The status of nuclear data uncertainty libraries

and the problem of too small uncertainties on differential data and too large uncertainties on integral data

V. Sobes, BJ Marshall, D. Wiarda,
F. Bostelmann, A. Holcomb, B.T. Rearden

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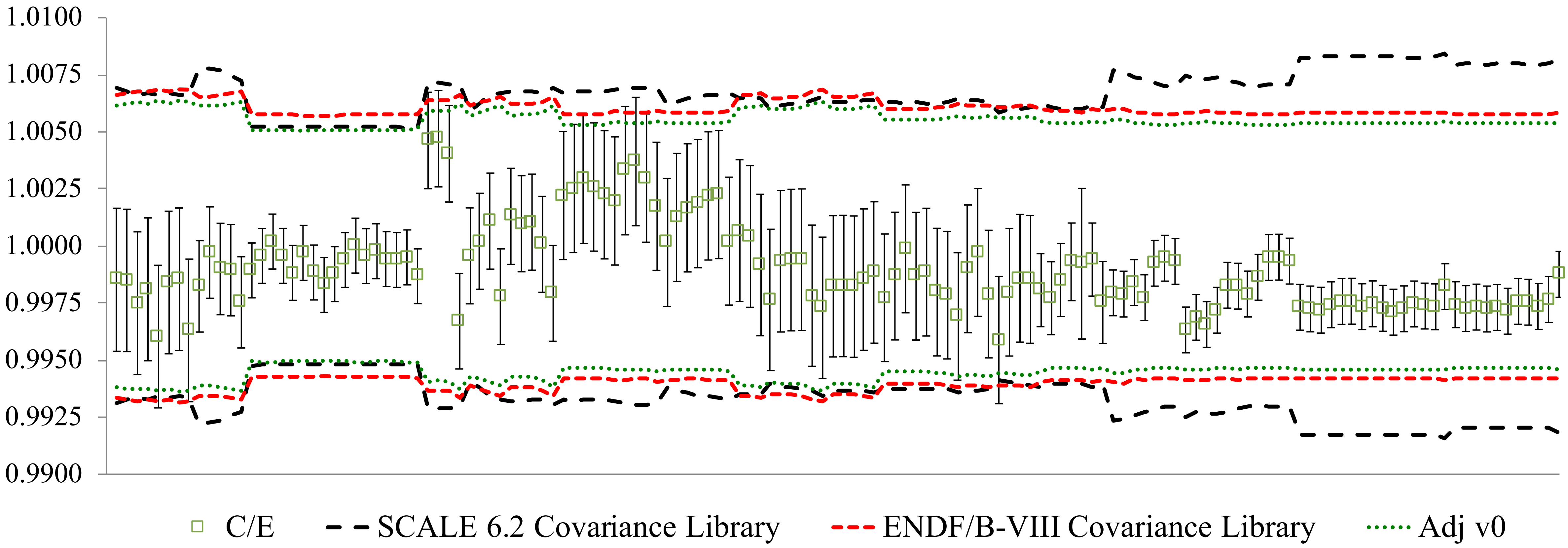
Washington

Difference between predicted and measured criticality is much smaller than predicted by nuclear data uncertainty



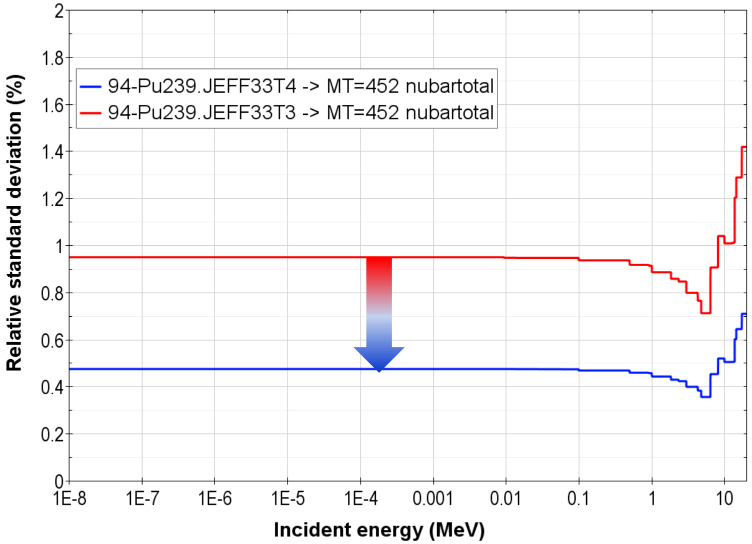
The response from the European nuclear data community to large propagated uncertainties

Nuclear Energy Agency

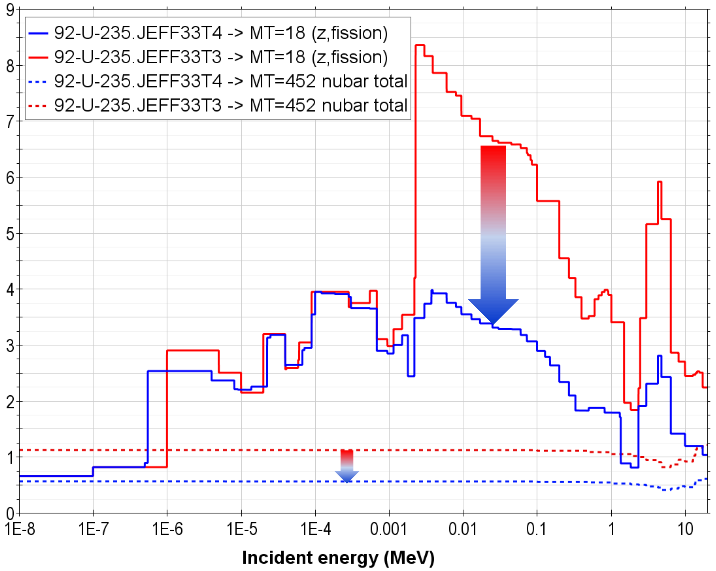
❑ Differences between JEFF-3.3T4 and JEFF-3.3T3

- **JEFF-3.3T3:** uncertainty in the fast range was based on microscopic experiment only.
  See files at: http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T3/neutrons/
- **JEFF-3.3T4:** reduced uncertainties to reflect adjustment (e.g. fast range to JEZEBEL).
  See files at: http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T4/neutrons/

Incident neutron data / / MAT9437 / MT=452 : nubar total / Covariances data (BOXER) Relative standard deviation

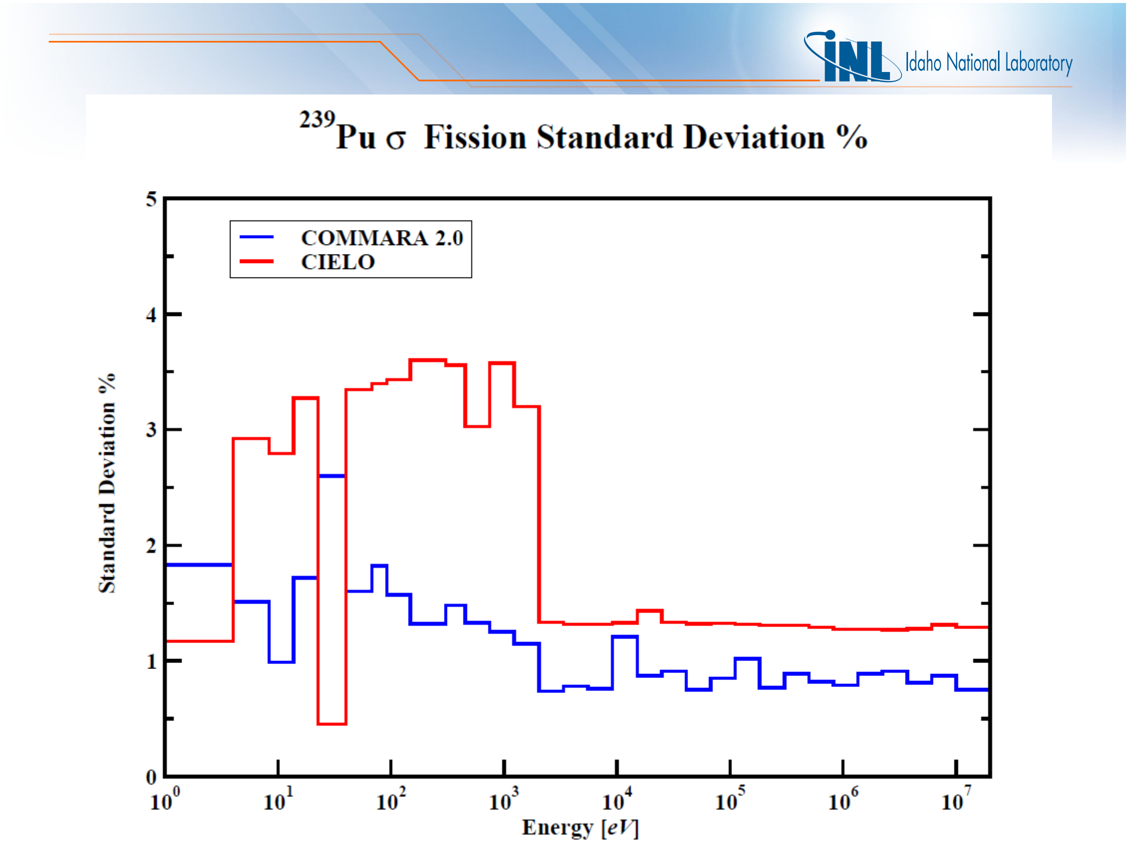


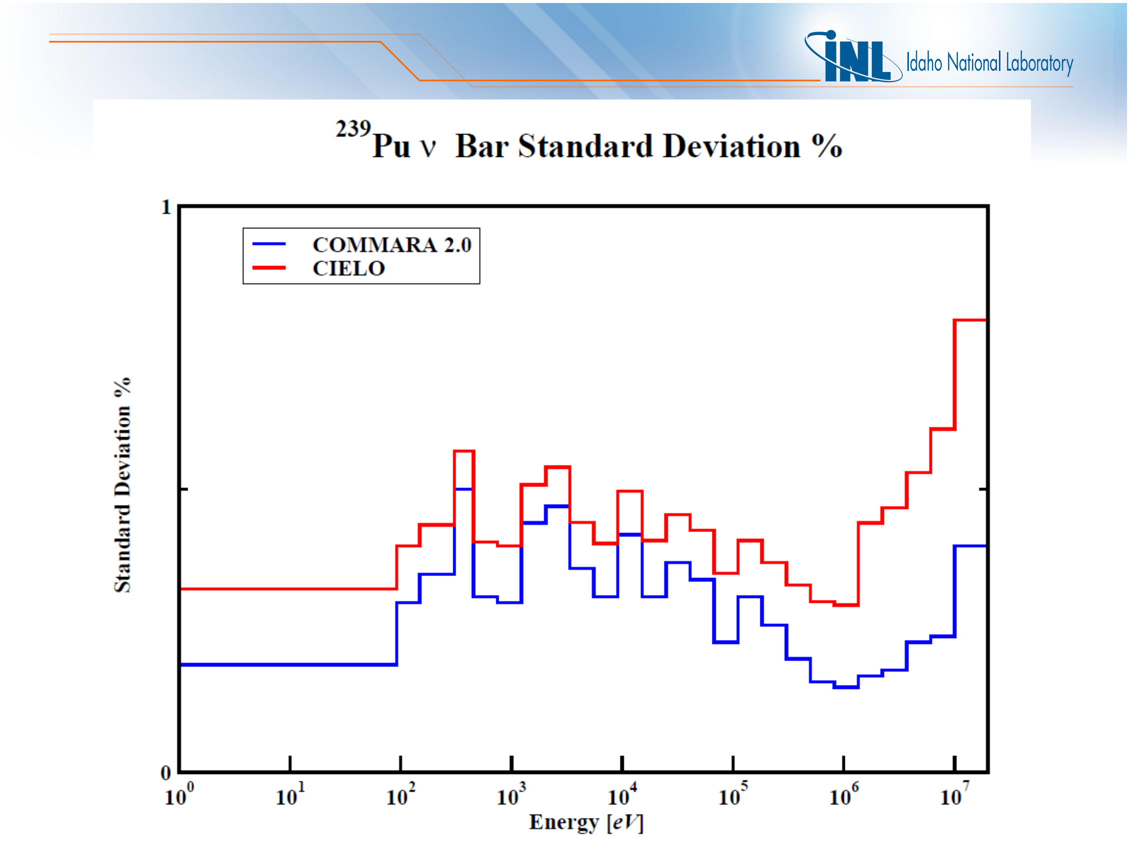
Incident neutron data / / MAT9228 / / Covariances data (BOXER) Relative standard deviation



Slide from O. Cabellos, CW2017

The US nuclear data community has (generally) increased uncertainties in the new library (red)





Slides from P. Palmiotti, WPEC 2018

The current official guidance from the US nuclear data center

Comments about the covariance in current ENDF evaluations

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1. The covariance data in the ENDF evaluations represents uncertainties and correlations in differential data.

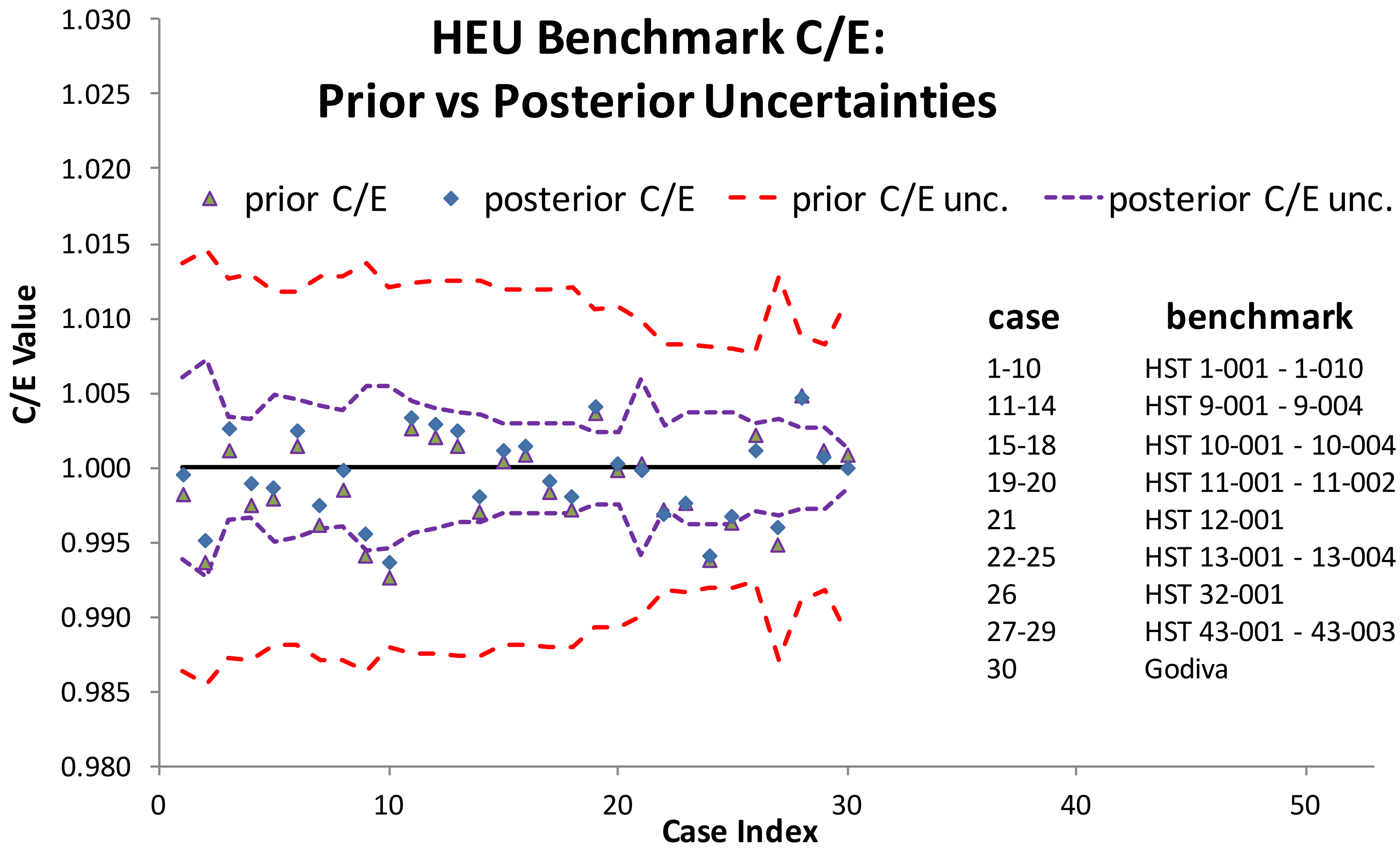
2. The use of this covariance to calculate uncertainties for integral quantities such as Keff will usually result in an overestimate of the uncertainty. That said, comparisons to integral data are essential during the evaluation process and users should not be surprised if the *mean value* nuclear data allow for the accurate prediction of Keff, even if the covariances to not reflect this consideration.

3. The recommended methodology to overcome this problem is to adjust the covariance to add information from set of integral data that represents the physics of the system for which the adjusted covariance will be used.

4. More information on this topic: https://www.oecd-nea.org/science/wpec/sg33/

5. CSEWG is currently studying the best covariance representation for future releases.

HEU Benchmark C/E: Prior vs Posterior Uncertainties



case	benchmark
1-10	HST 1-001 - 1-010
11-14	HST 9-001 - 9-004
15-18	HST 10-001 - 10-004
19-20	HST 11-001 - 11-002
21	HST 12-001
22-25	HST 13-001 - 13-004
26	HST 32-001
27-29	HST 43-001 - 43-003
30	Godiva

Slide from
M. Williams,
CSEWG 2017

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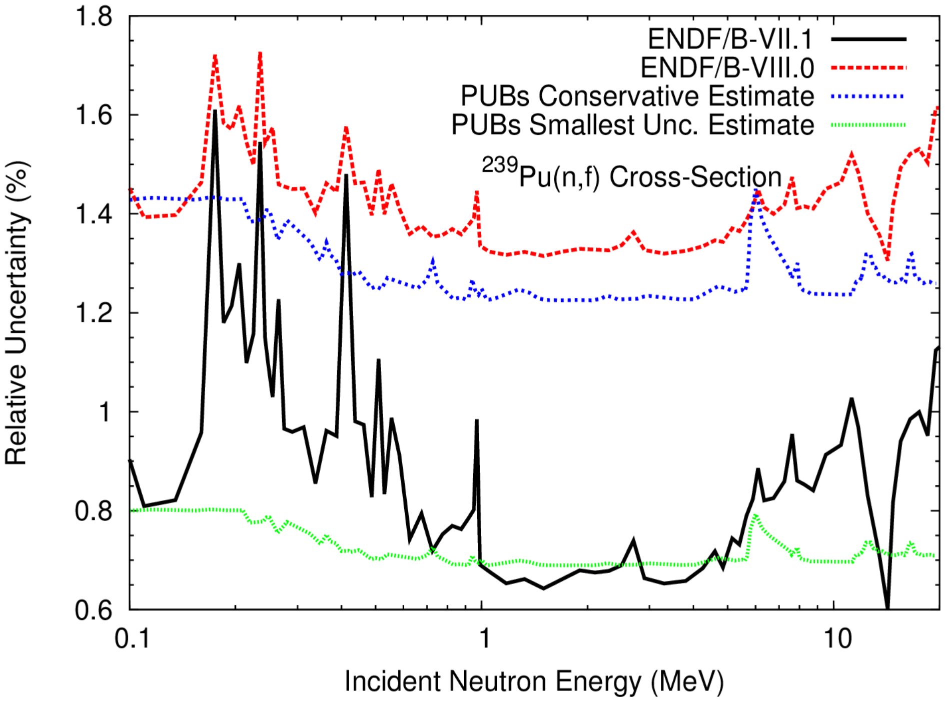
There are minimum bounds on realistic uncertainty estimates and adjustment methodologies often violate these

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.

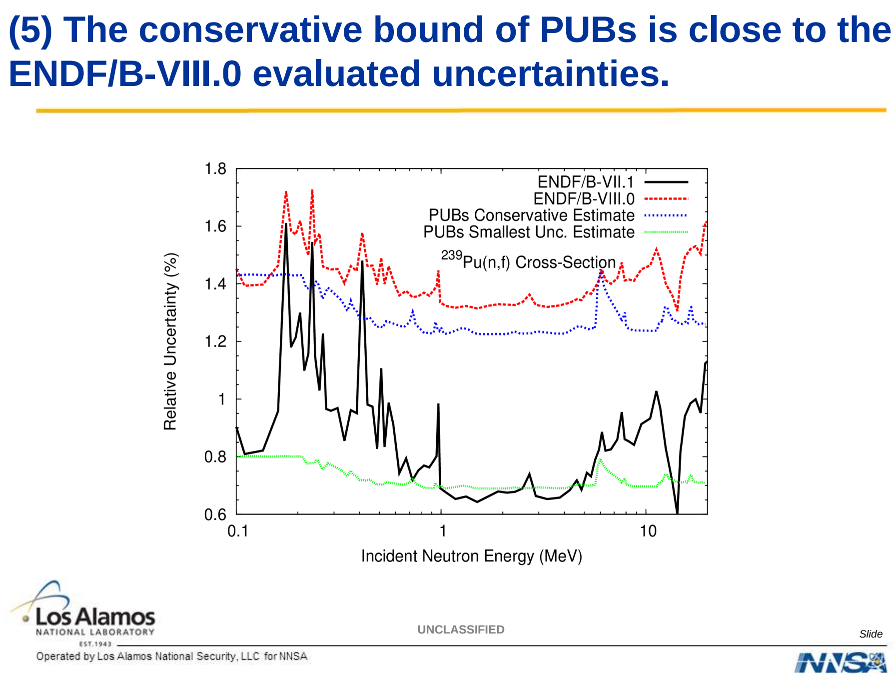


PUBs: Physical Uncertainty Boundaries

Slide from D. Neudecker, WPEC 2018

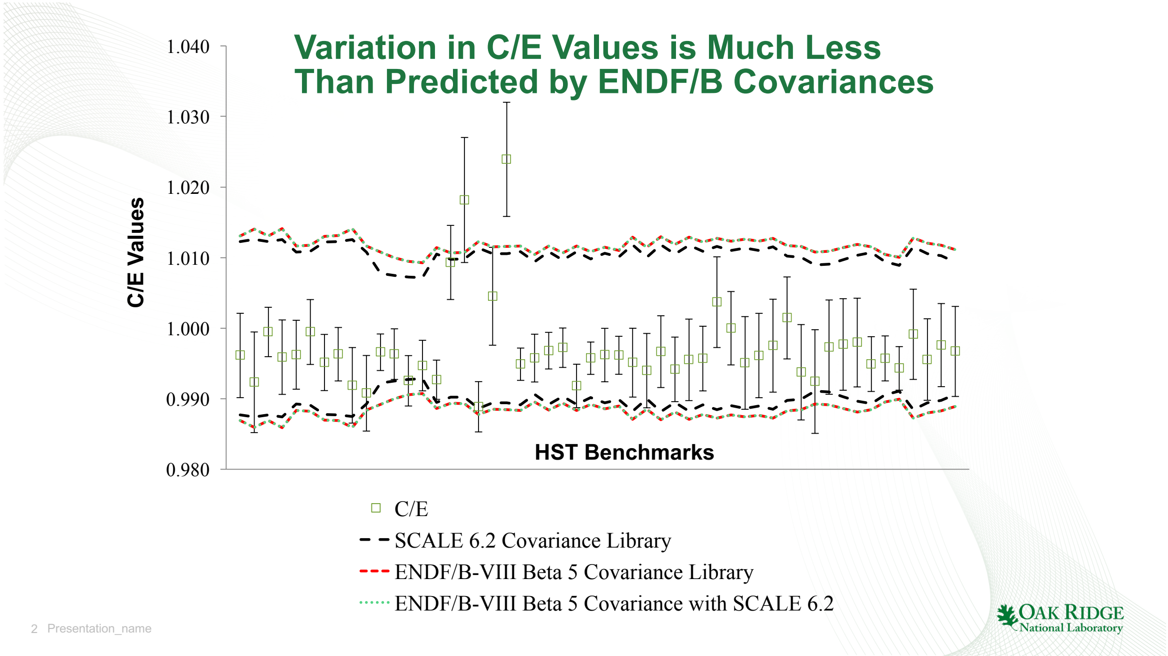
The problem of too small uncertainties on differential data and too large uncertainties on integral data

Nuclear data uncertainties are in danger of being smaller than what can be measured experimentally



Slide from of D. Neudecker, WPEC 2018

Nuclear data uncertainties are too large to reflect how well we actually know critical systems



Slide from of M. Williams, CSEWG 2017

Have your cake and eat it too: solving the discrepancy with nuclear data correlations

We cannot experimentally measure nuclear data to precision below 1%,

$$\delta\bar{\nu} > 1\%, \qquad \delta\sigma_f > 1\%$$

But, only 1% uncertainty in $\bar{\nu}$ results in 1% uncertainty in k_{eff} (more than $1 of reactivity),

$$k_\infty = \frac{(\bar{\nu} \pm 1\%)\,\Sigma_f}{\Sigma_a} \rightarrow 1\% \text{ uncertainty in } k_\infty$$

However, the ability to predict k_{eff} with better accuracy than 1% **does not imply** the knowledge of the cross sections to better than 1%.

It only says that we know the integral of the cross sections (in the appropriate spectra) to better than 1%.

Approach philosophy

- The discrepancy comes from non-systematic treatment
- The solution will be non-systematic, (no one mathemagical equation)
- However, **we promise** to
  1. Document exactly what is done, therefore, everything will be reproducible
  2. Test and iterate with the nuclear data community and users

The first iteration

Philosophy

1. 20/80 rule, start with only on the most impactful cross-correlations
2. Augment the ENDF/B-VIII.0 covariance matrix (not adjust)
3. Estimate the bulk correlation coefficient (coarse group structure)

Realization

1. ^{239}Pu, ^{235}U, ^{238}U $\sigma_{fis} - \bar{\nu}$
2. Only add new cross-correlations, do not adjust variances or existing correlations
3. | | | |
   |---|---|---|
   | Fast group | 20 MeV | - 50 keV* |
   | Inter. group | 50 keV | - 0.625 eV |
   | Thermal group | 0.625 eV | - 10^{-5} eV |

The goal of the first iteration was not to "solve" the problem outright, but to show conservative progress in the right direction

*Selected to match the boundary of the SCALE 56-group structure

Future development

Philosophy

1. 20/80 rule
2. Do not change uncertainty on differential data
3. Include benchmarks beyond ICSBEP (e.g. shielding and transmission)
4. Iterate with testing community frequently. Increase the number of cross-correlations and fidelity in energy domain.
5. Do not aspire to reduce propagated uncertainty to level of C/E discrepancy in integral data

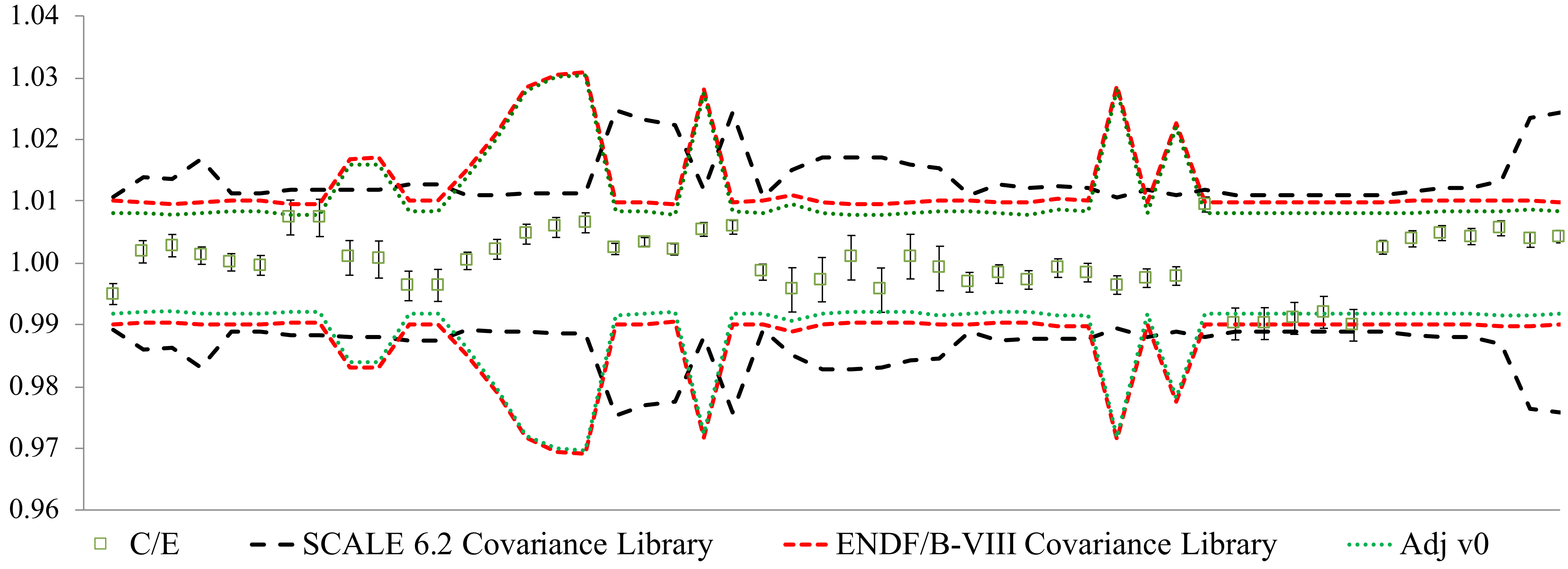
Realization

1. Prioritize work on only the most impactful cross-correlations. The vision is not to have a full covariance matrix for the library
2. Only add cross-correlations, do not adjust variances
3. Collaboration with community
4. Test that uncertainty on "unstudied" integral systems is not significantly reduced
5. Reduce uncertainty as possible by realistic estimation of "generic" cross-correlations independent of integral system

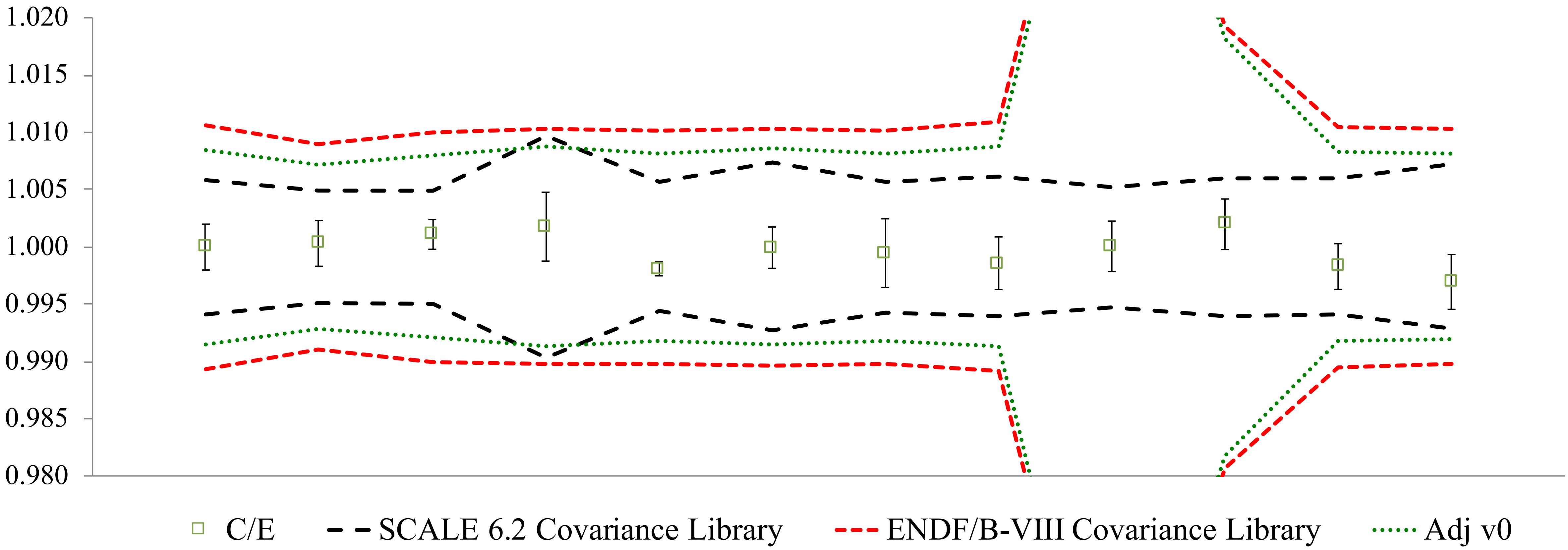
^{235}U $\sigma_{fis} - \bar{\nu}$ (bulk cross-correlations are only weakly dependent on choice of integral system)

INTER-MET-FAST (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-33	-37
fission intermediate	-28	-20	-23
fission thermal	-38	-26	-30
INTER-MET-FAST (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-34	-38
fission intermediate	-28	-20	-23
fission thermal	-39	-27	-31
LEU-COMP-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-10	-8	-13
fission intermediate	-24	-17	-32
fission thermal	-23	-13	-36
LEU-COMP-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-9	-9	-11
fission intermediate	-23	-18	-30
fission thermal	-23	-13	-36

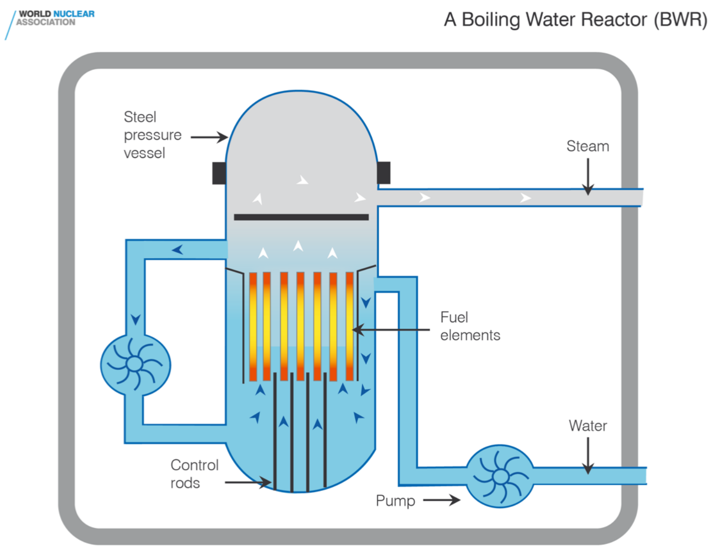
Results for HEU-MET-FAST systems

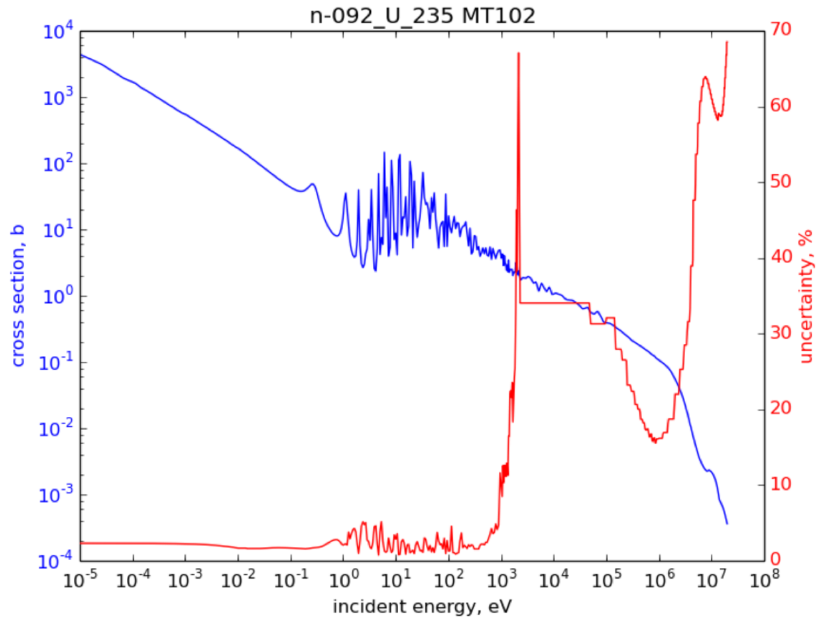


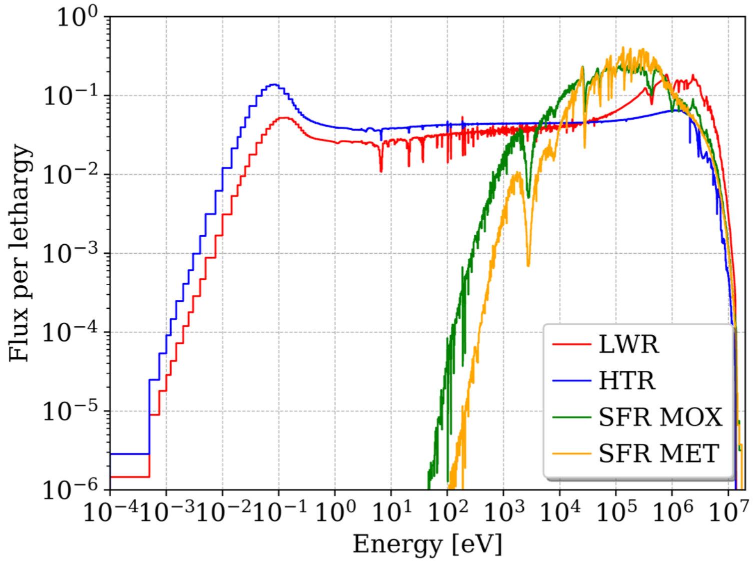
Results for PU-MET-FAST systems

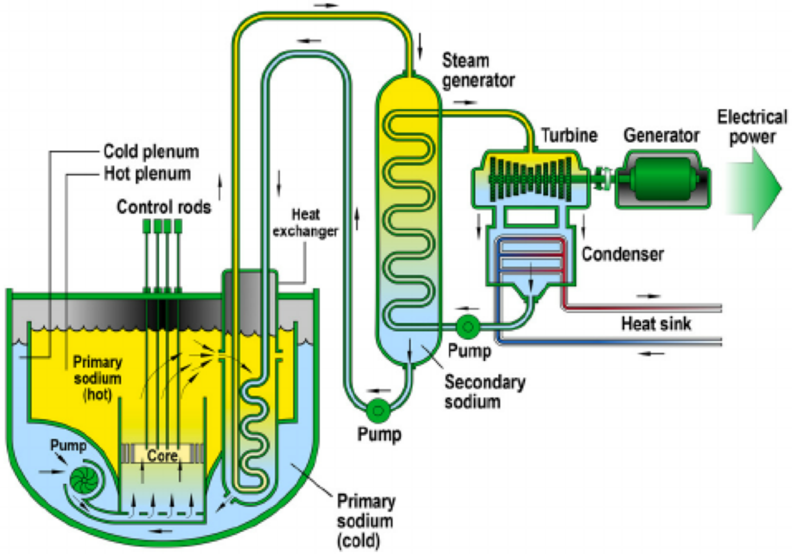


Through a careful examination of nuclear data correlations (energy, reaction, isotope), propagated uncertainties for well known systems can be small and large for systems without vast validation data









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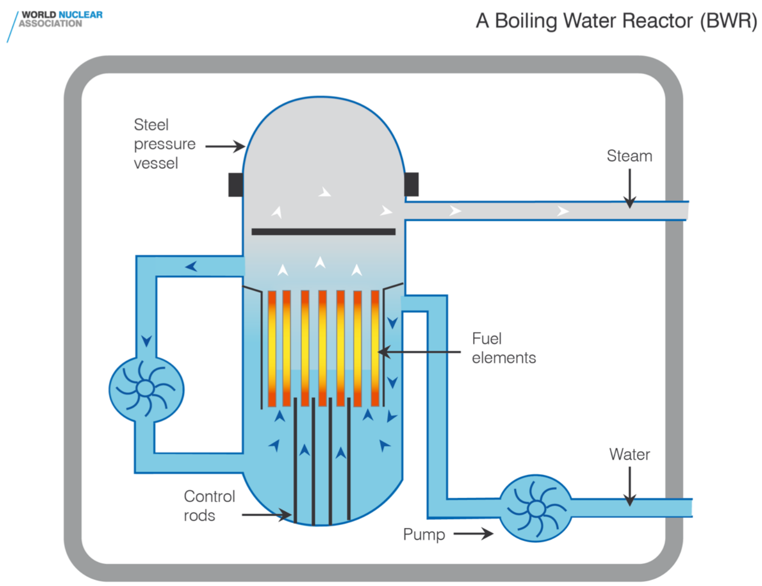
Concluding remarks

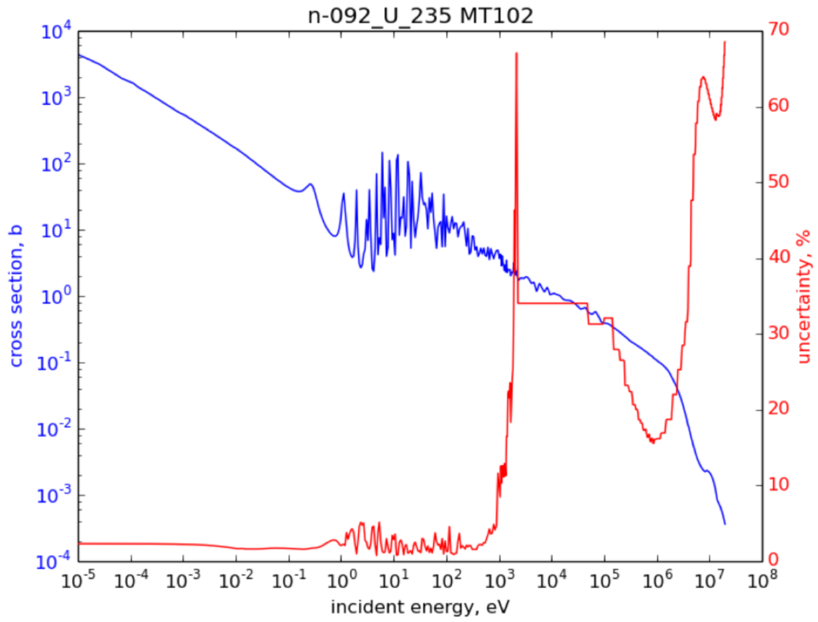
ENDF/B-VIII.0 augmented uncertainty data

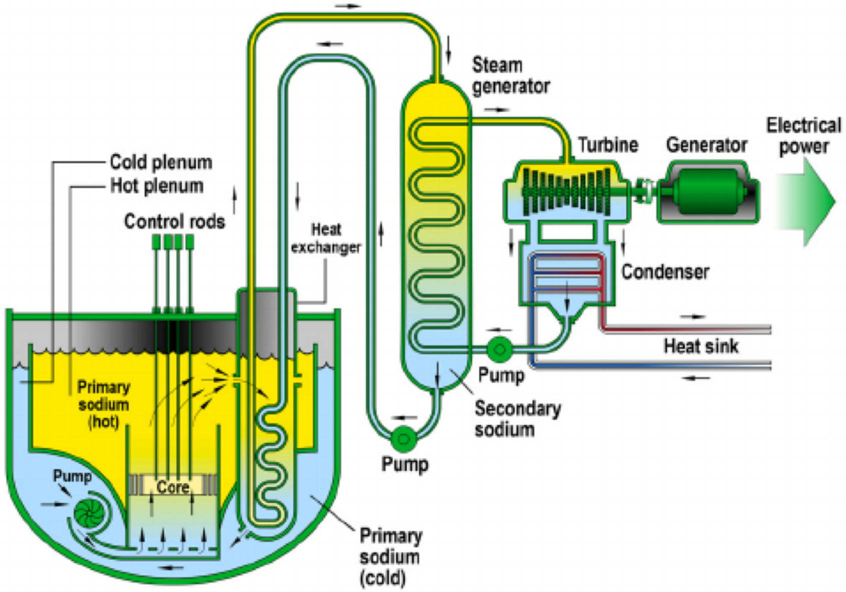
- The first demonstration augmented ENDF/B-VIII.0 uncertainty data make progress in the right direction
- More work and collaboration with the international community is necessary for further progress

Thermal Scattering Law uncertainty data

- Currently there is no uncertainty data for thermal scattering in ENDF and the impact on applications is unknown
- University of Michigan and ORNL are developing a format for TLS covariance in new nuclear data format (GNDS)







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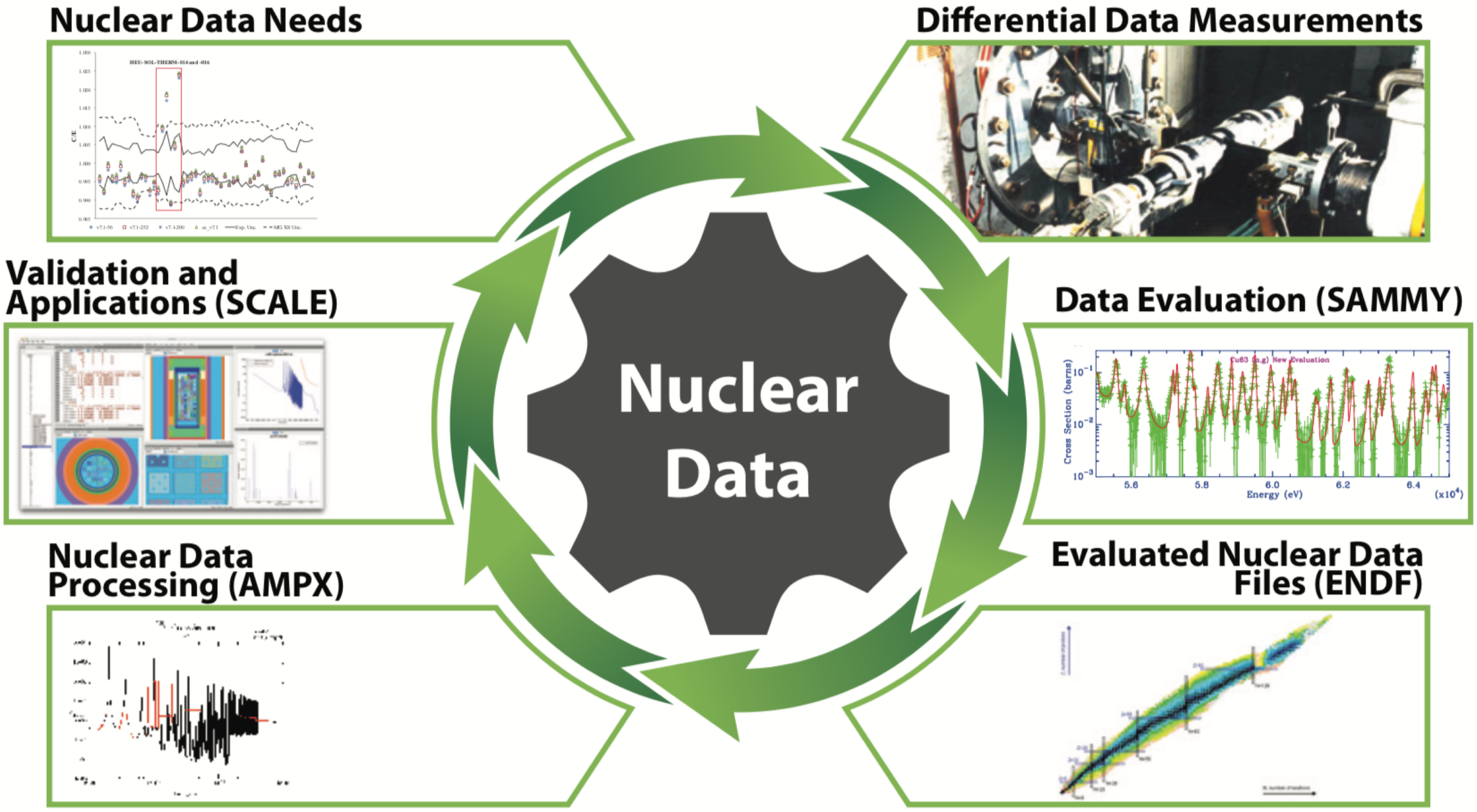
Nuclear data cycle



EXFOR data base: *http://www-nds.indcentre.org.in/exfor/exfor.htm*

Help » Manual PDF | Lexfor | NNDC-Help | Output | Plot+ | R33 Databases » ENDF | CINDA | IBANDL CD-ROM » EXFOR-CINDA | CD-Catalog

NNDC NRDC

Experimental Nuclear Reaction Data (EXFOR)

Database Version of 2018-12-07

Software Version of 2018-07-11

The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively.
The EXFOR library contains data from 22353 experiments (see statistics and recent database updates).
EXFOR Reference Paper: Nucl. Data Sheets 120(2014)272
EXFOR Web Database & Tools Paper: NIM A 888 (2018) 31. Mirror-sites

Search: Go ?

Examples of requests: 1|2|3|4|5|6|7|...
1| Cross section σ(E) /updates/ More examples...

Request Submit Reset Help

Target
Reaction
Quantity
Product
Energy from to eV
Author(s)
Publication year
Last modified
Accession #

Extended
Keywords
Expert

Submit Reset

Go to: [upload your data]

Options

- Exclude superseded data
- No reaction combinations (ratios,..)
- Exclude evaluated data
- Enhanced search of Products
- Retrieve listing only
- Disable Prompt-Help

Sort by: reaction publication
View: basic extended

Ranges (Z,A)
Reaction Sub-Fields
Feedback and User's Input
Clone Request: CINDA ENDF

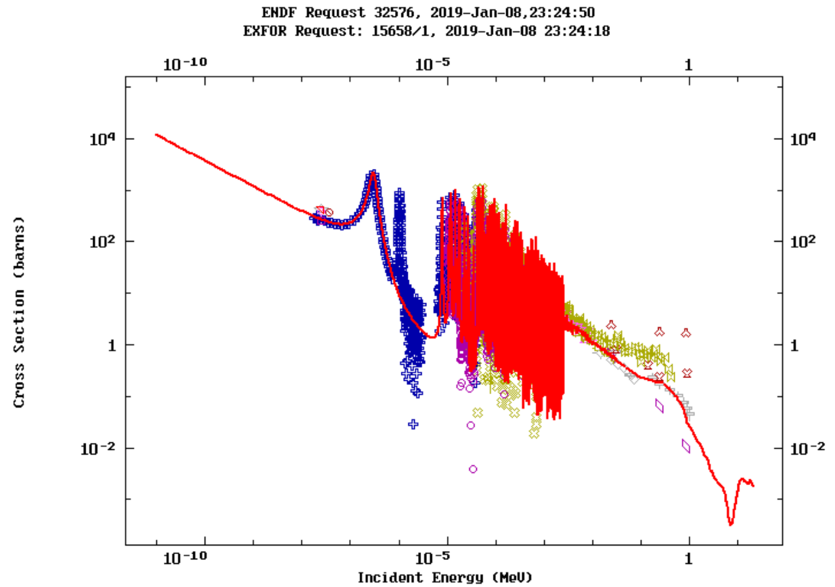
More Web Tools

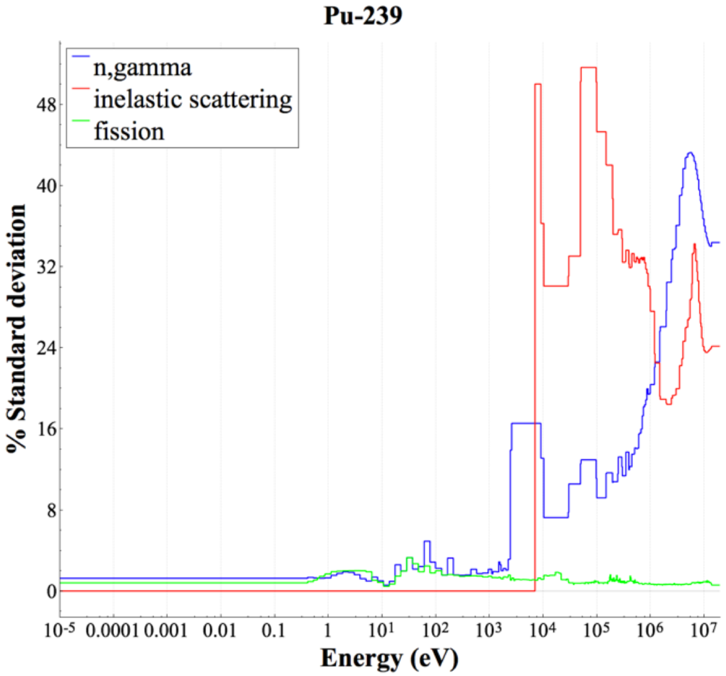
Plotting. See also: [video-guide]

Note:
- all criteria are optional (selected by checking ☑)
- selected criteria are combined for search with logical AND
- criteria separated in a field by ";" are combined with logical OR
- criteria starting with "^" will be used as logical NOT
- wildcards (*) and intervals (..) are available

Statistics of usage: visits: 630, data search: 15657, since 23-Jul-2018

Database Manager: Viktor Zerkin, NDS, International Atomic Energy Agency (V.Zerkin@iaea.org)
Web and Database Programming: Viktor Zerkin, NDS, International Atomic Energy Agency (V.Zerkin@iaea.org) 2018-07-11
Data Source: Network of Nuclear Reaction Data Centres (NRDC)





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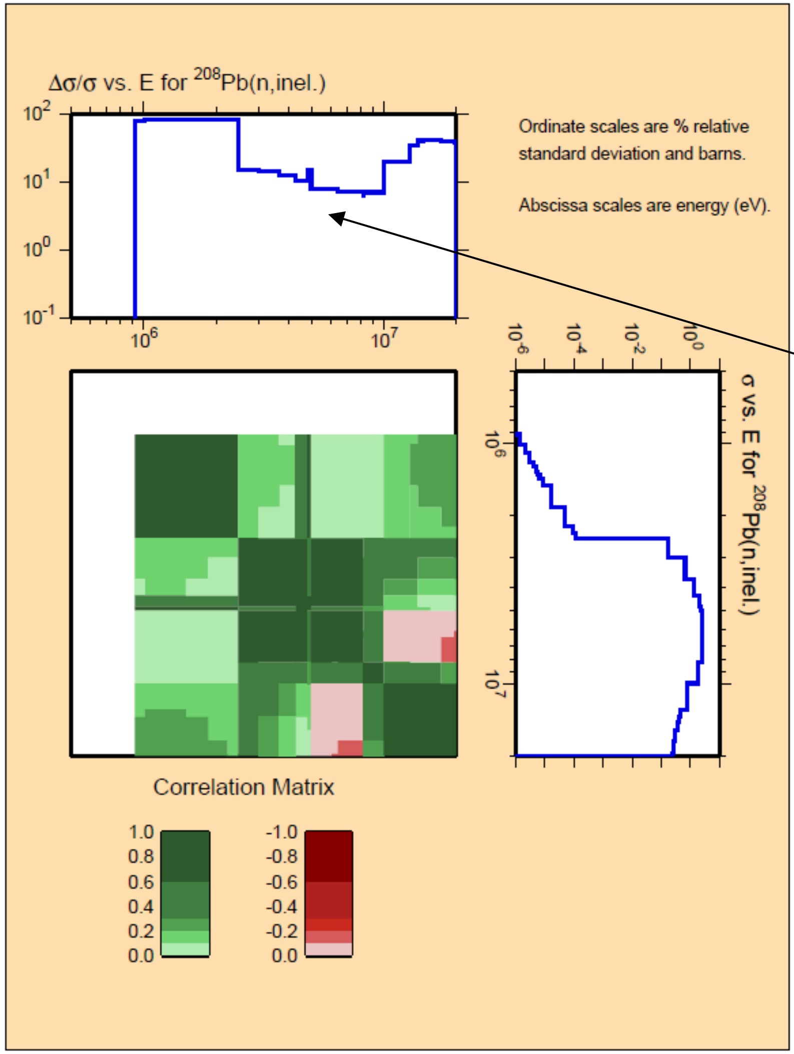
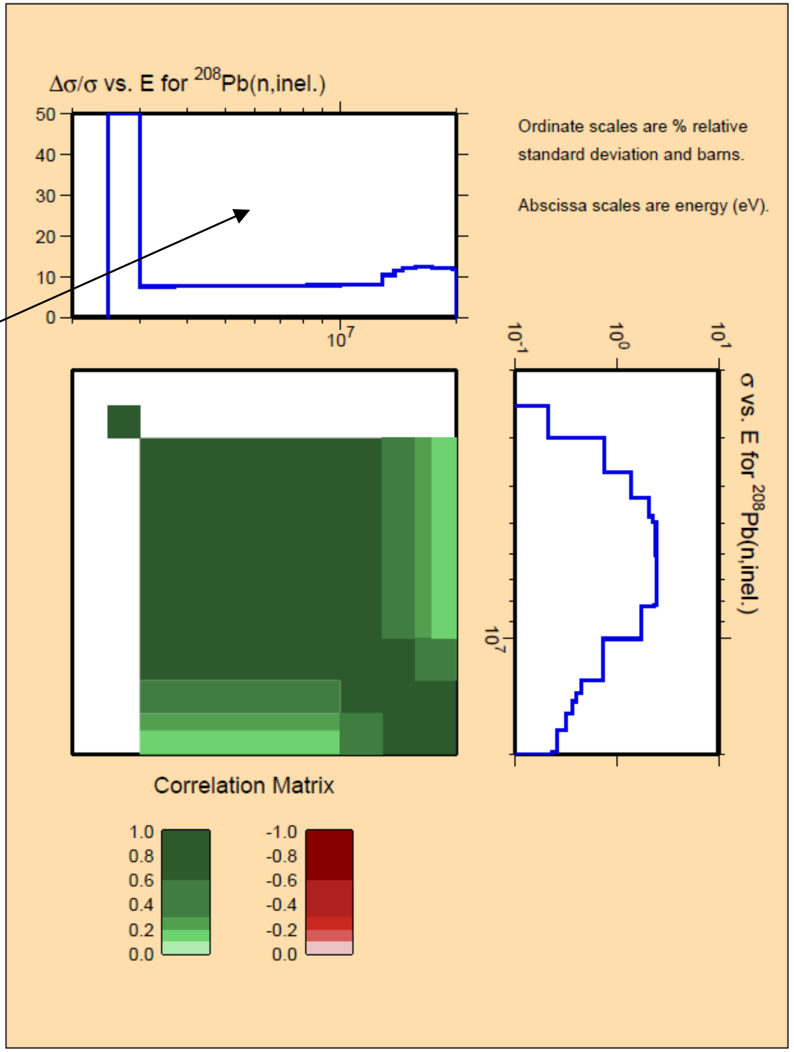
JEFF-3.3

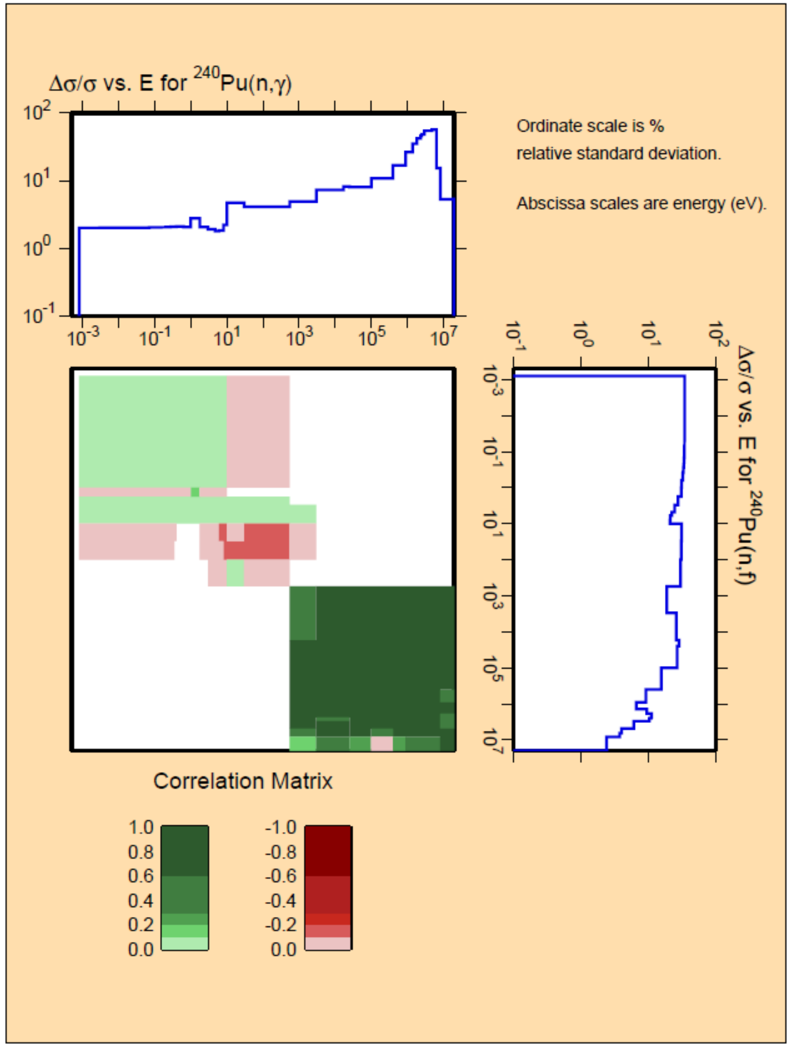


ENDF/B-VIII.0

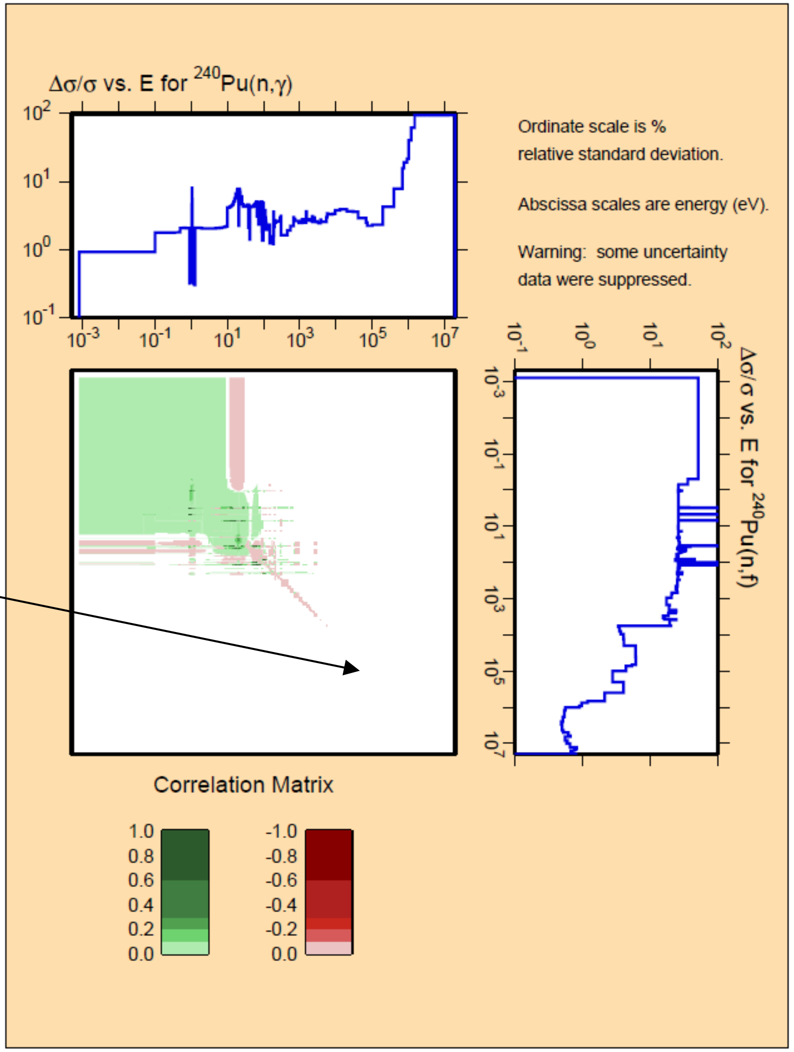


Different cross section uncertainty

JEFF-3.3

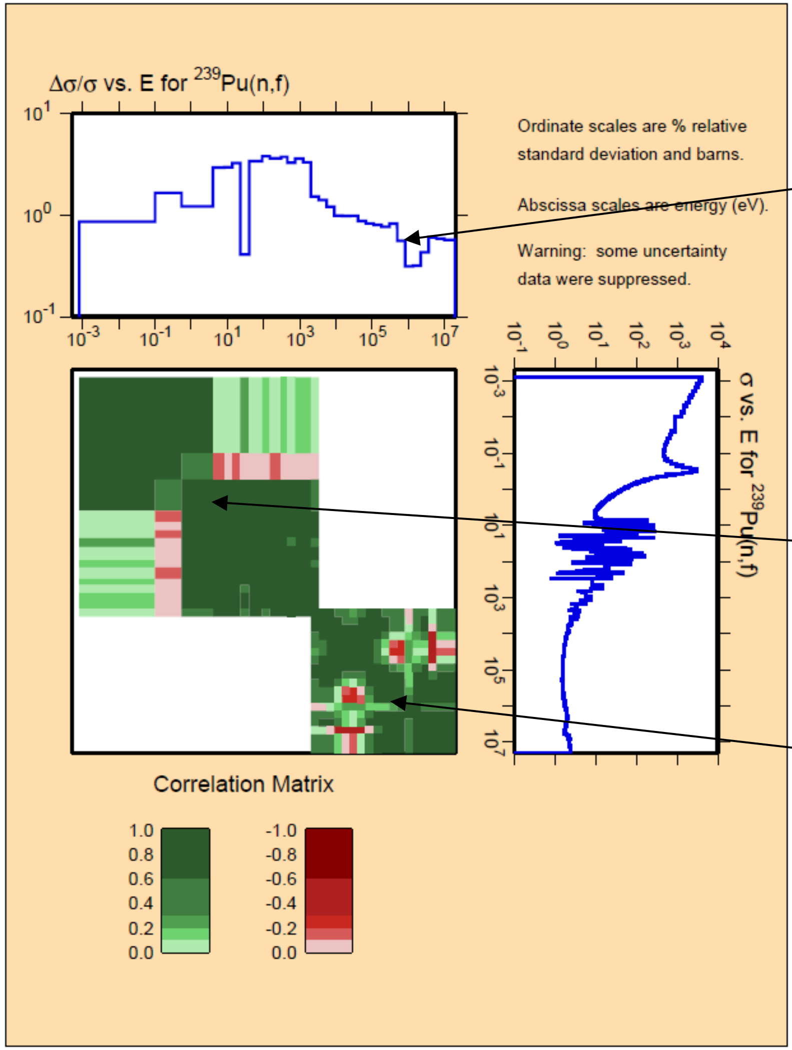


ENDF/B-VIII.0

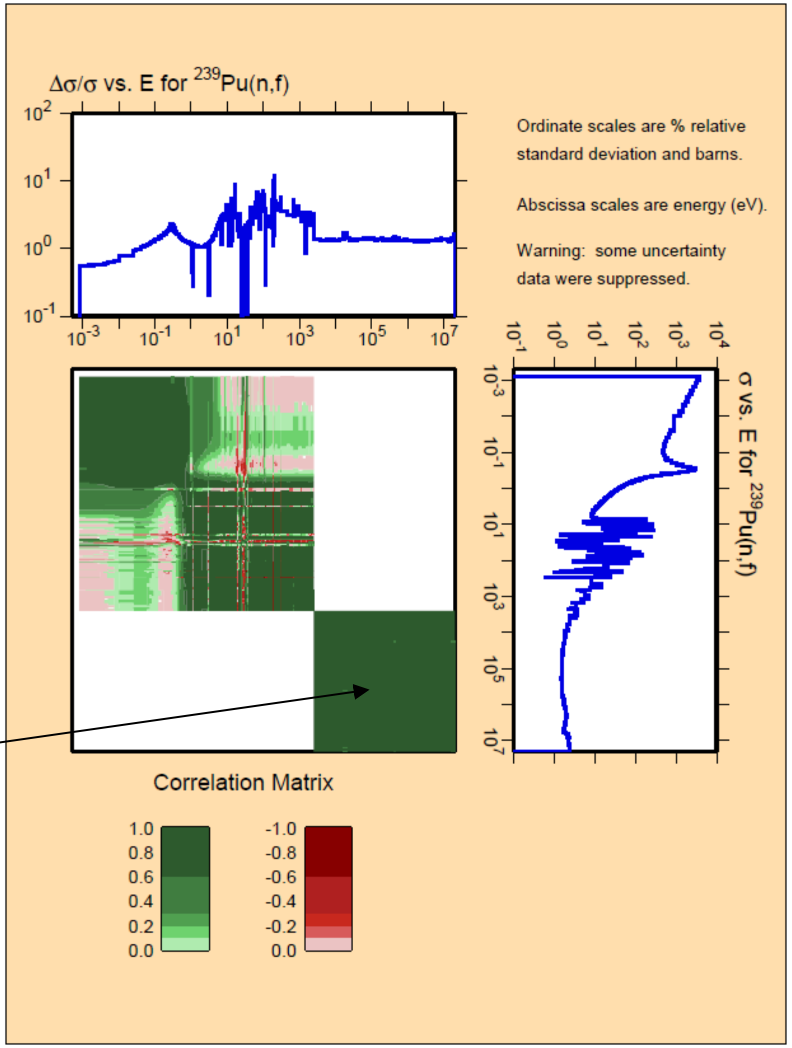


Missing correlations

JEFF-3.3



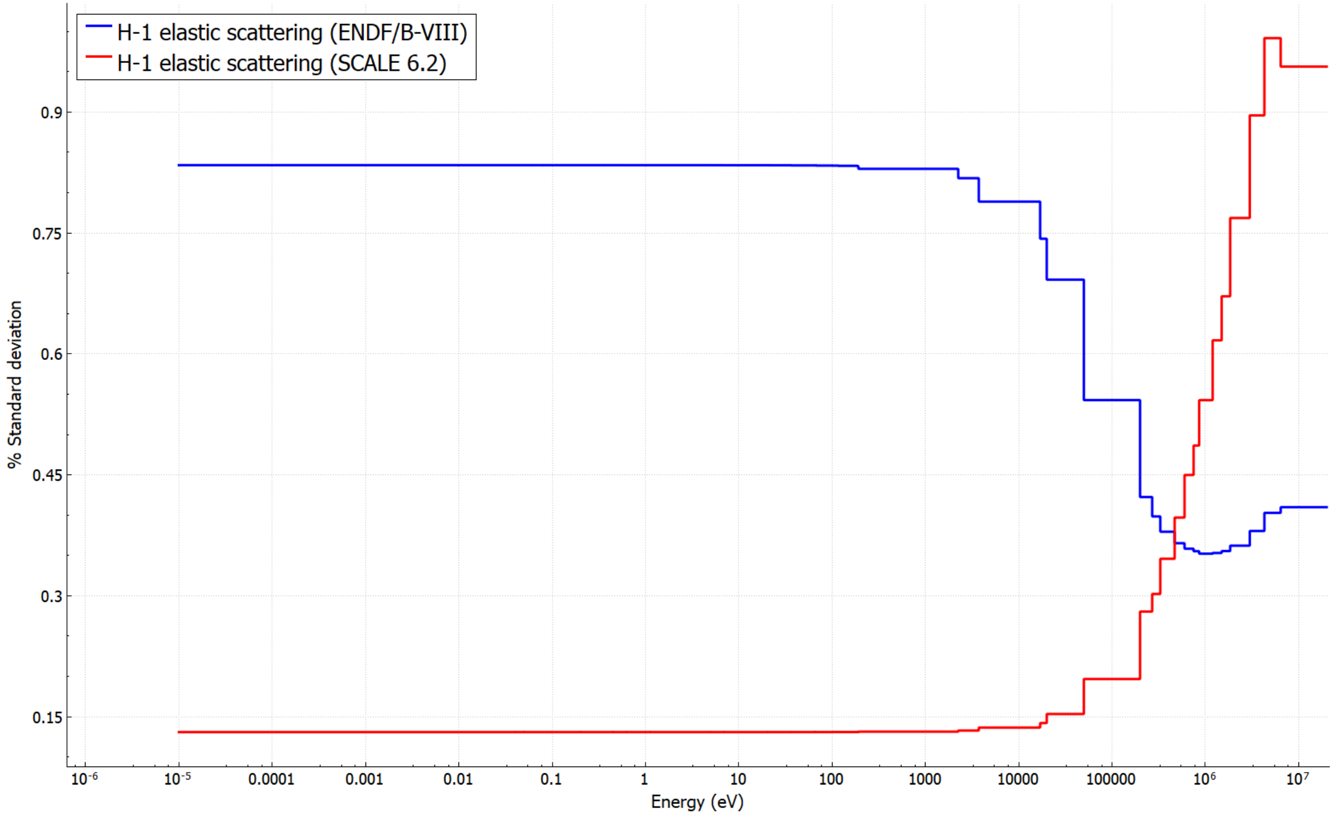
ENDF/B-VIII.0



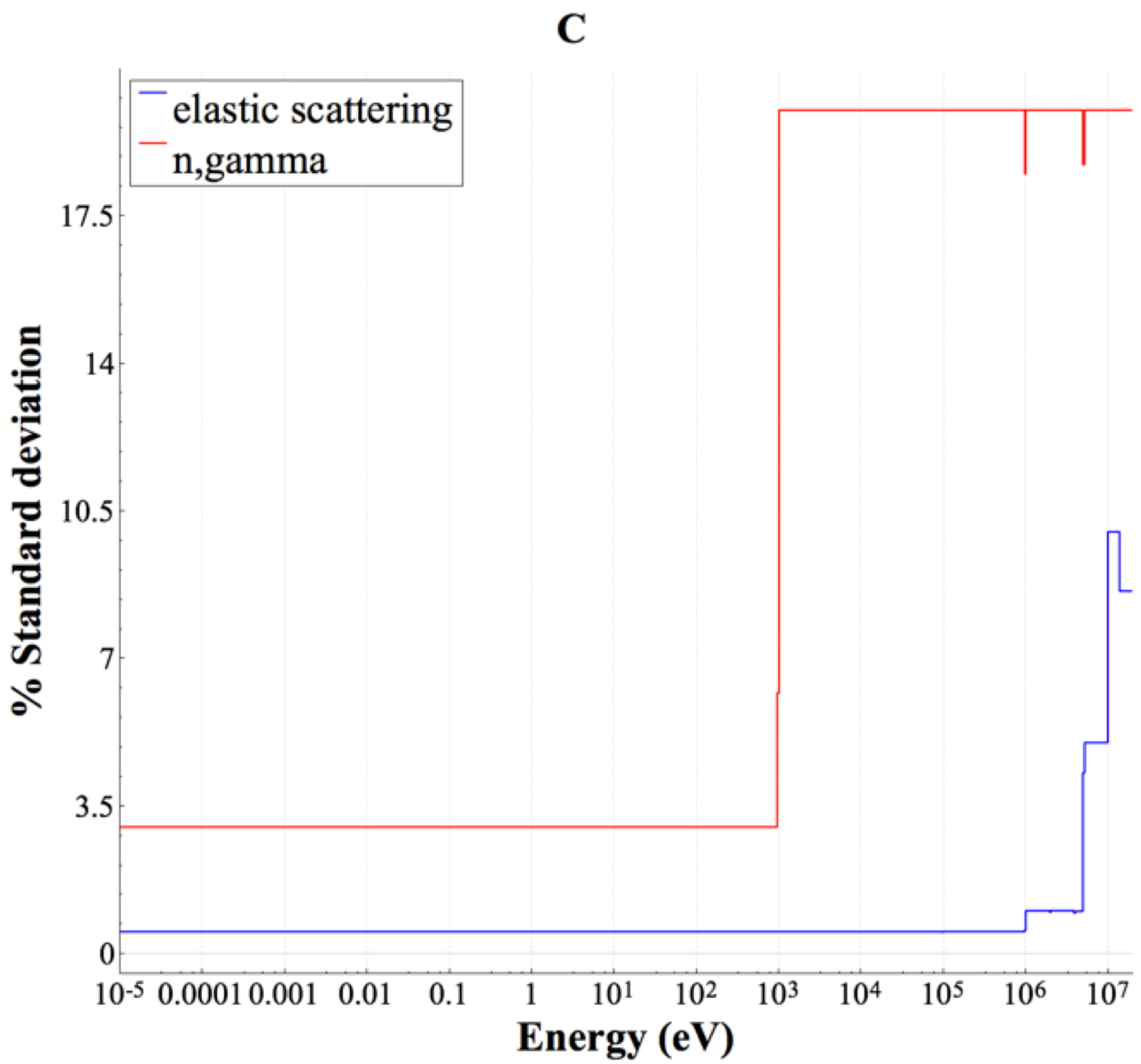
Uncertainty drop?

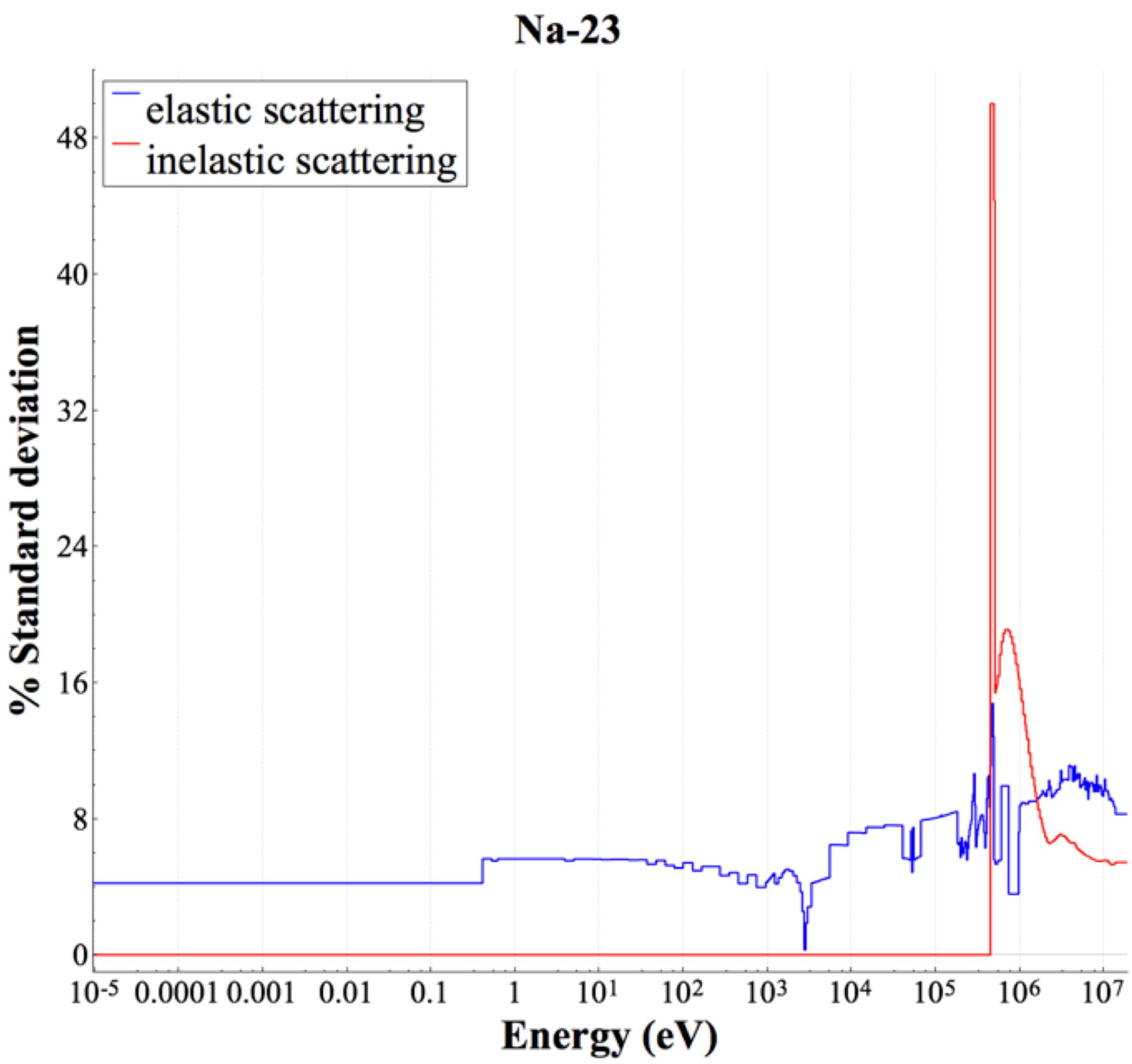
33g energy grid

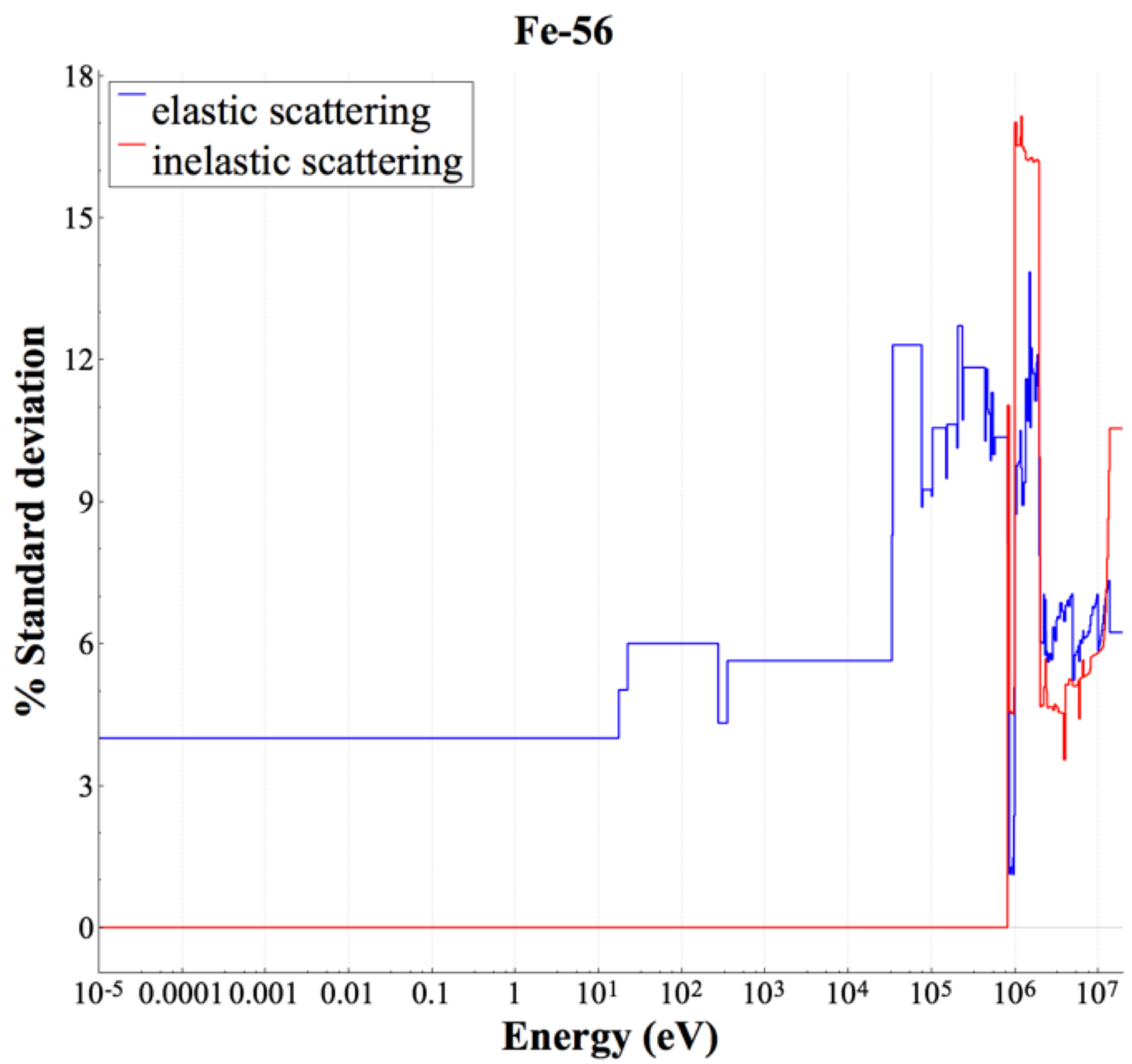
Different correlations

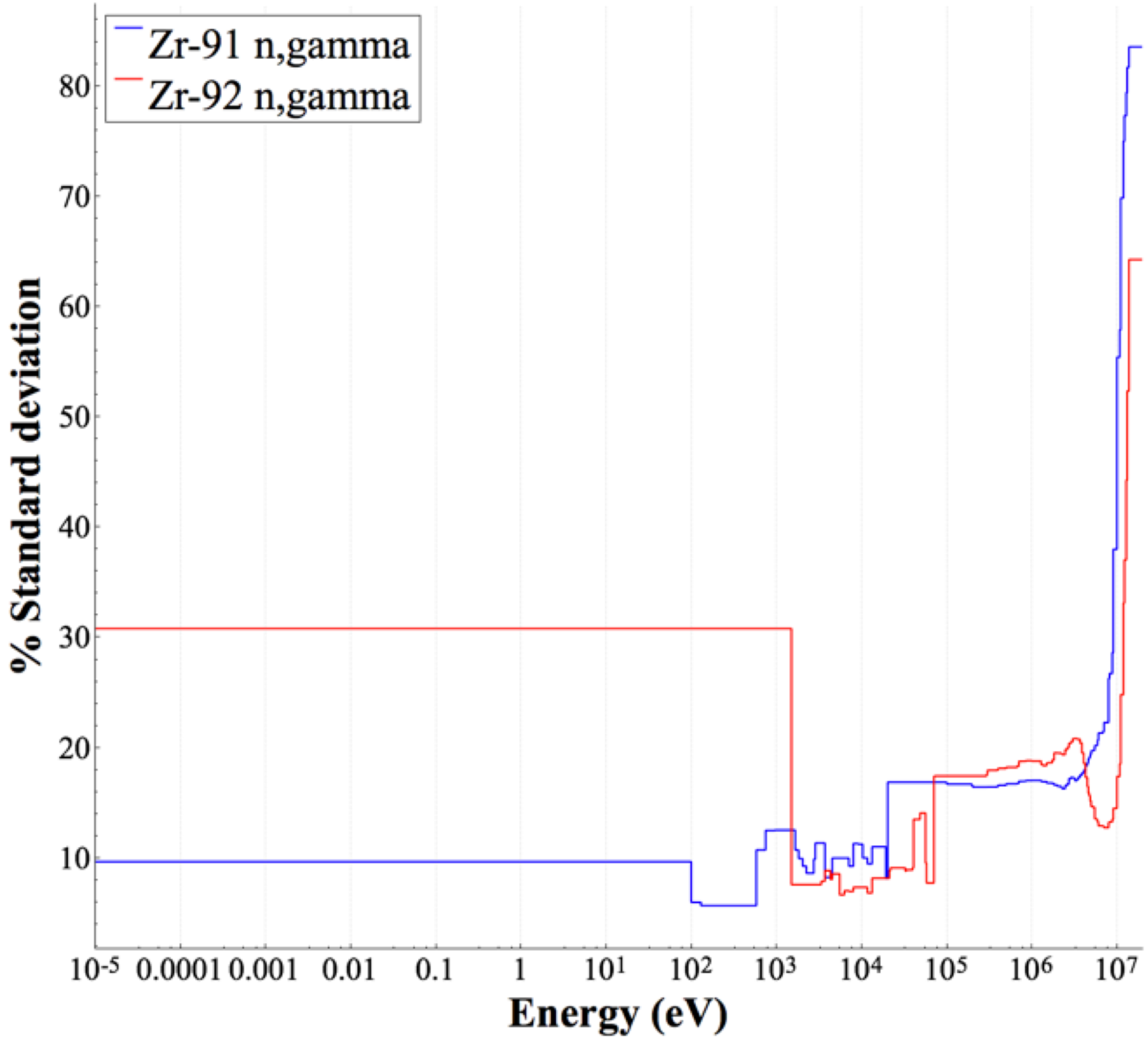


H-1 elastic scattering (ENDF/B-VIII)
H-1 elastic scattering (SCALE 6.2)
% Standard deviation
0.9
0.75
0.6
0.45
0.3
0.15
10^{-6}
10^{-5}
0.0001
0.001
0.01
0.1
1
10
100
1000
10000
100000
10^{6}
10^{7}
Energy (eV)

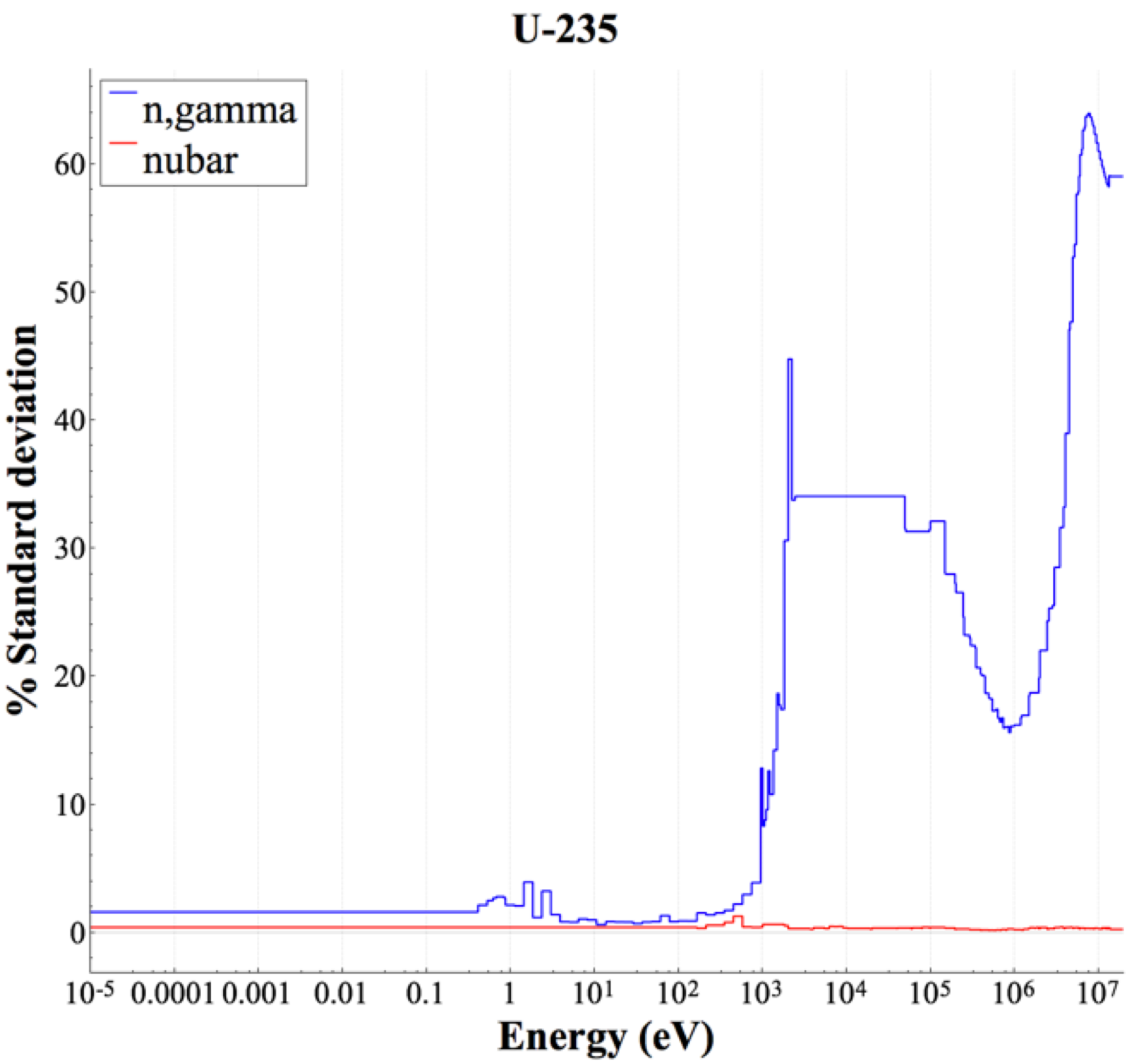

C
elastic scattering
n,gamma
% Standard deviation
17.5
14
10.5
7
3.5
0
10-5 0.0001 0.001 0.01 0.1 1 101 102 103 104 105 106 107
Energy (eV)

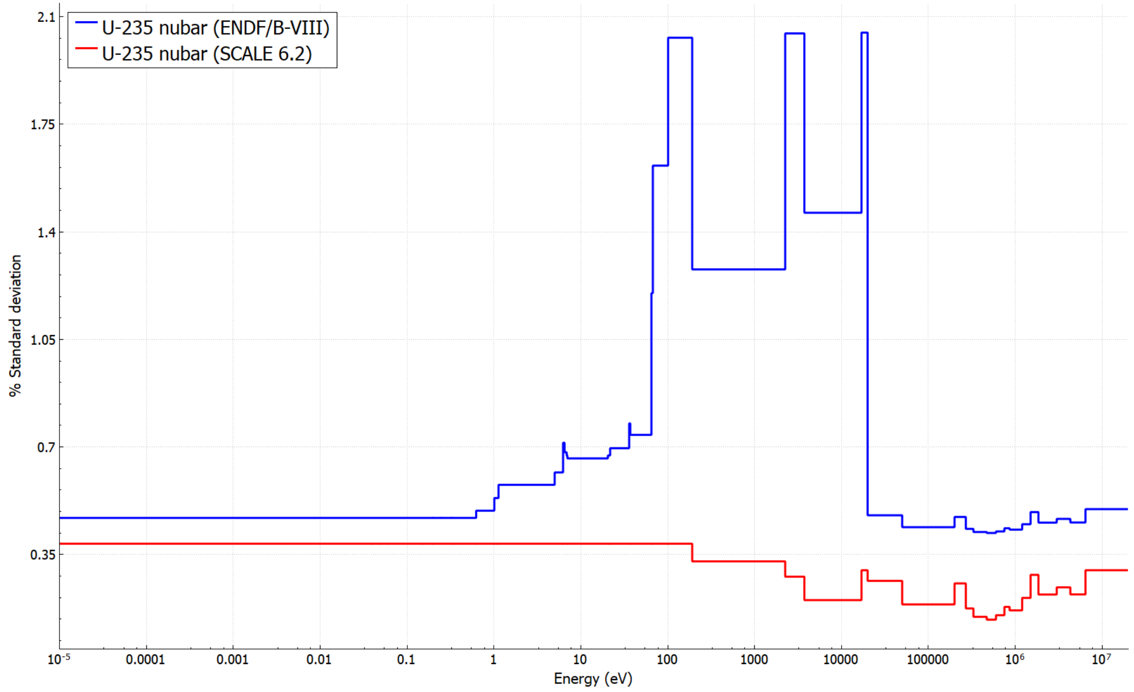

Na-23
elastic scattering
inelastic scattering
48
40
32
24
16
8
0
% Standard deviation
10-5 0.0001 0.001 0.01 0.1 1 10¹ 10² 10³ 10⁴ 10⁵ 10⁶ 10⁷
Energy (eV)

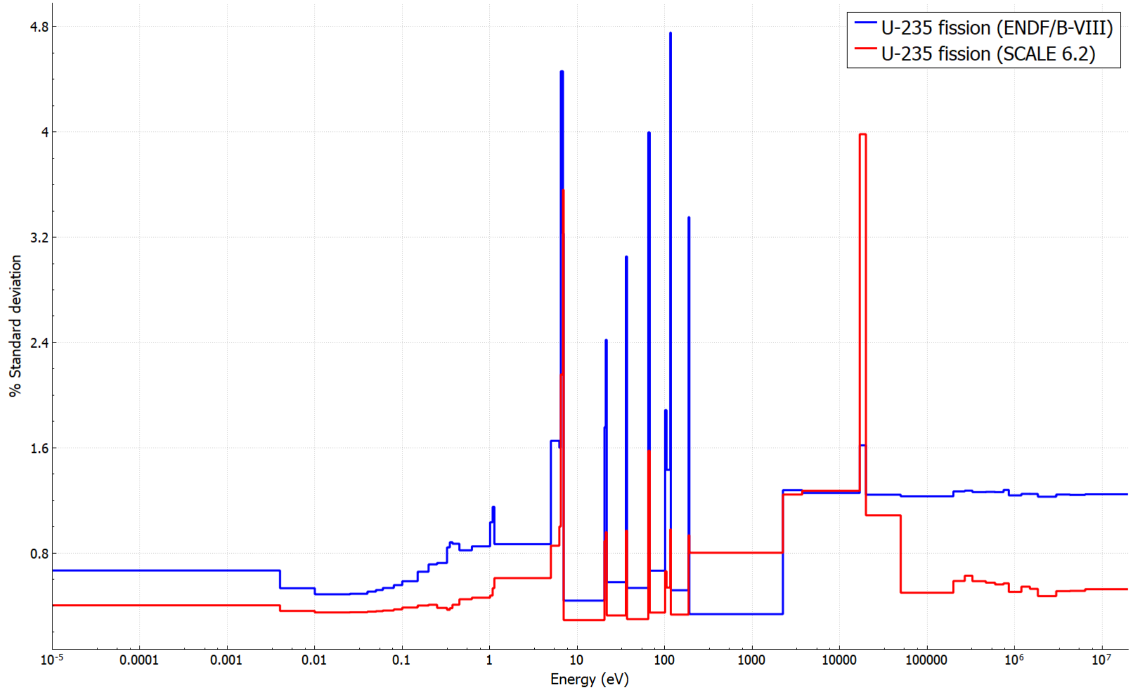

Fe-56
elastic scattering
inelastic scattering
% Standard deviation
18
15
12
9
6
3
0
10-5
0.0001
0.001
0.01
0.1
1
10¹
10²
10³
10⁴
10⁵
10⁶
10⁷
Energy (eV)

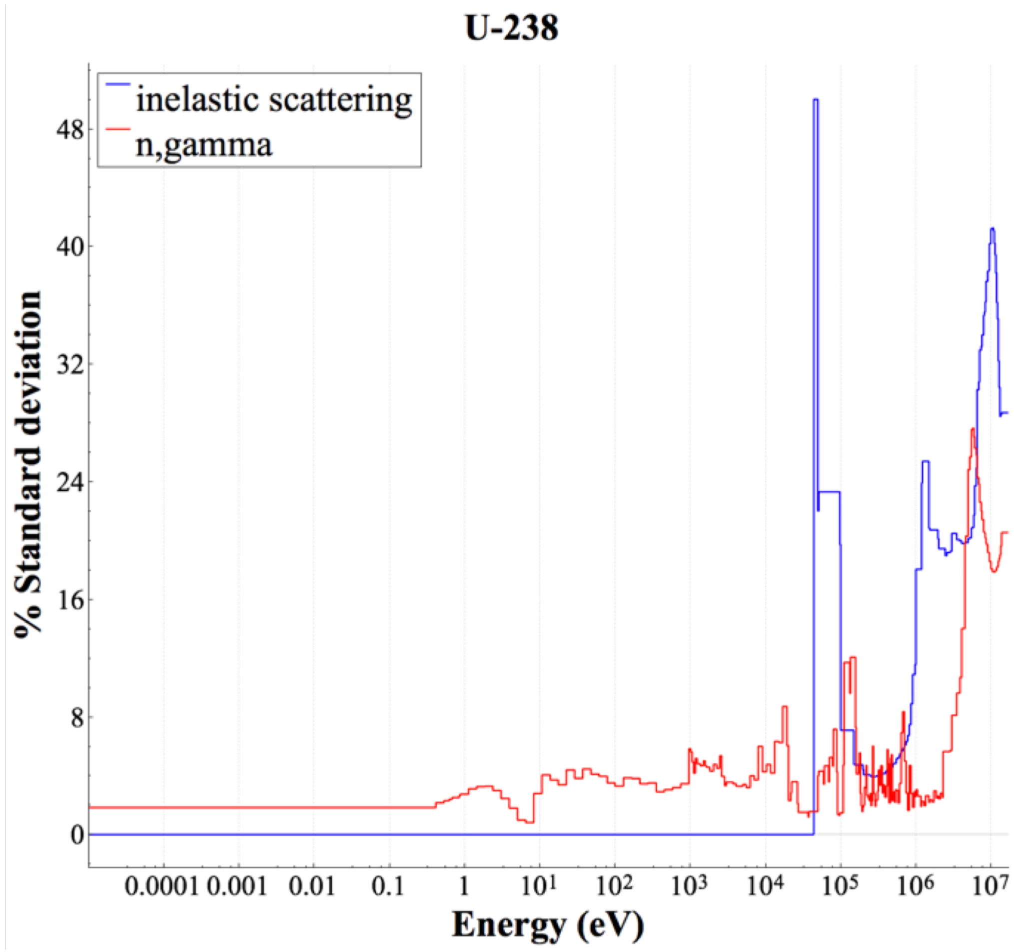


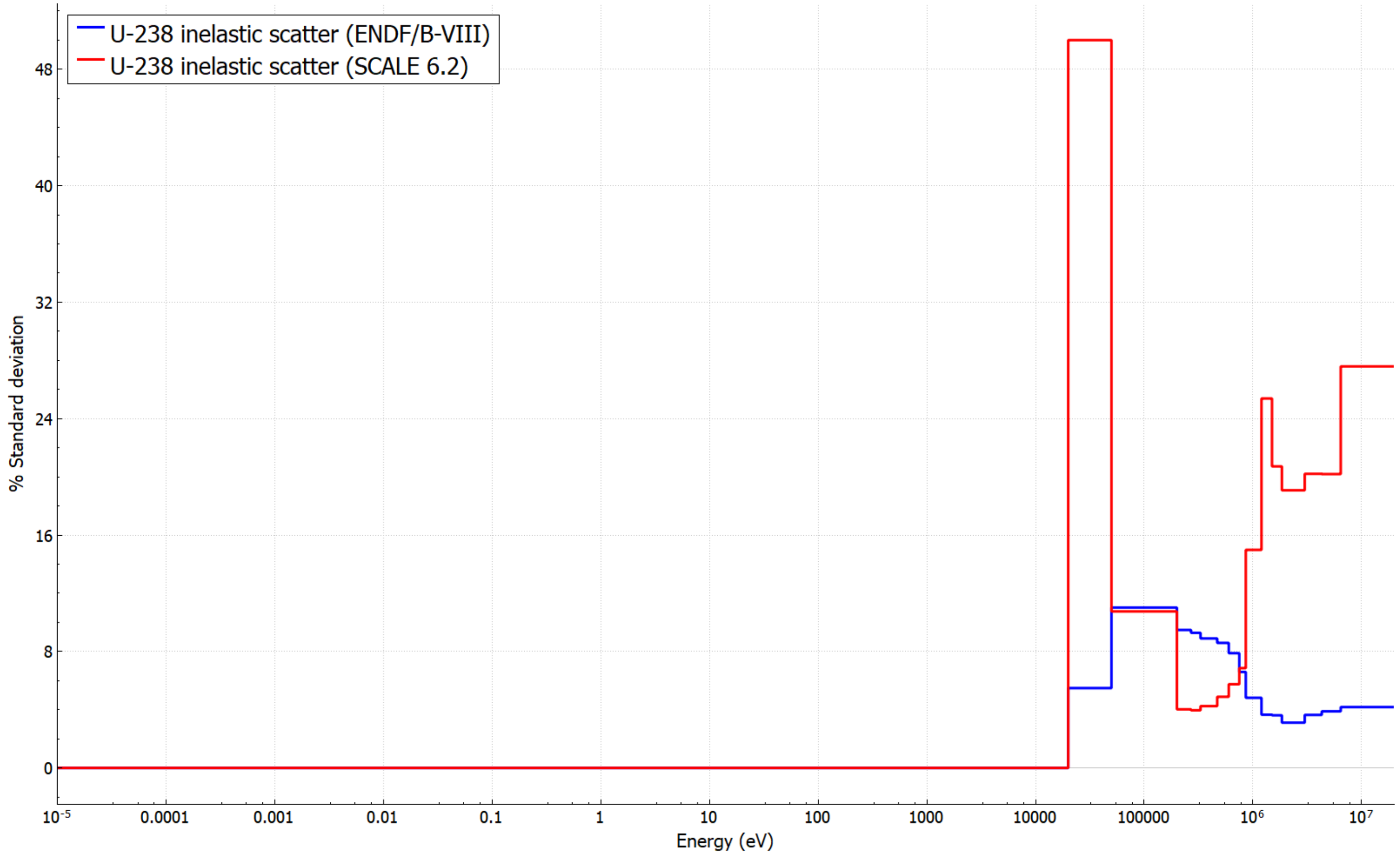
Zr-91 n,gamma
Zr-92 n,gamma
% Standard deviation
10
20
30
40
50
60
70
80
10-5 0.0001 0.001 0.01 0.1 1 10¹ 10² 10³ 10⁴ 10⁵ 10⁶ 10⁷
Energy (eV)

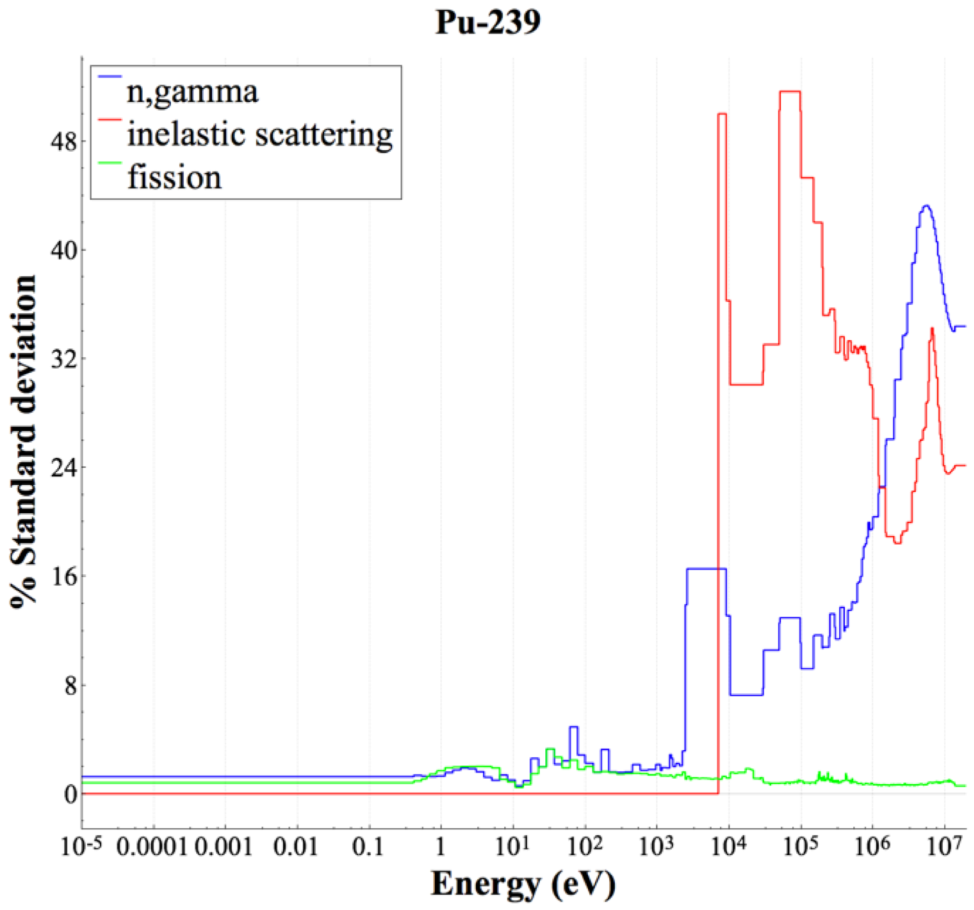

U-235
n,gamma
nubar
% Standard deviation
Energy (eV)

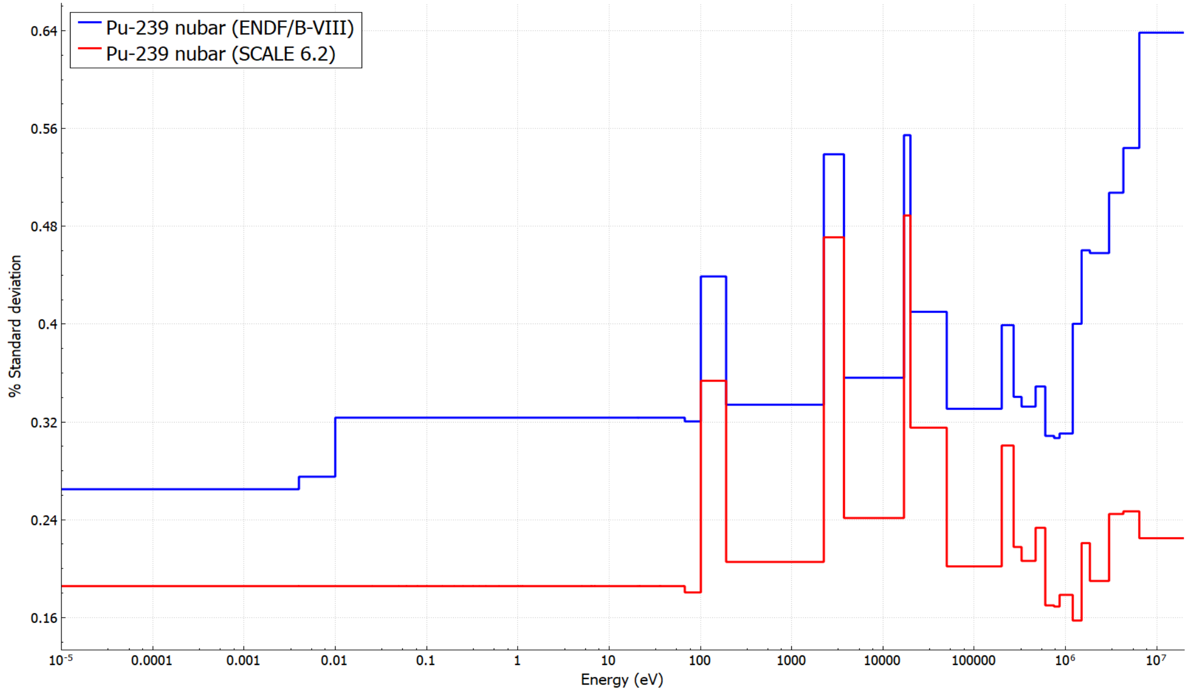

U-235 nubar (ENDF/B-VIII)
U-235 nubar (SCALE 6.2)
% Standard deviation
Energy (eV)

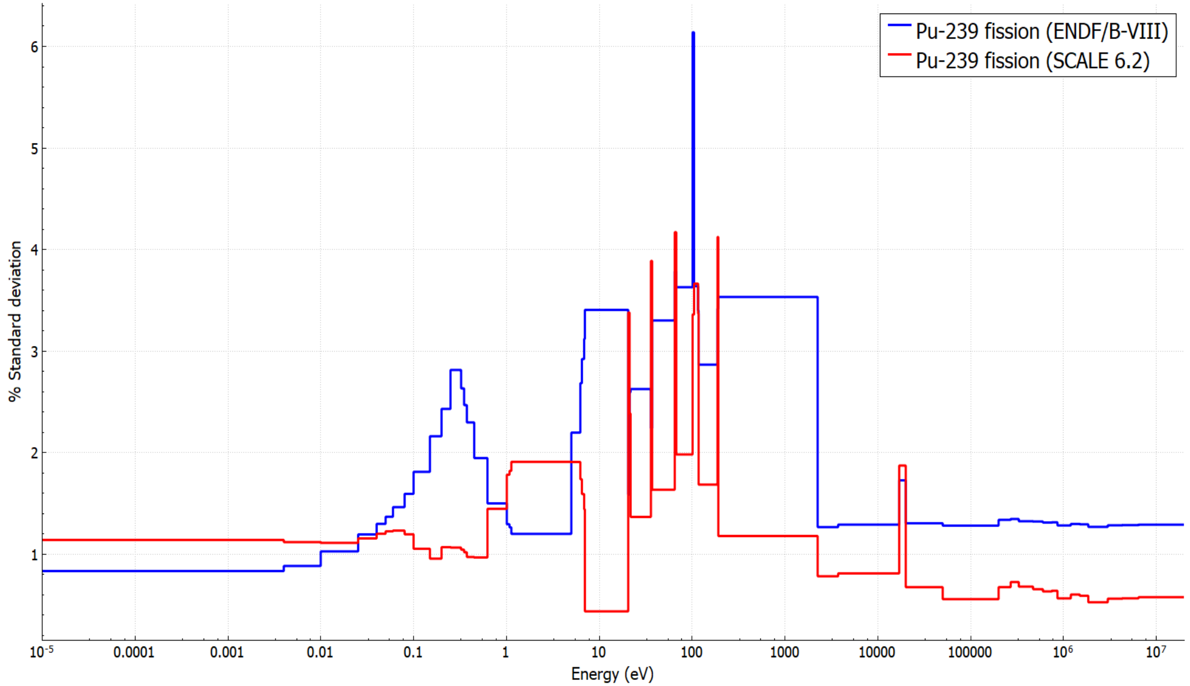

U-235 fission (ENDF/B-VIII)
U-235 fission (SCALE 6.2)
% Standard deviation
Energy (eV)


U-238
inelastic scattering
n,gamma
% Standard deviation
0
8
16
24
32
40
48
0.0001 0.001 0.01 0.1 1 10¹ 10² 10³ 10⁴ 10⁵ 10⁶ 10⁷
Energy (eV)


U-238 inelastic scatter (ENDF/B-VIII)
U-238 inelastic scatter (SCALE 6.2)
% Standard deviation
0
8
16
24
32
40
48
10⁻⁵ 0.0001 0.001 0.01 0.1 1 10 100 1000 10000 100000 10⁶ 10⁷
Energy (eV)


Pu-239
n,gamma
inelastic scattering
fission
% Standard deviation
Energy (eV)


Pu-239 nubar (ENDF/B-VIII)
Pu-239 nubar (SCALE 6.2)
% Standard deviation
Energy (eV)


Pu-239 fission (ENDF/B-VIII)
Pu-239 fission (SCALE 6.2)
% Standard deviation
Energy (eV)

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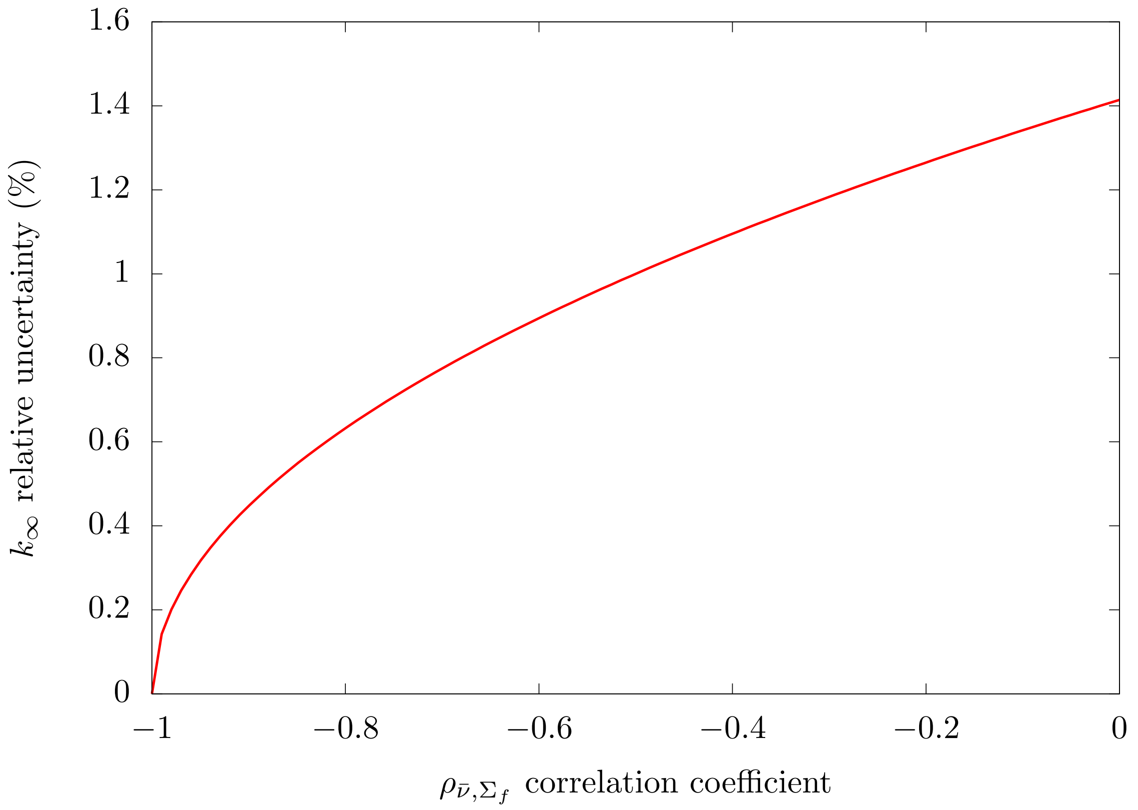
Have your cake and eat it too: solving the discrepancy with nuclear data correlations

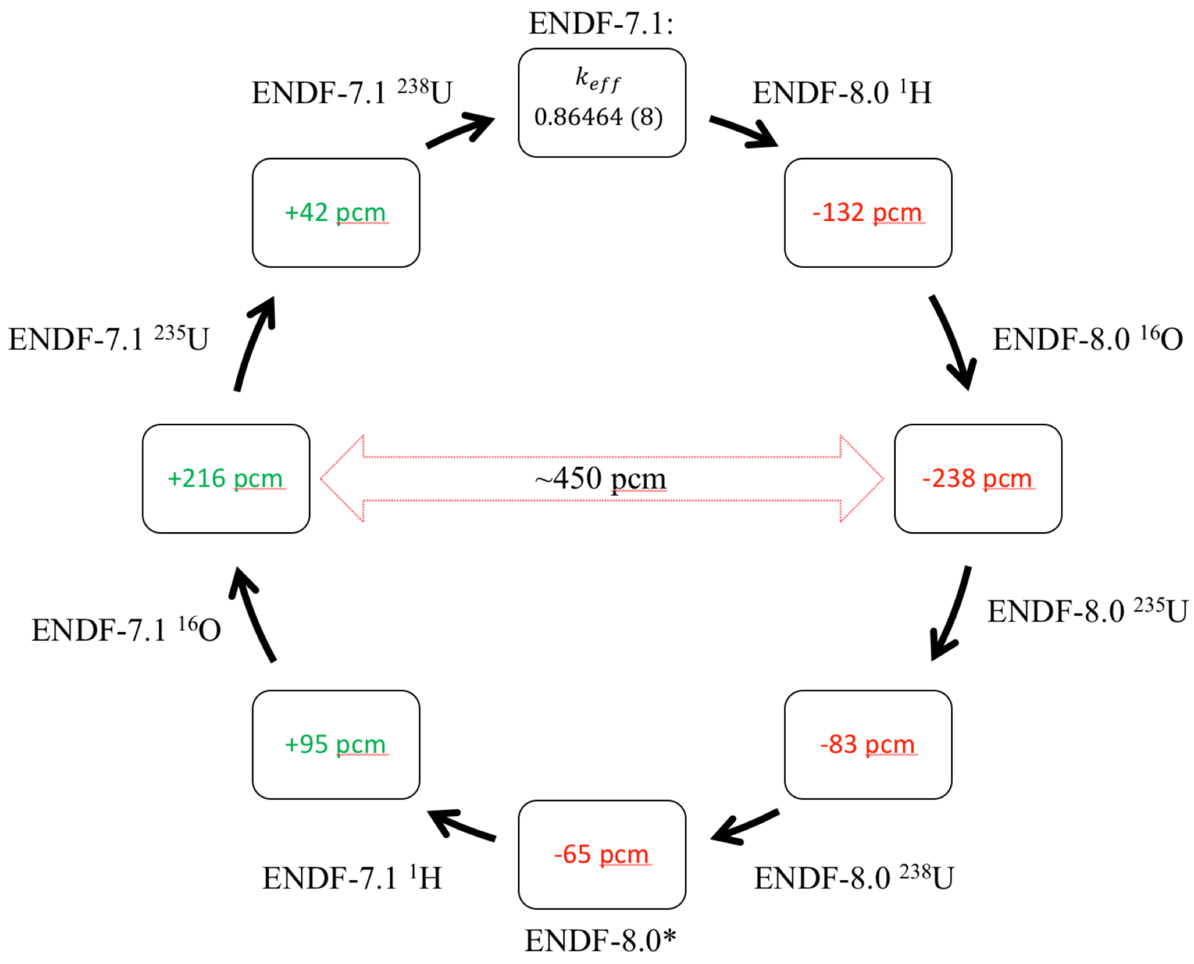
- A negative correlation coefficient between multiplicative terms allows you to keep realistic uncertainties for differential nuclear data which will propagate to realistic uncertainties on integral applications.

- Example:

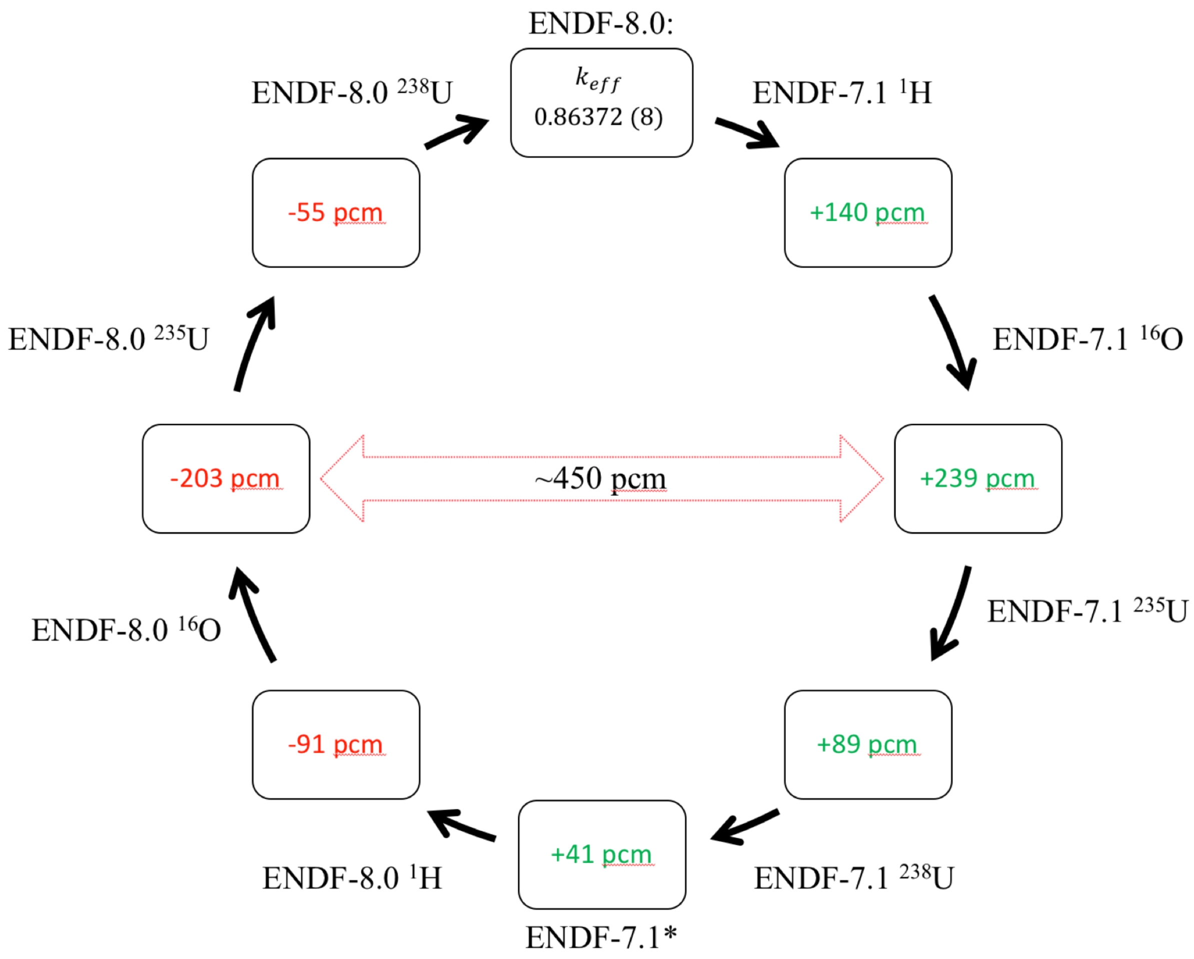
$$k_\infty = \frac{\bar{\nu}\,\Sigma_f}{\Sigma_a}, \qquad \frac{\delta\bar{\nu}}{\bar{\nu}} = 1\%, \qquad \frac{\delta\Sigma_f}{\Sigma_f} = 1\%$$



$$\frac{\delta k_\infty}{k_\infty} = \sqrt{\left(\frac{\delta\bar{\nu}}{\bar{\nu}}\right)^2 + \left(\frac{\delta\Sigma_f}{\Sigma_f}\right)^2 - 2\rho_{\bar{\nu},\Sigma_f}\left(\frac{\delta\bar{\nu}}{\bar{\nu}}\right)\left(\frac{\delta\Sigma_f}{\Sigma_f}\right)}$$



ENDF-7.1:
k_{eff}
0.86464 (8)
ENDF-8.0 ^{1}H
-132 pcm
ENDF-8.0 ^{16}O
-238 pcm
ENDF-8.0 ^{235}U
-83 pcm
ENDF-8.0 ^{238}U
-65 pcm
ENDF-8.0*
ENDF-7.1 ^{1}H
+95 pcm
ENDF-7.1 ^{16}O
+216 pcm
ENDF-7.1 ^{235}U
+42 pcm
ENDF-7.1 ^{238}U
~450 pcm



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