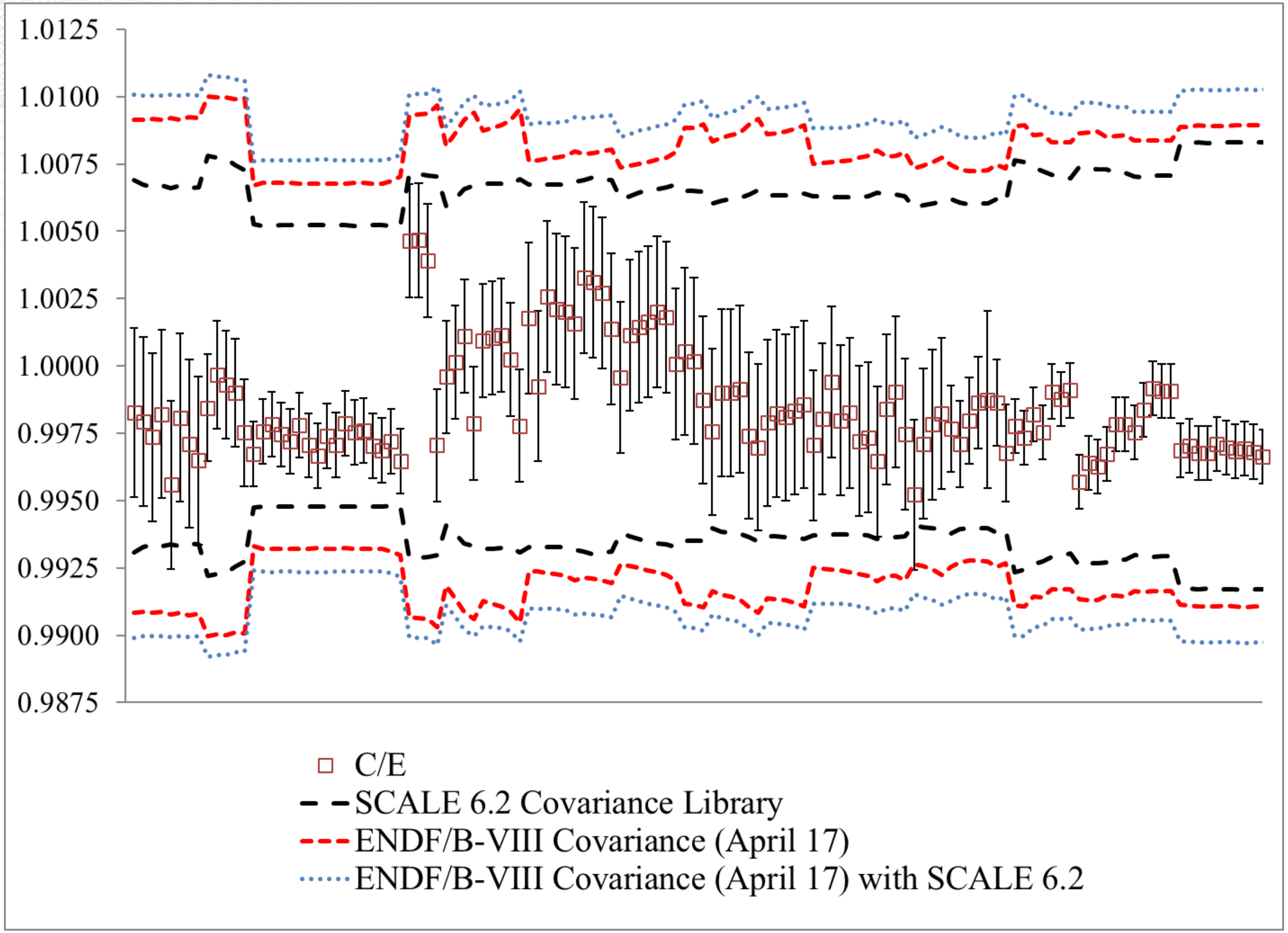
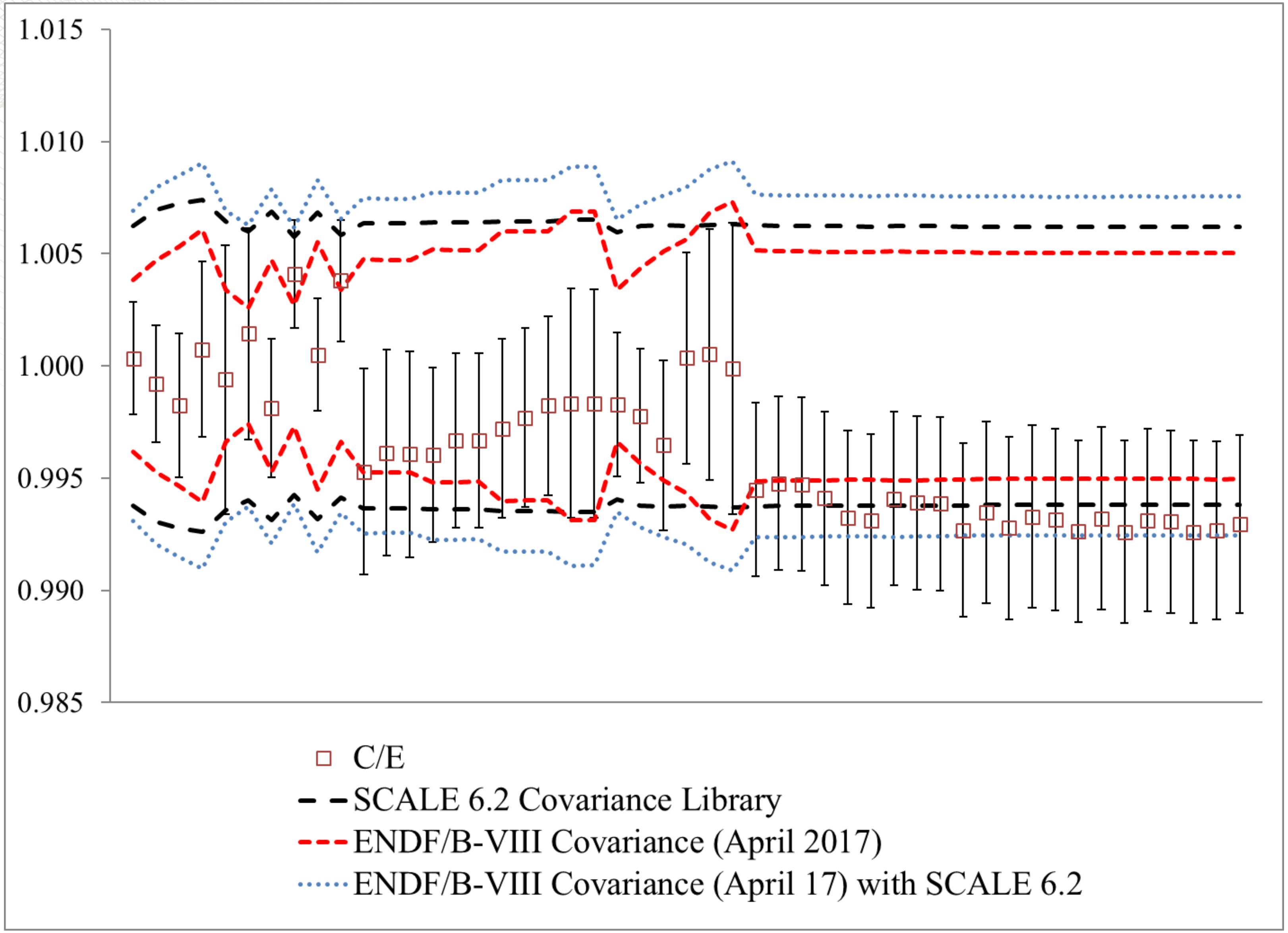
Results: LEU-COMP-THERM



- 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 ^{1}H capture and scatter
  - Reintroduction of errors identified in ENDF/B-VII.1 data during preparation and testing of SCALE 6.2 covariance library

Results: MIX-COMP-THERM



- 49 critical configurations
- New zigzag in the middle of the data is caused by ^{1}H capture
- Generally fewer points outside 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 ^{1}H problem?

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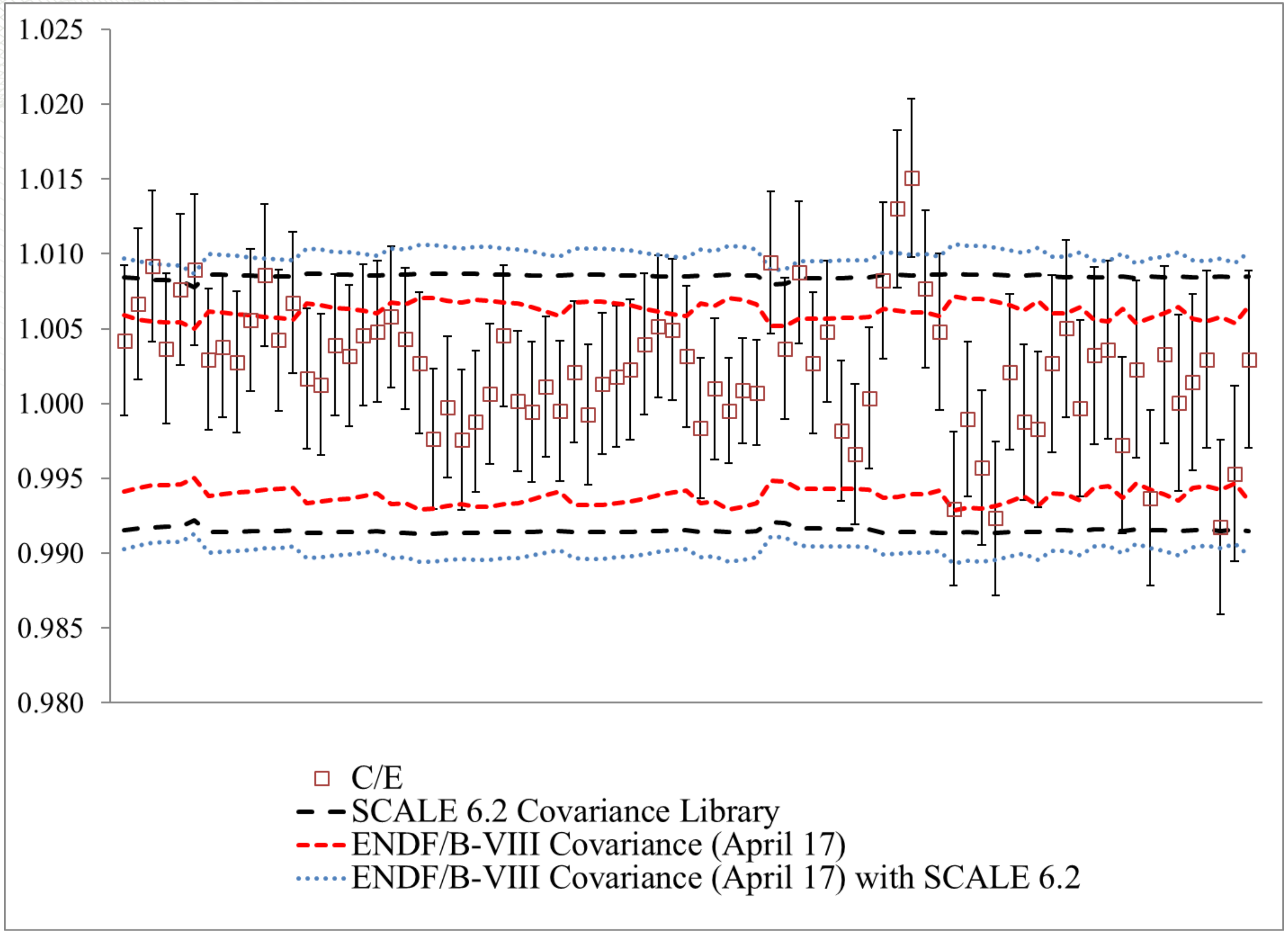
Results: PU-SOL-THERM



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

Results: Summary Table

Category	Number of Cases	Avg C/E (CE_V7.1)	Avg Exp. Unc.	St. Dev. Of C/Es	Avg 1σ 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 observed variability.

Questions before we move on?

Cross section uncertainty for SNF

- Purpose:
  - Determine k_{eff} uncertainty for each isotope in an SNF storage/transportation configuration, then also combine into specific groups
  - Major/minor/other actinides, major/other fission products, else/structural
  - Supported NRC Interim Staff Guidance 8, Revision 3 (ISG-8R3): PWR BUC
- Methodology:
  - TSUNAMI-IP will calculate k_{eff} uncertainty resulting from covariance data for each element in the covariance matrix (isotope/reaction pair and cross terms)
    - "uncert_long" keyword in parameters block
  - AWK script combines uncertainty components for each isotope
  - Spreadsheet used to collect information by category

Results

Category	PWR Spent Fuel Pool Model				PWR Spent Fuel Cask Model				BWR SFP Model	
	10 GWd/MTU		40 GWd/MTU		10 GWd/MTU		40 GWd/MTU		11 GWd/MTU	
	6.2	E8+	6.2	E8+	6.2	E8+	6.2	E8+	6.2	E8+
Maj. Act.	0.00437	0.00586	0.00378	0.00493	0.00414	0.00549	0.00368	0.00474	0.00427	0.00588
Min. Act	0.00007	0.00007	0.00022	0.00022	0.00007	0.00007	0.00022	0.00022	0.00011	0.00011
Maj. FP	0.00022	0.00059	0.00054	0.00091	0.00024	0.00063	0.00055	0.00091	0.00024	0.00045
Other Act	0.00006	0.00006	0.00006	0.00006	0.00000	0.00000	0.00001	0.00001	0.00000	0.00000
Other FP	0.00021	0.00031	0.00063	0.00084	0.00015	0.00017	0.00047	0.00050	0.00025	0.00045
Else	0.00123	0.00254	0.00102	0.00203	0.00144	0.00267	0.00127	0.00224	0.00099	0.00161
ALL	0.00455	0.00643	0.00401	0.00548	0.00440	0.00614	0.00396	0.00535	0.00440	0.00613
ALL % Diff (E8-6.2)/6.2		41.3		36.6		40.0		35.0		39.3

Results: Isotopes that caused differences

- Major actinides: ^{235}U and ^{240}Pu
- Major fission products: ^{149}Sm and ^{151}Sm; ^{103}Rh to a lesser extent
- Other actinides: ^{233}U (11,000% to 25,000% increase)
- Other fission products: ^{147}Pm (Almost a factor of 4)
- Else/structural: ^{1}H

Questions before we move on?

c_k (similarity) assessment

- Purpose:
  - Calculate c_k parameter for each experiment in a reference set compared to 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: $\mathbf{C_{kk}} = \mathbf{S_k C_{\alpha\alpha} S_k^T}$ 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.): $c_k = \frac{\sigma_{ij}^2}{(\sigma_i \sigma_j)}$ Where:

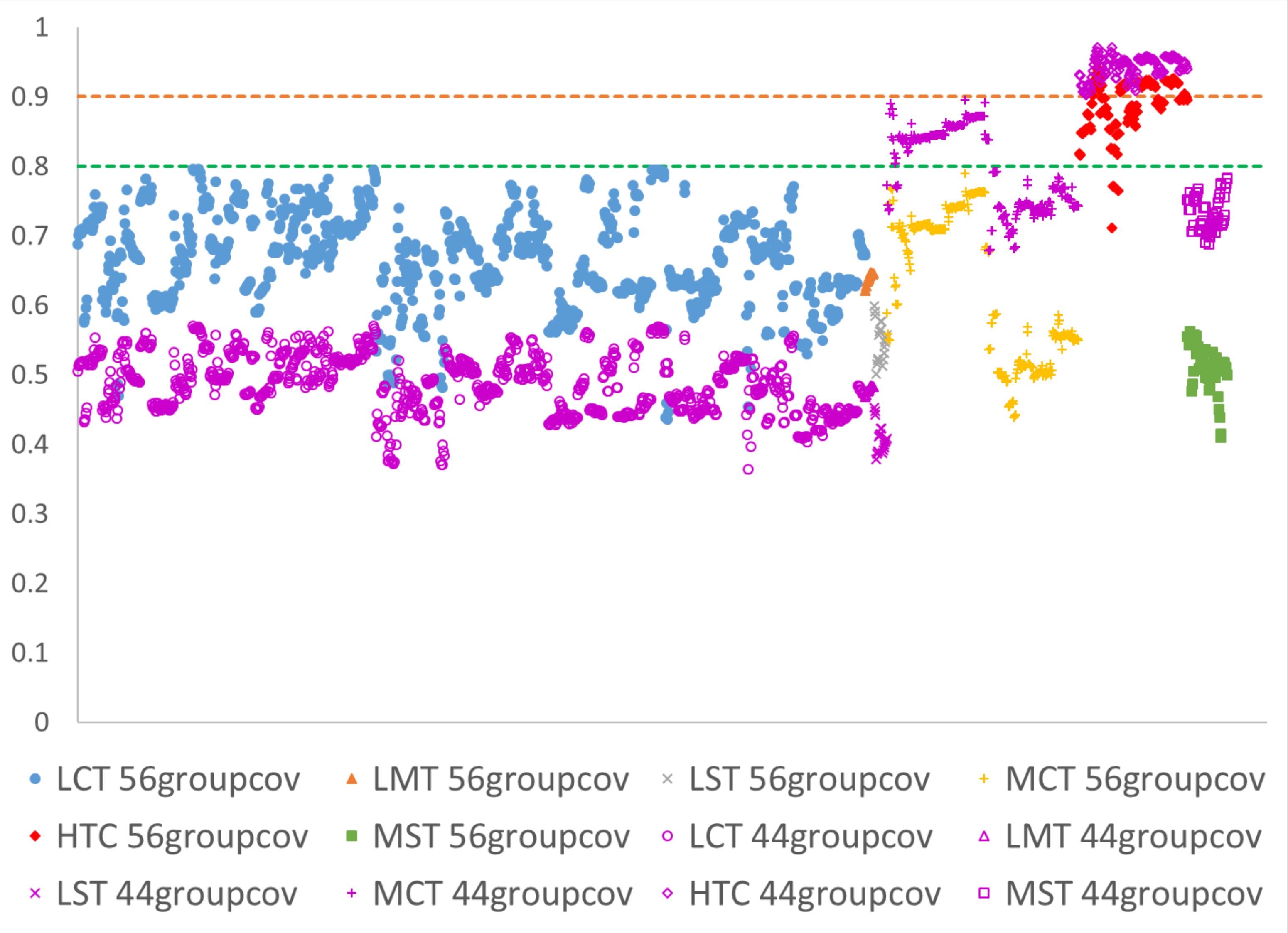
σ_{ij}^2 is off-diagonal term of $\mathbf{C_{kk}}$ matrix (aka covariance)

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

c_k (similarity) assessment (2)

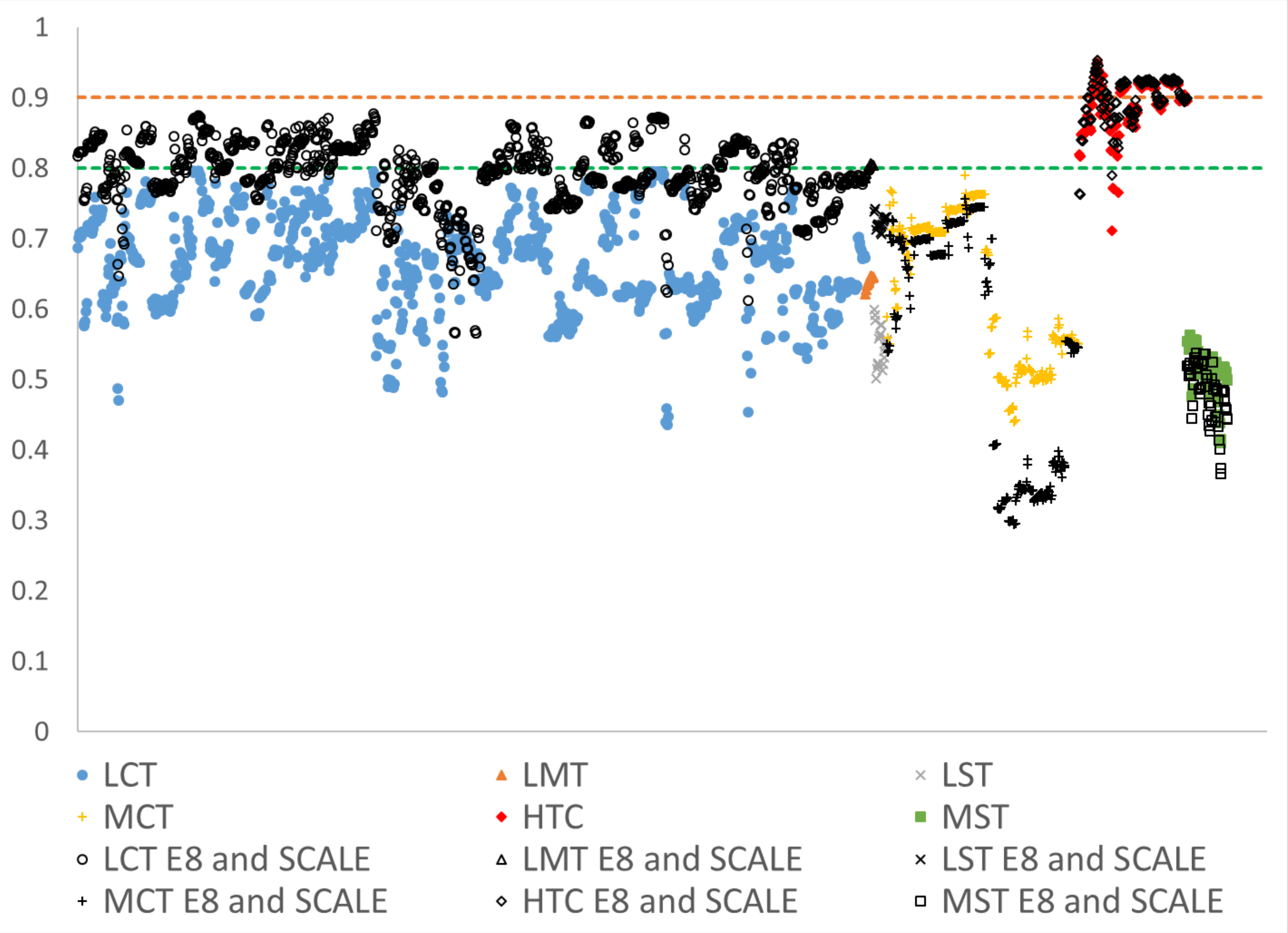
- Purpose (continued):
  - How is it useful in covariance testing?
    - c_k can indicate which covariance data are important in determining similarity
    - Results should be explicable result of composition of systems
    - Especially helpful for comparison of primary fissile species uncertainty data
- Methodology:
  - TSUNAMI-IP calculates c_k provided sensitivity data files (SDFs) 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
- 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)

Overall testing summary & conclusions

- ^{235}U nubar and ^{1}H covariance data has regressed to incorrect values included in ENDF/B-VII.1 and previously identified by ORNL
- There was no ^{239}Pu covariance data in ENDF/B-VIII when Doro pulled the data, so the SCALE 6.2 value was used
  - No indication of how ENDF/B-VIII ^{239}Pu covariance data perform
- Uncertainty bands have historically been too wide, and still tend to increase and not decrease with each new release
- Inappropriate uncertainty bands undermine usefulness of S/U methods for criticality safety validation, reactor physics uncertainty quantification, and depletion calculation uncertainty quantification

This concludes my prepared remarks. Are there any additional questions at this time?

marshallwj@ornl.gov if you have additional questions at a later date.

Thank you for your attention!

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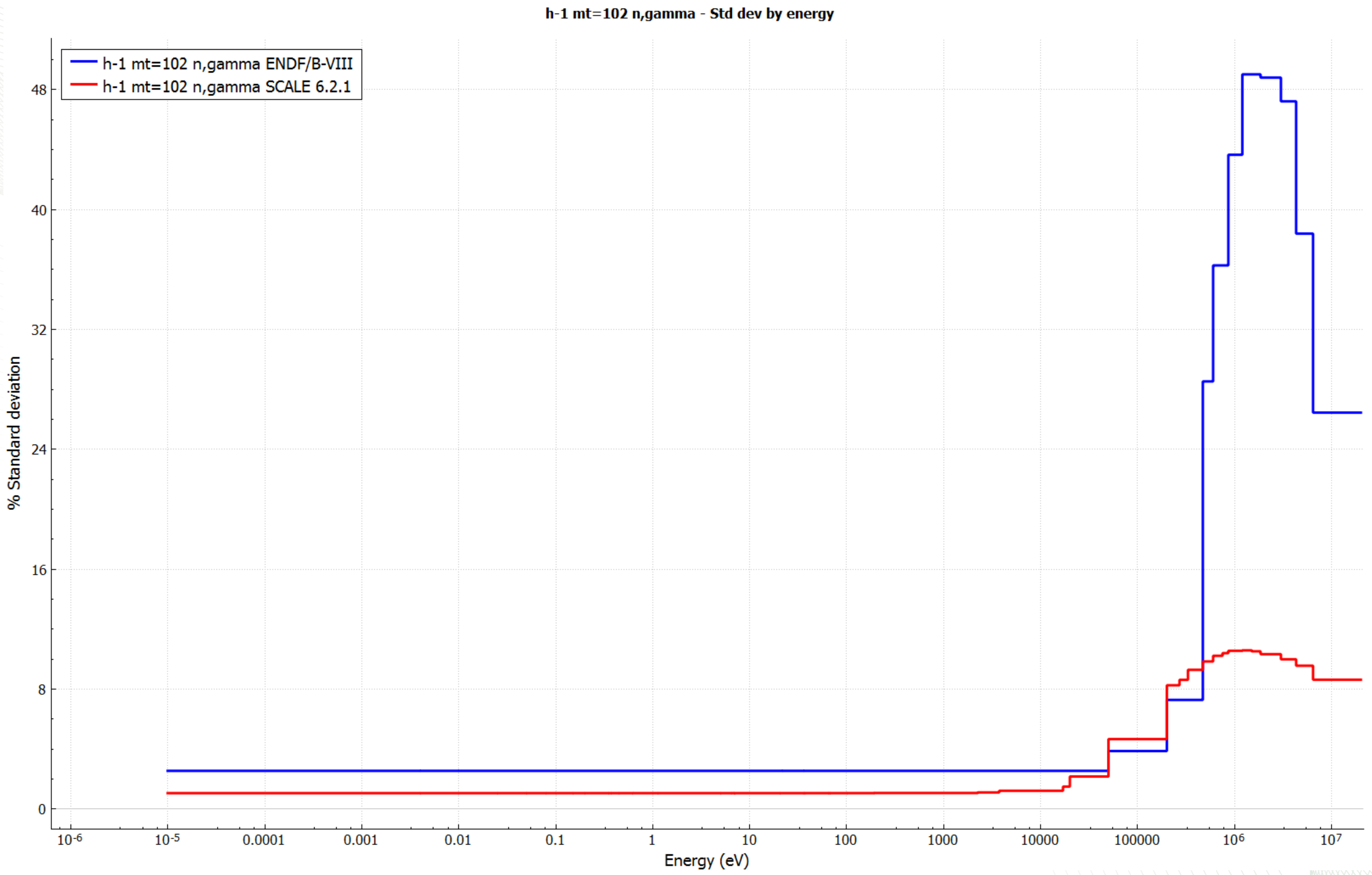
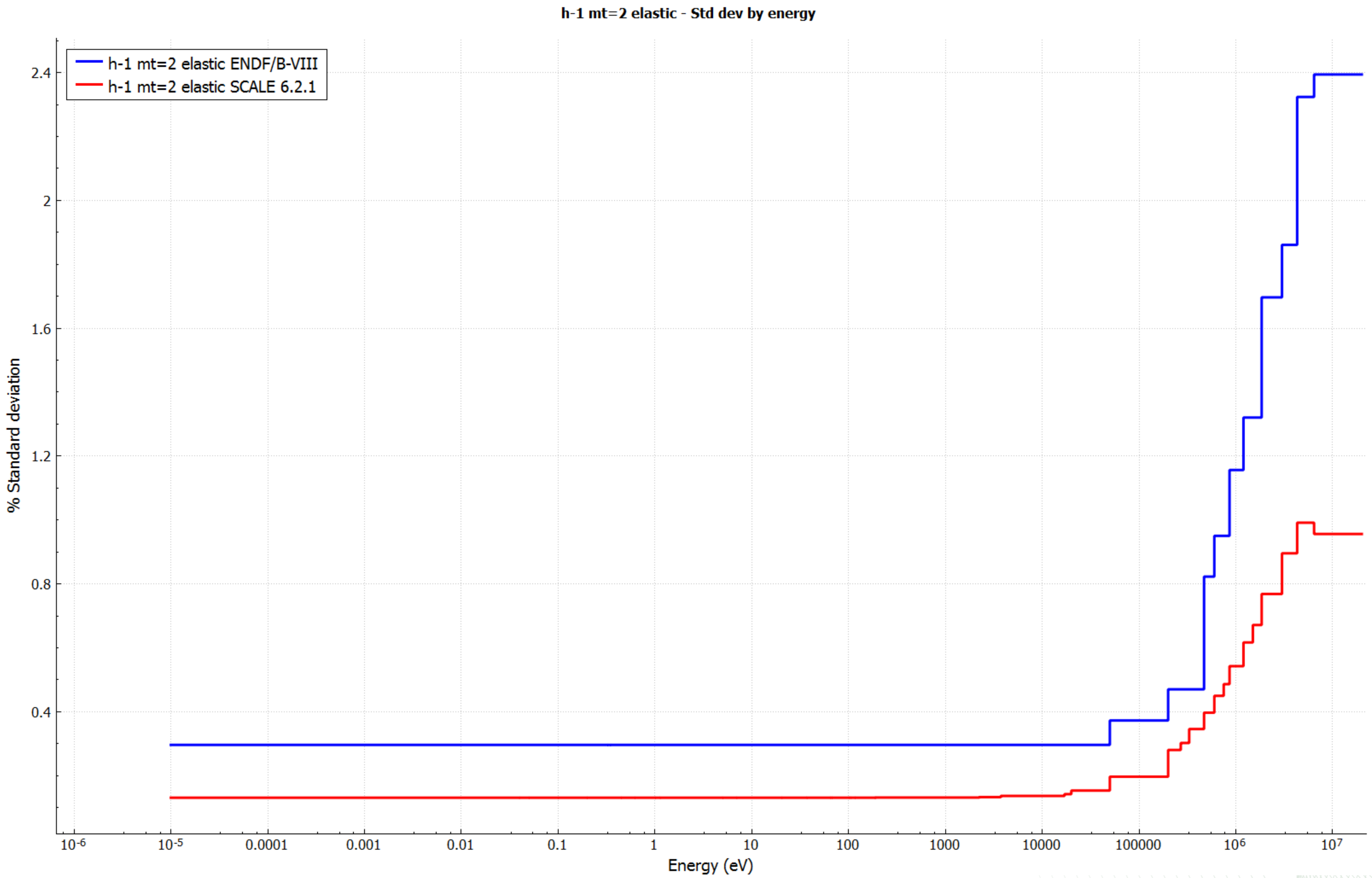
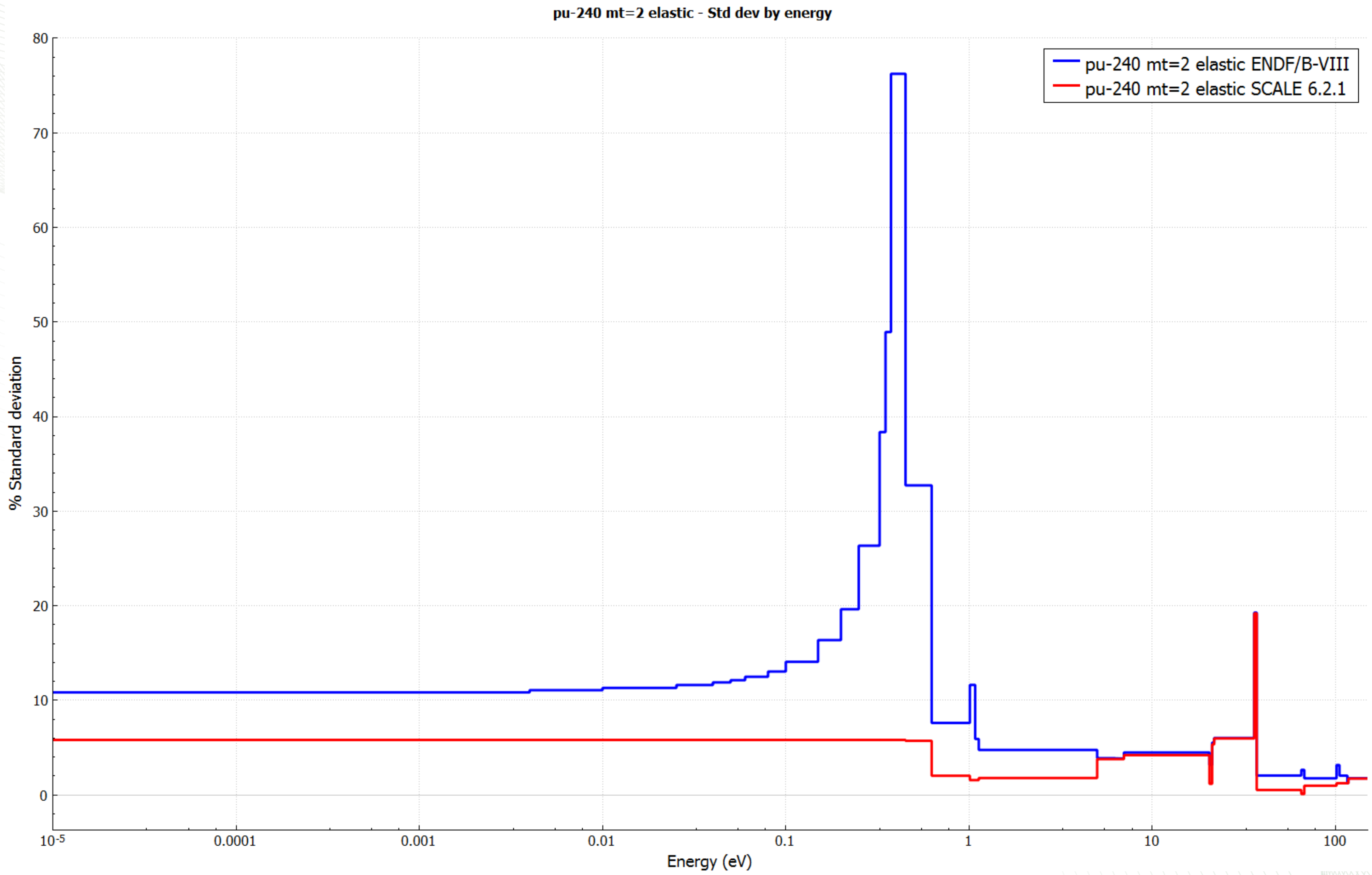
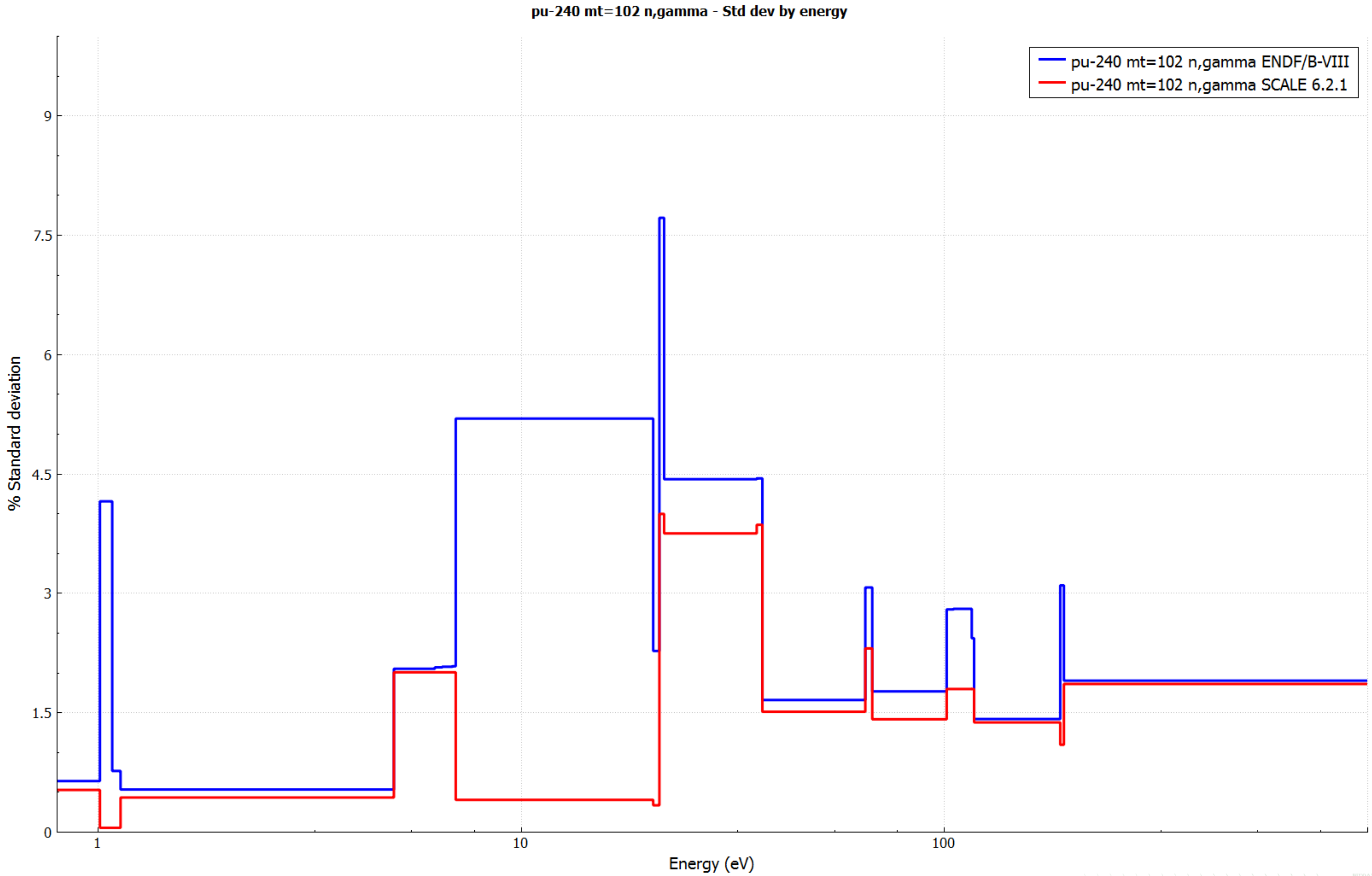

h-1 mt=102 n,gamma - Std dev by energy
h-1 mt=102 n,gamma ENDF/B-VIII
h-1 mt=102 n,gamma SCALE 6.2.1
% Standard deviation
48
40
32
24
16
8
0
10^{-6}
10^{-5}
0.0001
0.001
0.01
0.1
1
10
100
1000
10000
100000
10^{6}
10^{7}
Energy (eV)

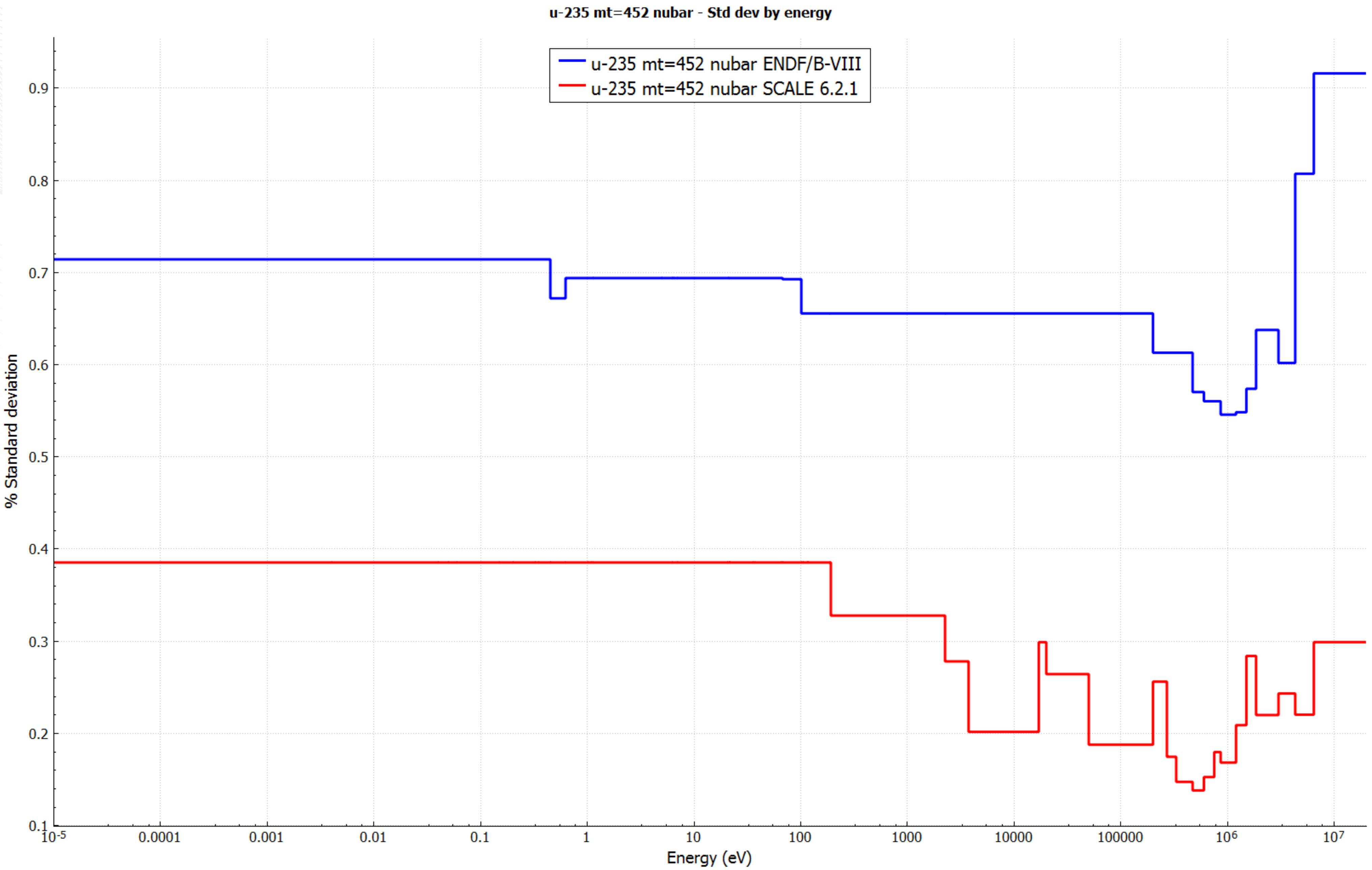

h-1 mt=2 elastic - Std dev by energy
h-1 mt=2 elastic ENDF/B-VIII
h-1 mt=2 elastic SCALE 6.2.1
% Standard deviation
2.4
2
1.6
1.2
0.8
0.4
10-6
10-5
0.0001
0.001
0.01
0.1
1
10
100
1000
10000
100000
106
107
Energy (eV)

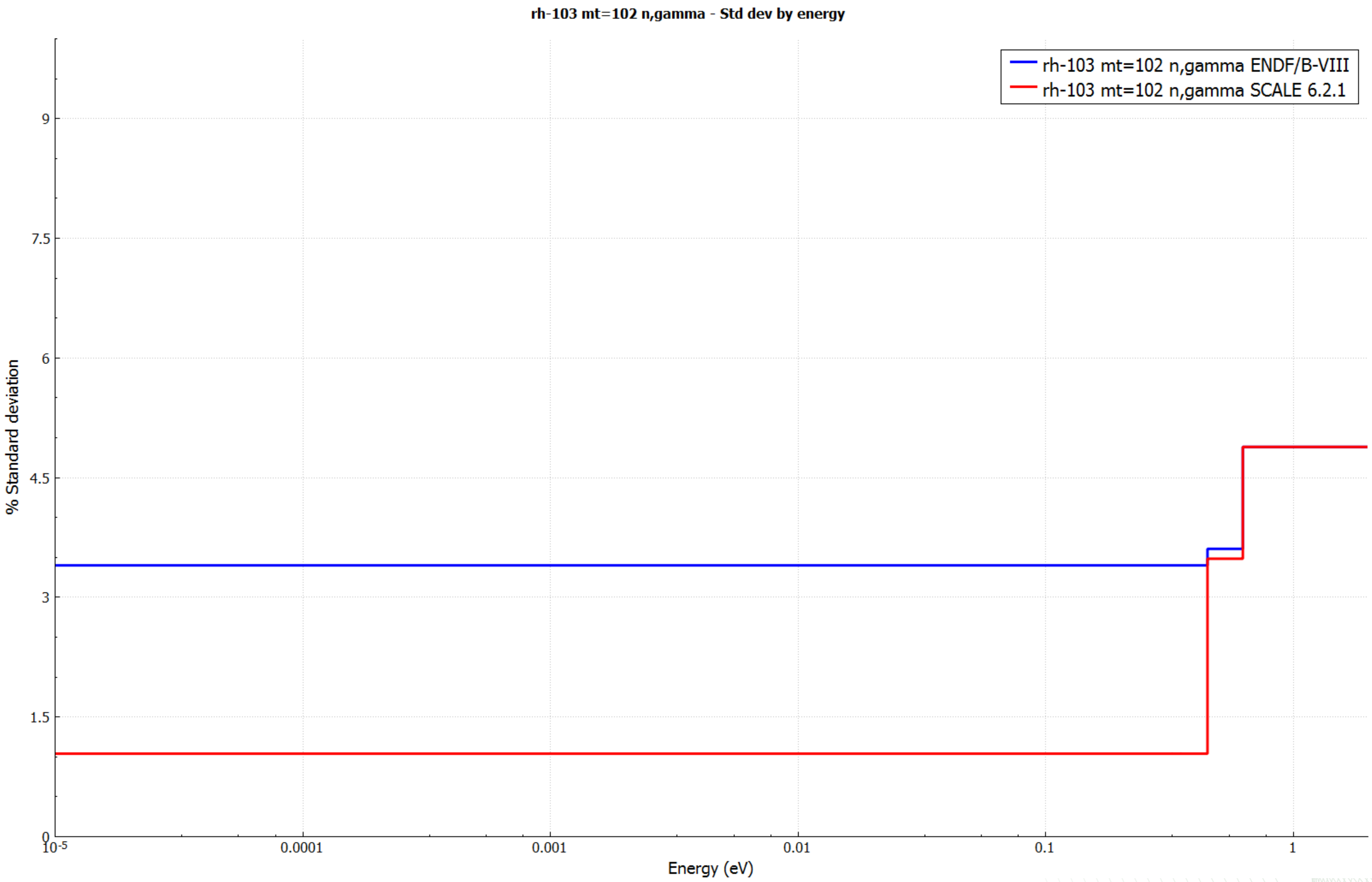


pu-240 mt=2 elastic - Std dev by energy
pu-240 mt=2 elastic ENDF/B-VIII
pu-240 mt=2 elastic SCALE 6.2.1
% Standard deviation
Energy (eV)
80
70
60
50
40
30
20
10
0
10^{-5}
0.0001
0.001
0.01
0.1
1
10
100



pu-240 mt=102 n,gamma - Std dev by energy
pu-240 mt=102 n,gamma ENDF/B-VIII
pu-240 mt=102 n,gamma SCALE 6.2.1
% Standard deviation
0
1.5
3
4.5
6
7.5
9
1
10
100
Energy (eV)


u-235 mt=452 nubar - Std dev by energy
u-235 mt=452 nubar ENDF/B-VIII
u-235 mt=452 nubar SCALE 6.2.1
% Standard deviation
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10-5
0.0001
0.001
0.01
0.1
1
10
100
1000
10000
100000
106
107
Energy (eV)


rh-103 mt=102 n,gamma - Std dev by energy
rh-103 mt=102 n,gamma ENDF/B-VIII
rh-103 mt=102 n,gamma SCALE 6.2.1
% Standard deviation
9
7.5
6
4.5
3
1.5
0
10-5
0.0001
0.001
0.01
0.1
1
Energy (eV)

Results: Summary Table χ^2

Category	Number of Cases	χ^2 Statistic (Should ≈Num. of Cases)	χ^2 P-Value
HMF	49	7.94	1.0000000000
HST	52	10.93	0.9999999996
IMF	13	2.62	0.9976738347
LCT	140	9.93	1.0000000000
LST	19	1.78	0.9999995703
MCT	49	15.89	0.9999966817
PMF	10	0.59	0.9999400415
PST	81	15.69	1.0000000000