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Atoms for Peace and Development

Verification and Validation of the ENDF/B-VIII.b5 Library

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Overview

- Consistency with measured data and Standards
  - Should be done at the evaluation stage
- Formal file correctness
  - ENDF checking codes
- QA on data processing
  - Focusing on ACE libraries for MC
  - Heating
  - TSL processing
  - Covariance plotting
- Bechmarking for validation
  - ICSBEP, IRPhE, SINBAD, …

Consistency with measured data and Standards

- Tuning of model parameters to achieve consistency as much as possible
- Replacement of cross sections and covariances with Standards in the final evaluation

Formal file correctness

- Apply standard checking codes: CHECKR, FIZCON, PSYCHE
- Check basic processability with PrePro
- Check for processing anomalies when making ACE files (QA procedure)
- Plot covariances with NJOY

QA on data processing

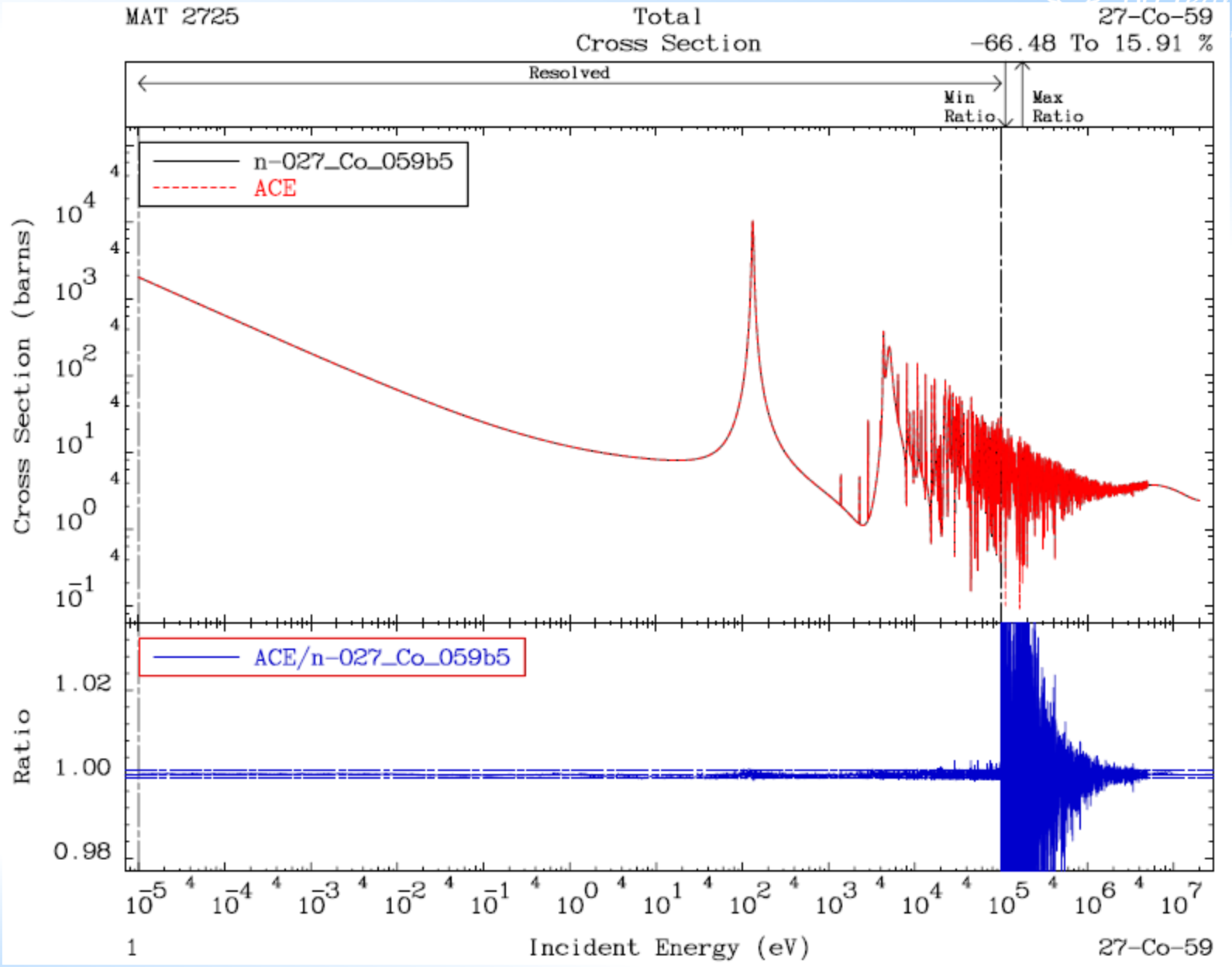
- Convert ACE back to ENDF (partial)
- Make equivalent PENDF with PrePro
- Compare converted ENDF with PENDF from PrePro using COMPLOT of PrePro

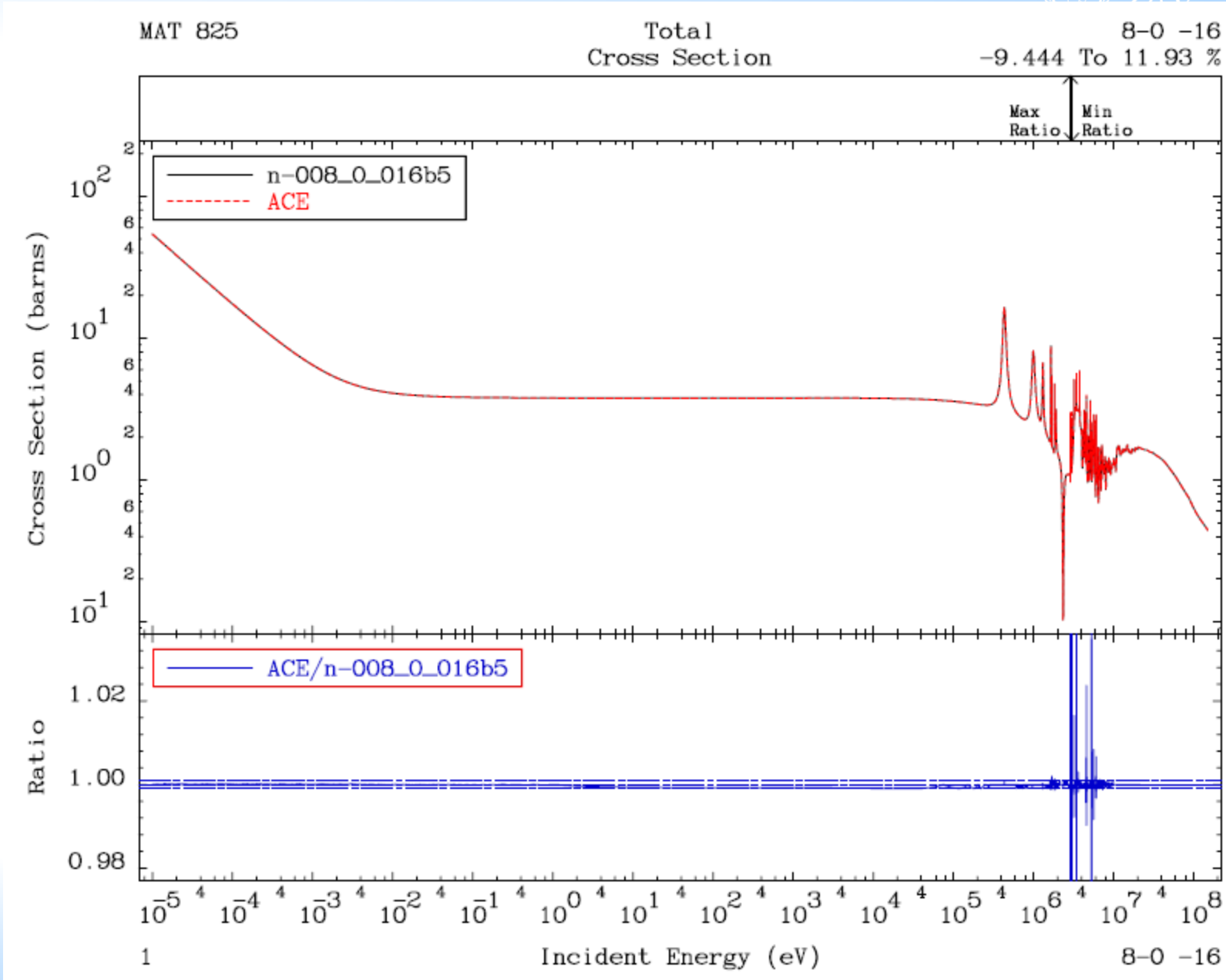
A number of problems were identified:

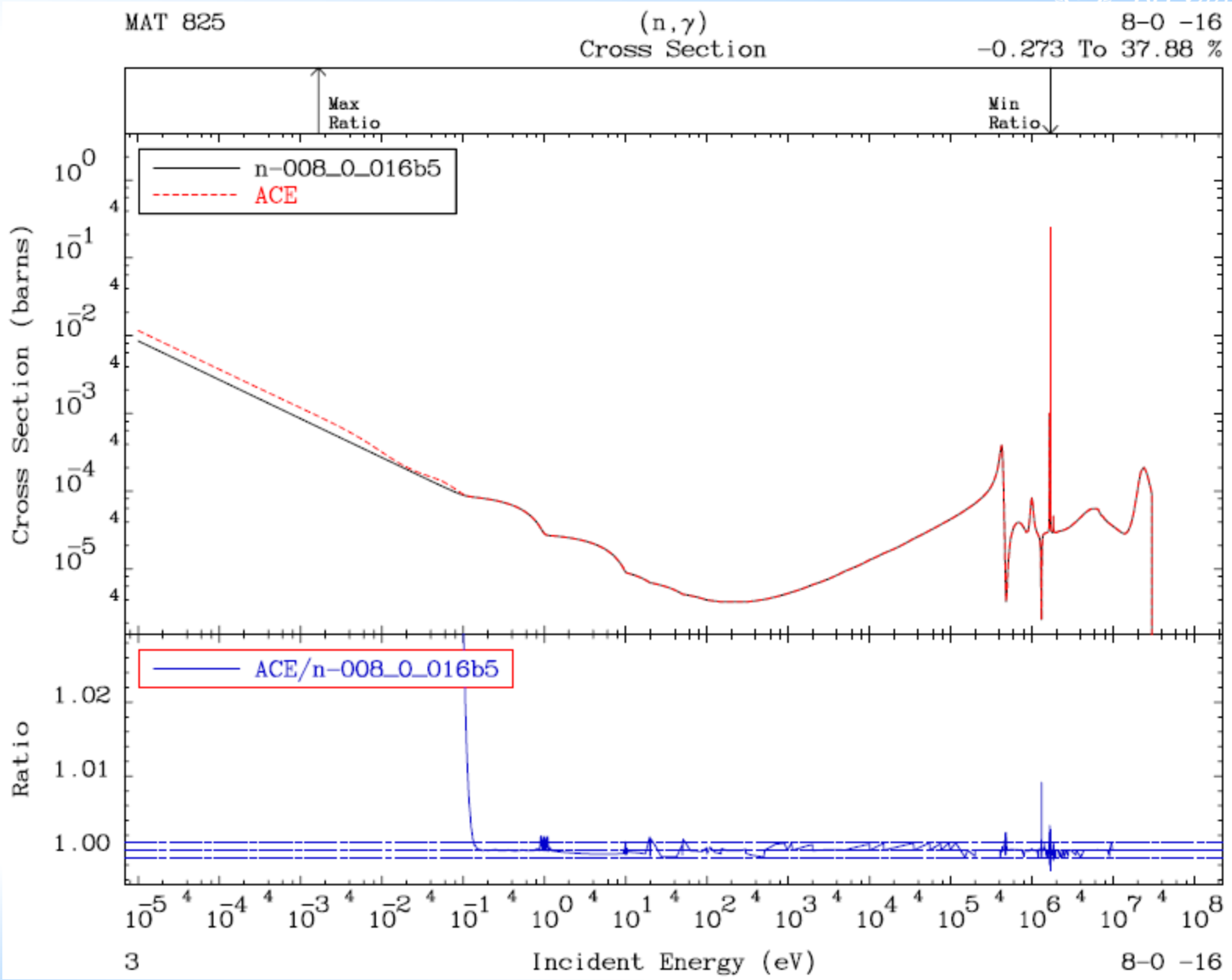
https://www-nds.iaea.org/CIELO/QA_Summary.html

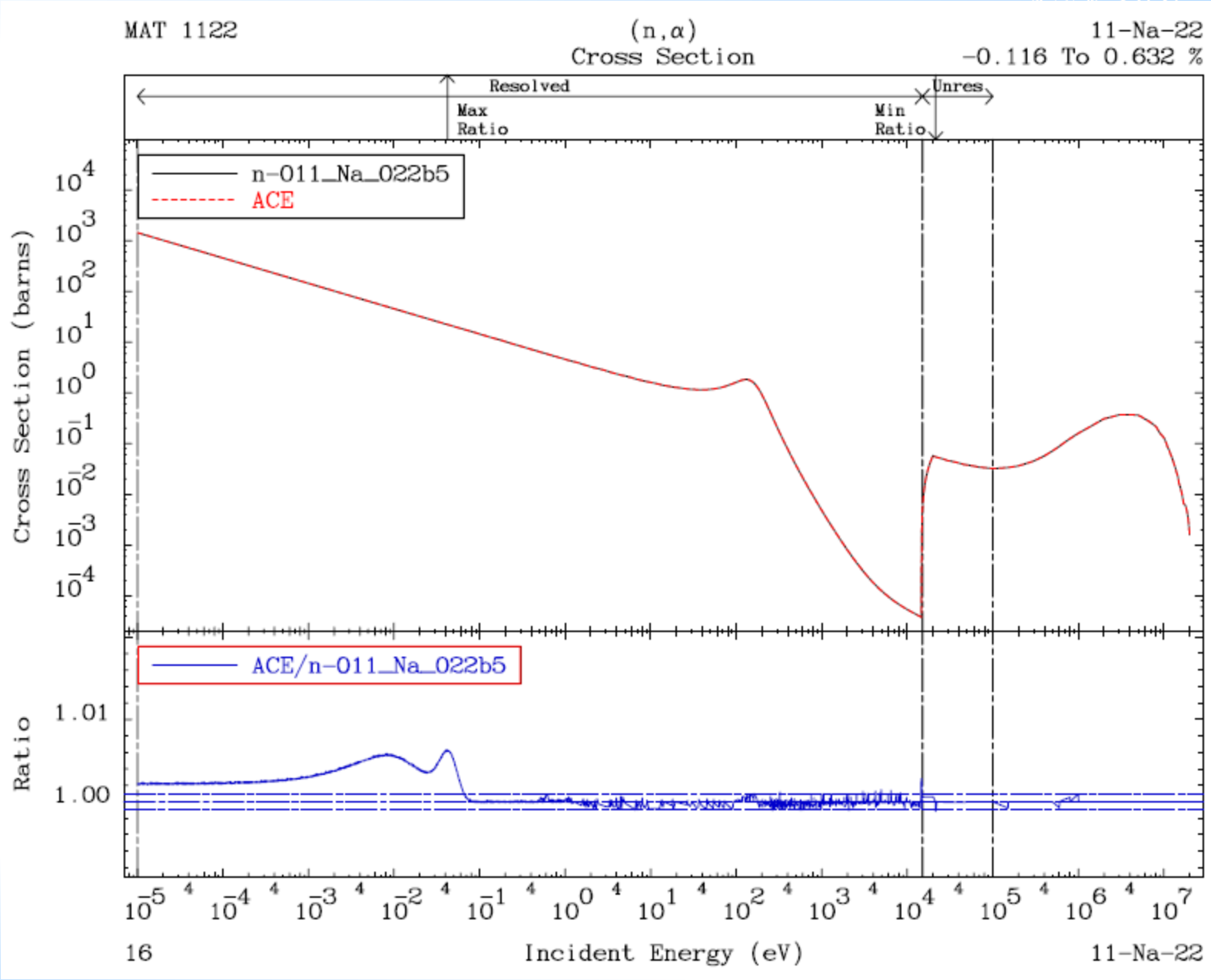
QA on data processing (Cont.)

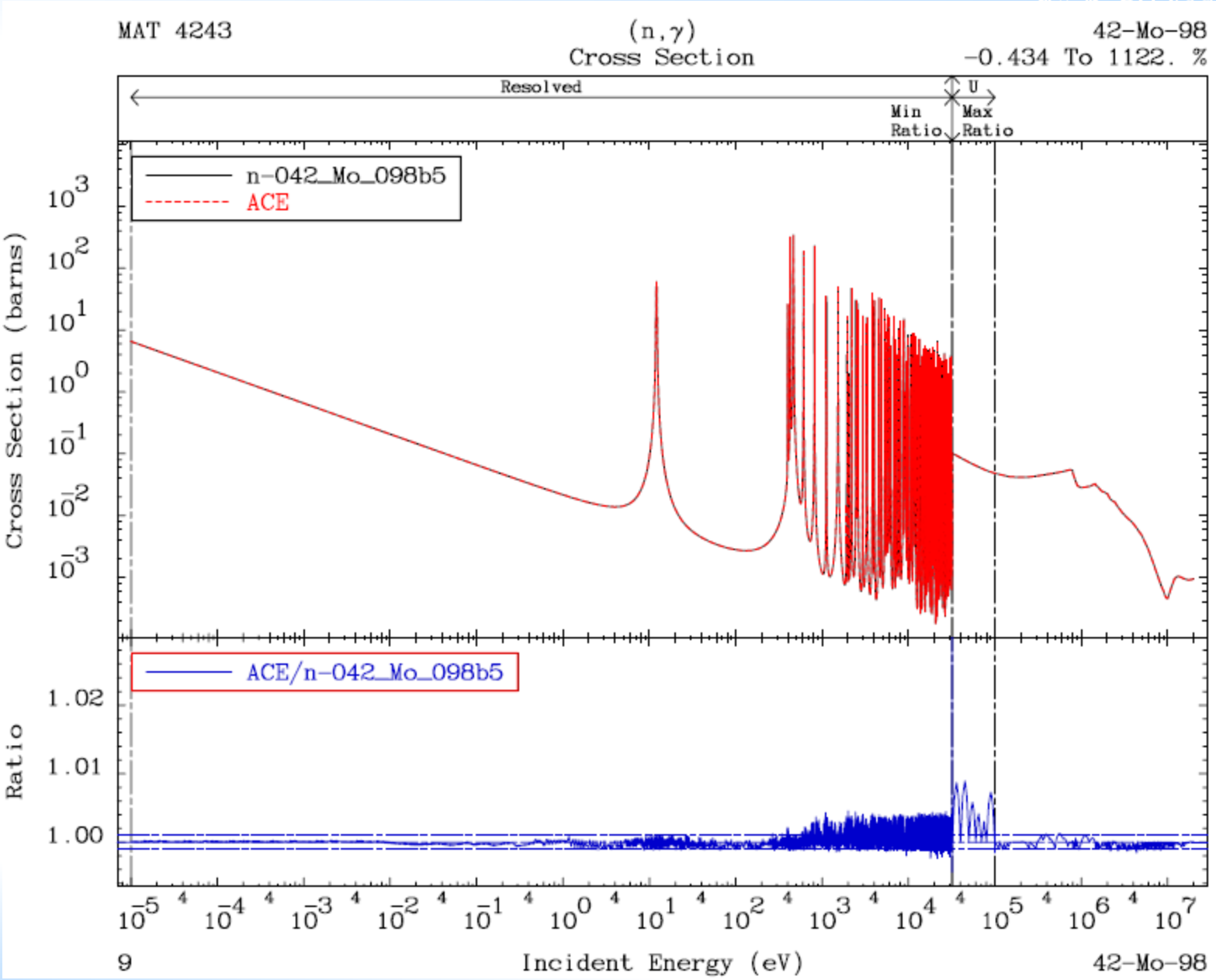
- PrePro and NJOY treat discontinuities differently (ignore)
- PrePro and NJOY use different criteria for the upper energy for Doppler broadening (ignore in most cases)
- Differences in the (minor) cross sections in the thermal range (criteria for Doppler broad.)
- Ripples and spikes in the unresolved resonance range (thinning criteria; URR interpolation still not precisely defined)


MAT 2725
Total
Cross Section
27-Co-59
-66.48 To 15.91 %
Resolved
Min Ratio
Max Ratio
n-027_Co_059b5
ACE
Cross Section (barns)
ACE/n-027_Co_059b5
Ratio
1.02
1.00
0.98
Incident Energy (eV)
27-Co-59


MAT 825
Total
Cross Section
8-0 -16
-9.444 To 11.93 %
Max Ratio
Min Ratio
n-008_0_016b5
ACE
Cross Section (barns)
ACE/n-008_0_016b5
Ratio
Incident Energy (eV)
8-0 -16


MAT 825
(n,γ)
Cross Section
8-0 -16
-0.273 To 37.88 %
Max Ratio
Min Ratio
n-008_0_016b5
ACE
Cross Section (barns)
ACE/n-008_0_016b5
Ratio
1.02
1.01
1.00
Incident Energy (eV)
3
8-0 -16


MAT 1122
(n,α)
Cross Section
11-Na-22
-0.116 To 0.632 %
Resolved
Unres
Max Ratio
Min Ratio
n-011_Na_022b5
ACE
Cross Section (barns)
ACE/n-011_Na_022b5
Ratio
1.01
1.00
Incident Energy (eV)
16
11-Na-22

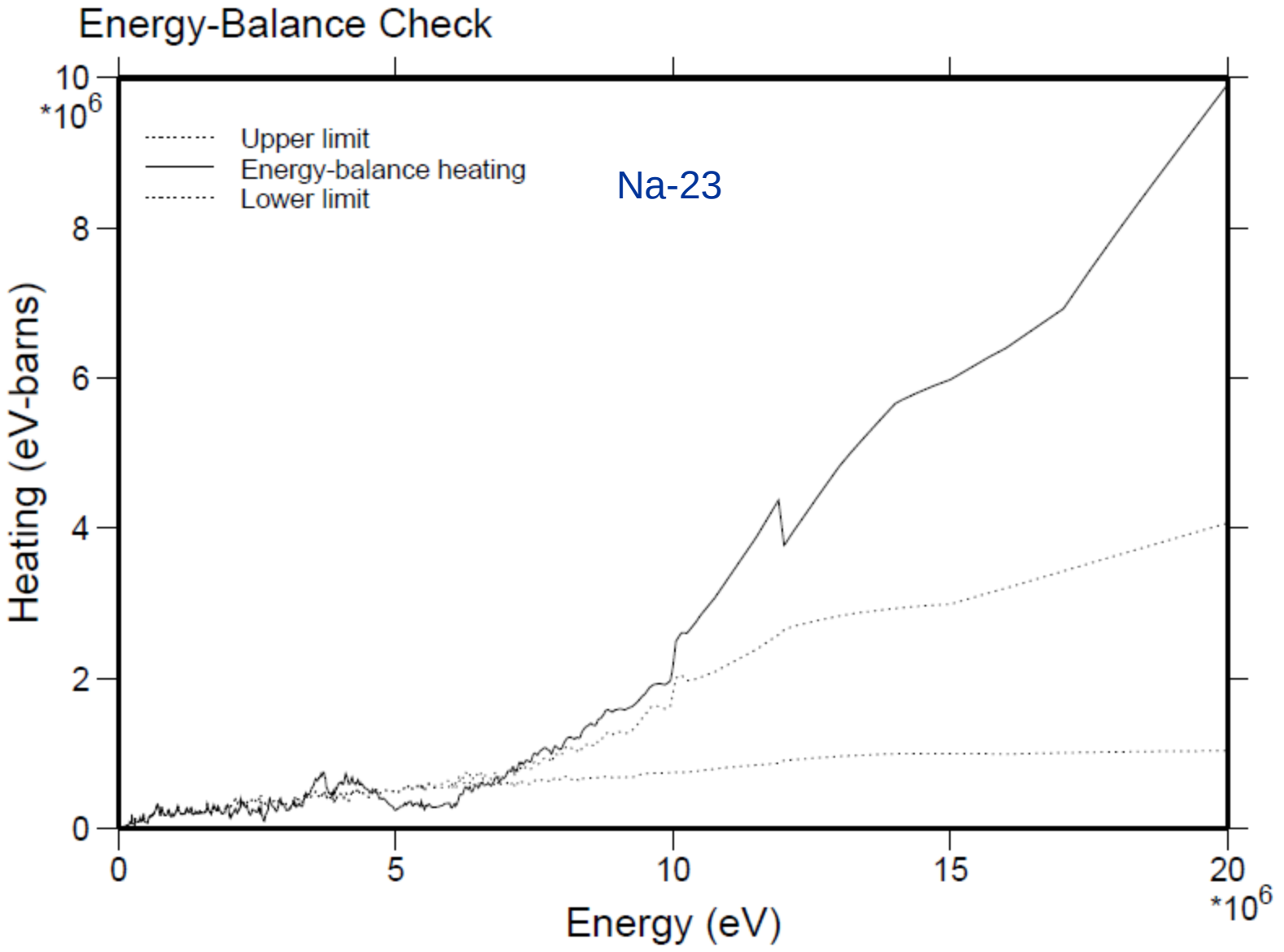

MAT 4243
(n,γ)
Cross Section
42-Mo-98
-0.434 To 1122. %
Resolved
U
Min Ratio
Max Ratio
n-042_Mo_098b5
ACE
Cross Section (barns)
ACE/n-042_Mo_098b5
Ratio
Incident Energy (eV)
9
42-Mo-98

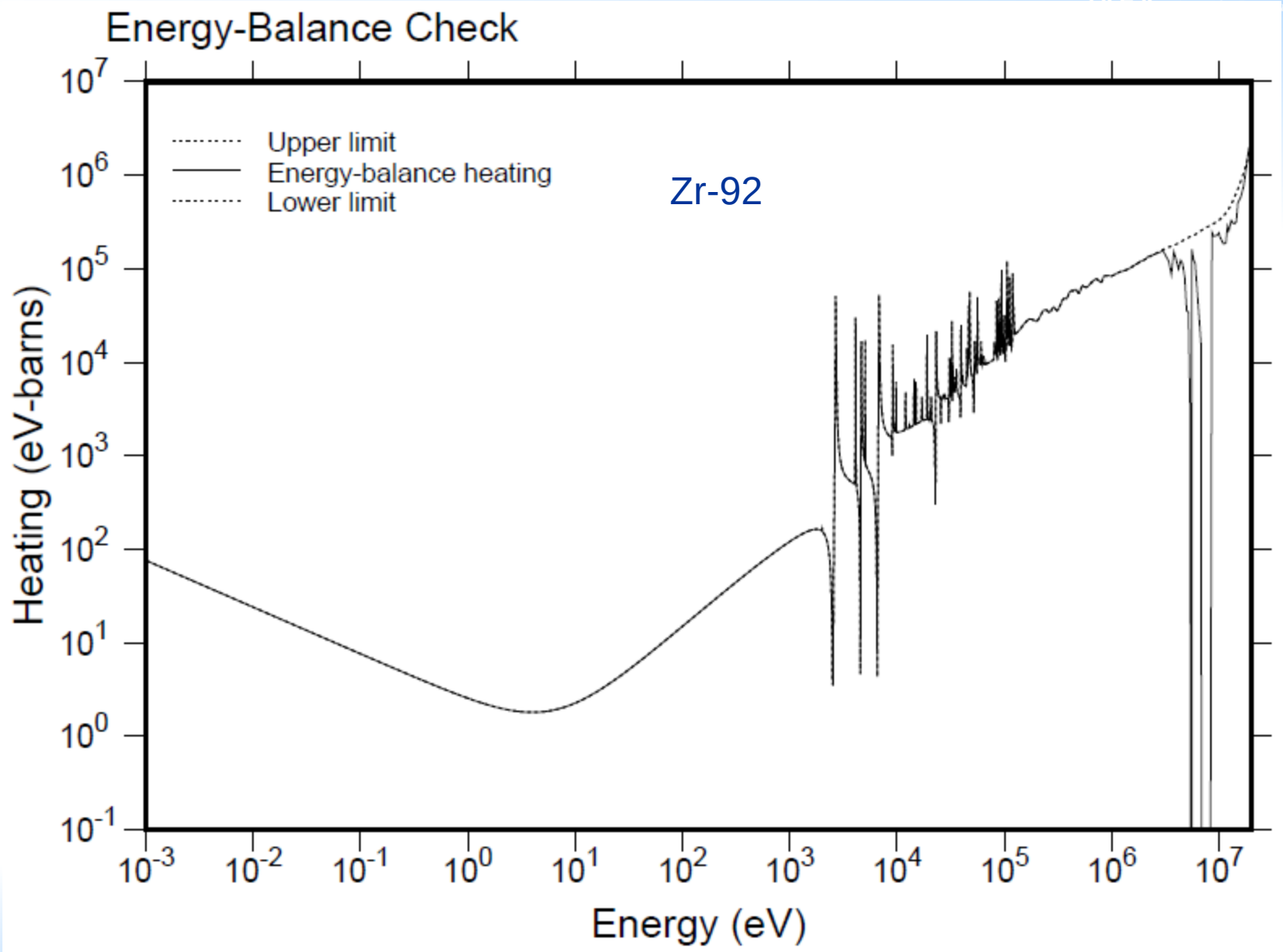
Heating

- Plots produced by HEATR were checked
  - Energy-balance heating is often outside the kinematic limits
  - Differences may amount to several orders of magnitude (no gamma-emission data?)
  - Most of the problems identified for ENDF/B-VII.1 http://t2.lanl.gov/nis/data/endf/ebalVII/summary.html remain in ENDF/B-VIII.

Full list of questionable cases in “beta5”:

https://www-nds.iaea.org/CIELO/Heating_Summary.html


Energy-Balance Check
Upper limit
Energy-balance heating
Lower limit
Na-23
Heating (eV-barns)
*10^6
10
8
6
4
2
0
0
5
10
15
20
*10^6
Energy (eV)


Energy-Balance Check
Upper limit
Energy-balance heating
Lower limit
Zr-92
Heating (eV-barns)
Energy (eV)
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7}

TSL processing

- Several warnings in THERMR about |cos|>1
  - Patched setting |cos|=1
- NJOY runs through, including ACER, but
- MCNP stops randomly with a message
  - Bad trouble … cos NaN
- Showstopper in producing reliable benchmark results

Covariance plotting

Processing issues:

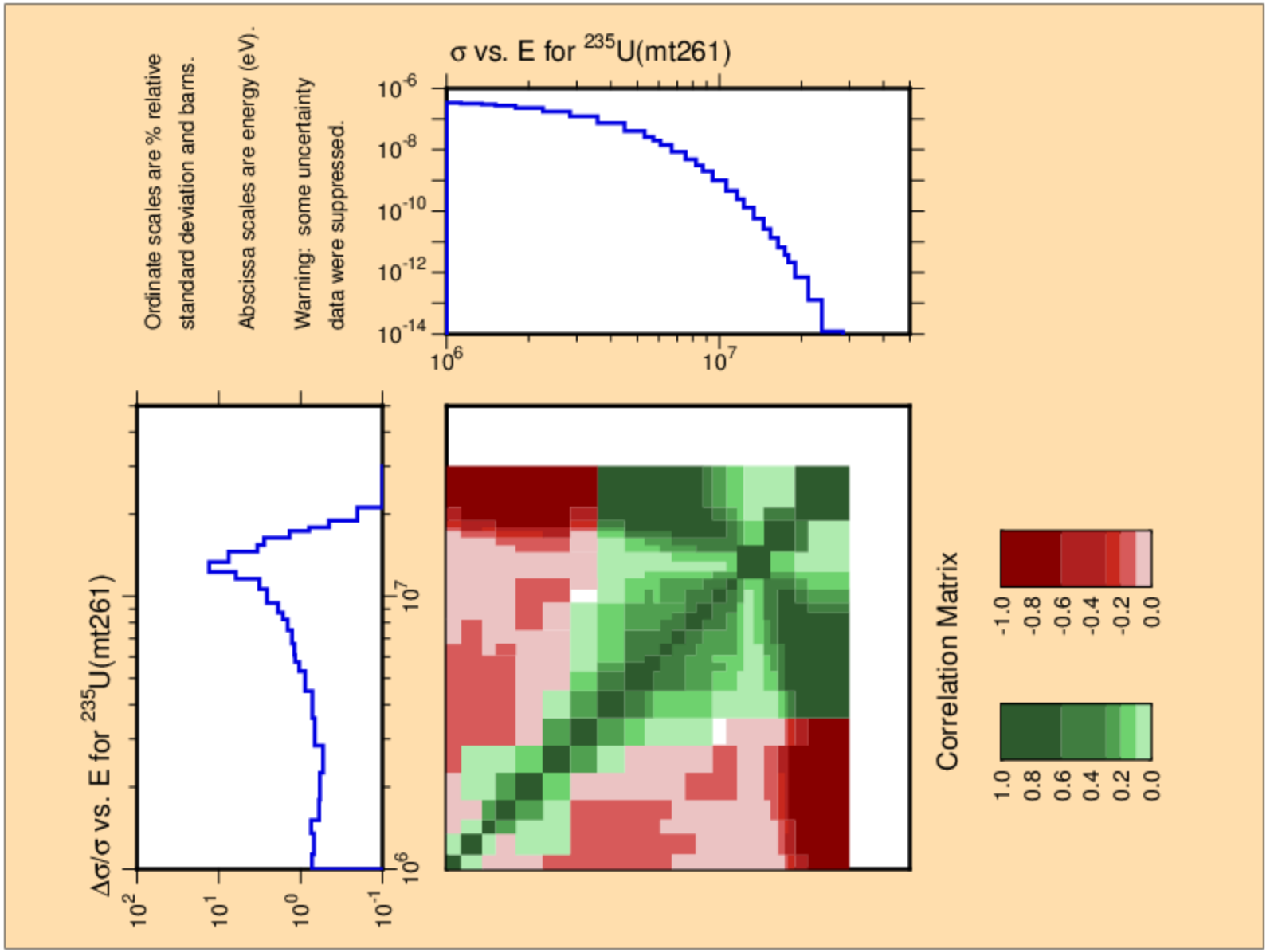
- Implementation of covariance processing of angular distributions is strictly limited to P_1(no correlations with P_0 allowed)
- ERRORR does not read binary ENDF on input
- At the high-energy end the processed covariance matrix is intuitively wrong

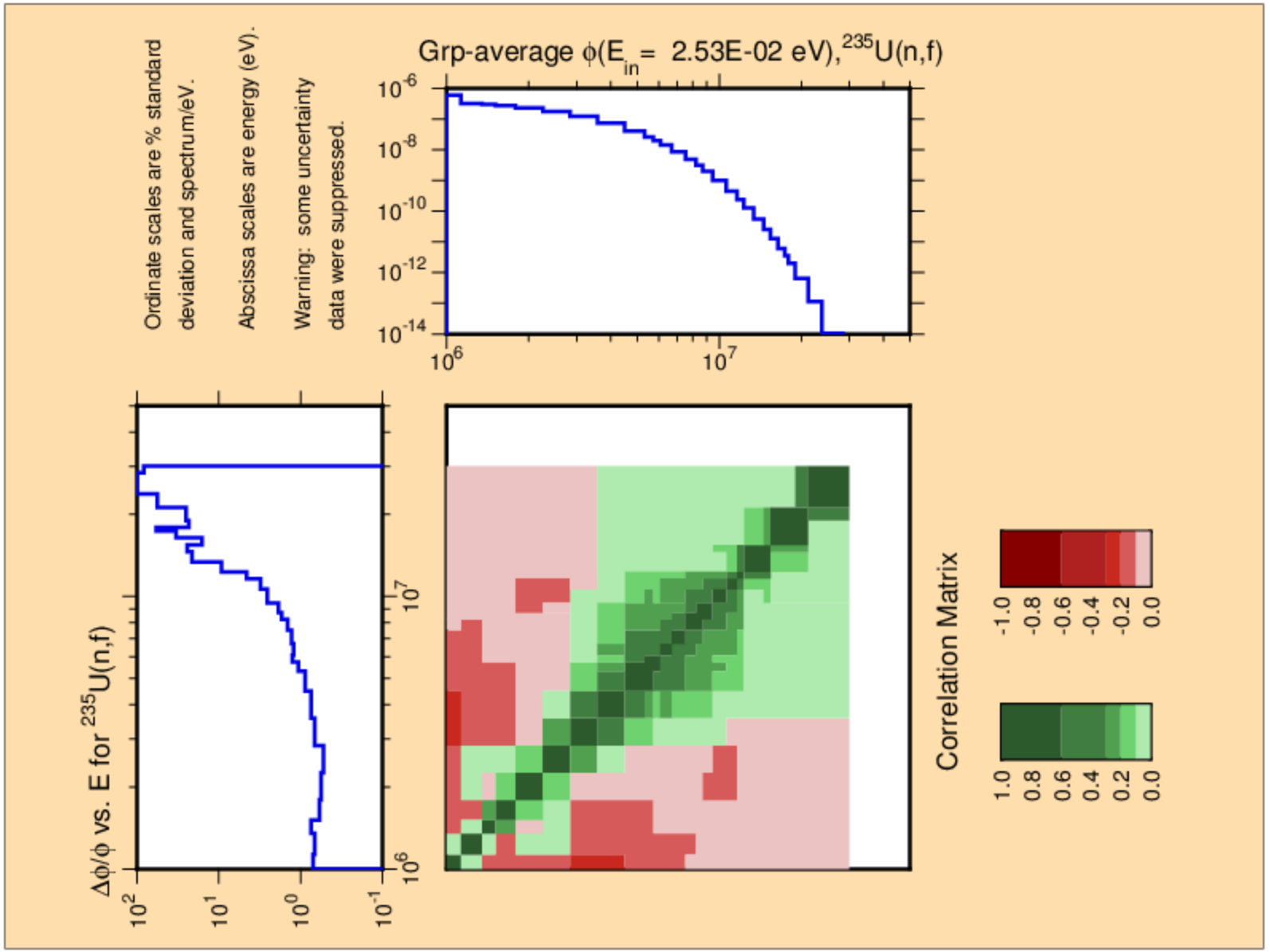
Covariance plotting (Cont.)

- Consider a quantity with a strong negative gradient, constant uncertainty 12% (12-15 MeV), 20% (15-20 MeV), 50% (>20 MeV)
  - Variance trend in MF 33 seems wrong
  - Opposite trend if MF 35, but this is due to group width (requires a dense covariance energy grid)

The full list of covariance plots is on

https://www-nds.iaea.org/CIELO/Covariance_Summary.html


σ vs. E for 235U(mt261)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
Δσ/σ vs. E for 235U(mt261)
Correlation Matrix
1.0
0.8
0.6
0.4
0.2
0.0
-1.0
-0.8
-0.6
-0.4
-0.2
0.0


Grp-average φ(E_in = 2.53E-02 eV), ^235U(n,f)
Ordinate scales are % standard deviation and spectrum/eV.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
Δφ/φ vs. E for ^235U(n,f)
Correlation Matrix

Processing issues to be addressed

- Checking THERMR (cos > 1) and ACER to track down the cause of “bad trouble” in MCNP (show-stopper for reliable benchmarking)
- Processing of P_l covariance data
- Checking the high-energy part of the cross section covariances

The full list of files/plots from processing is on

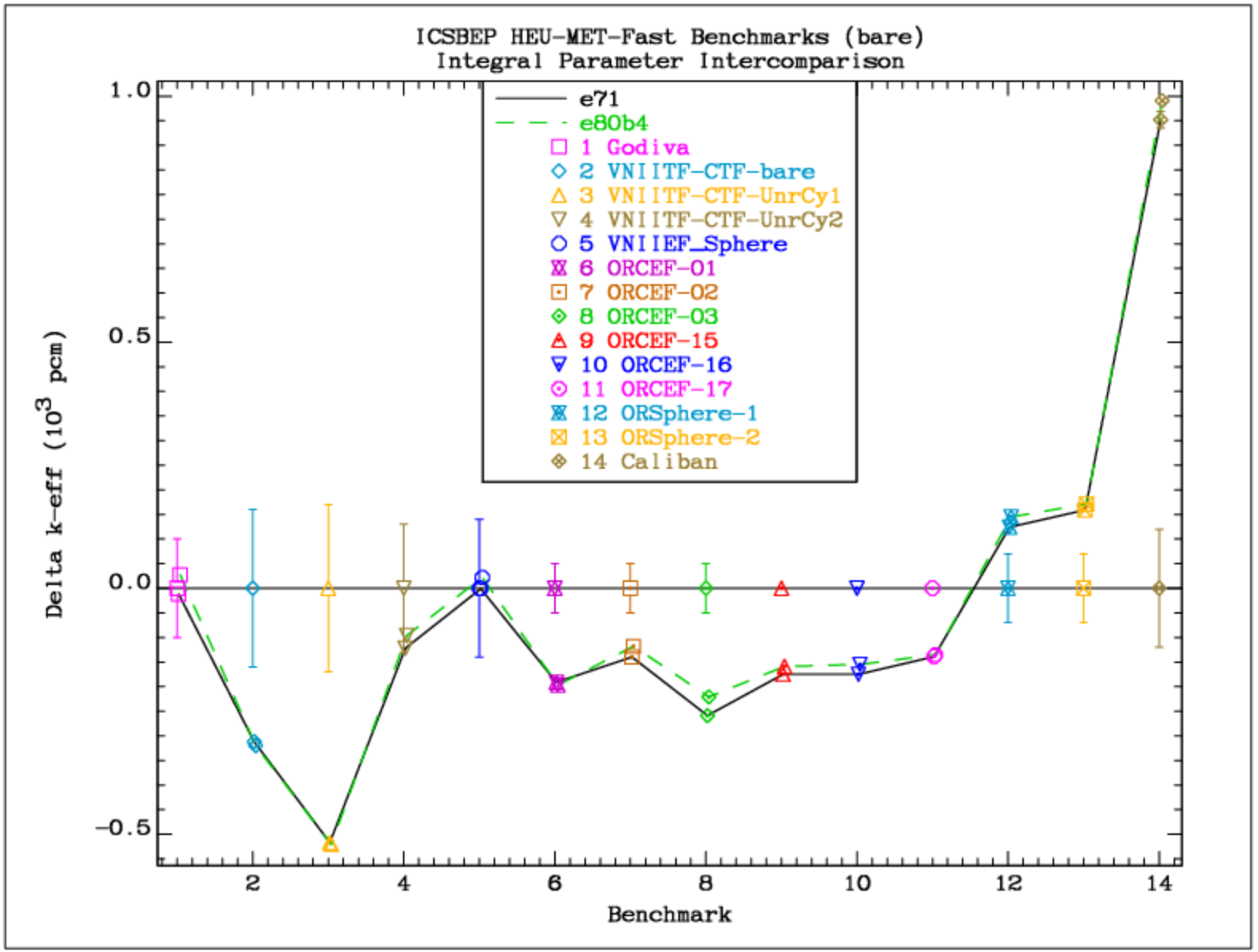
https://www-nds.iaea.org/CIELO/e80b5_list.html

Benchmarking

Validation requires reliable benchmarks

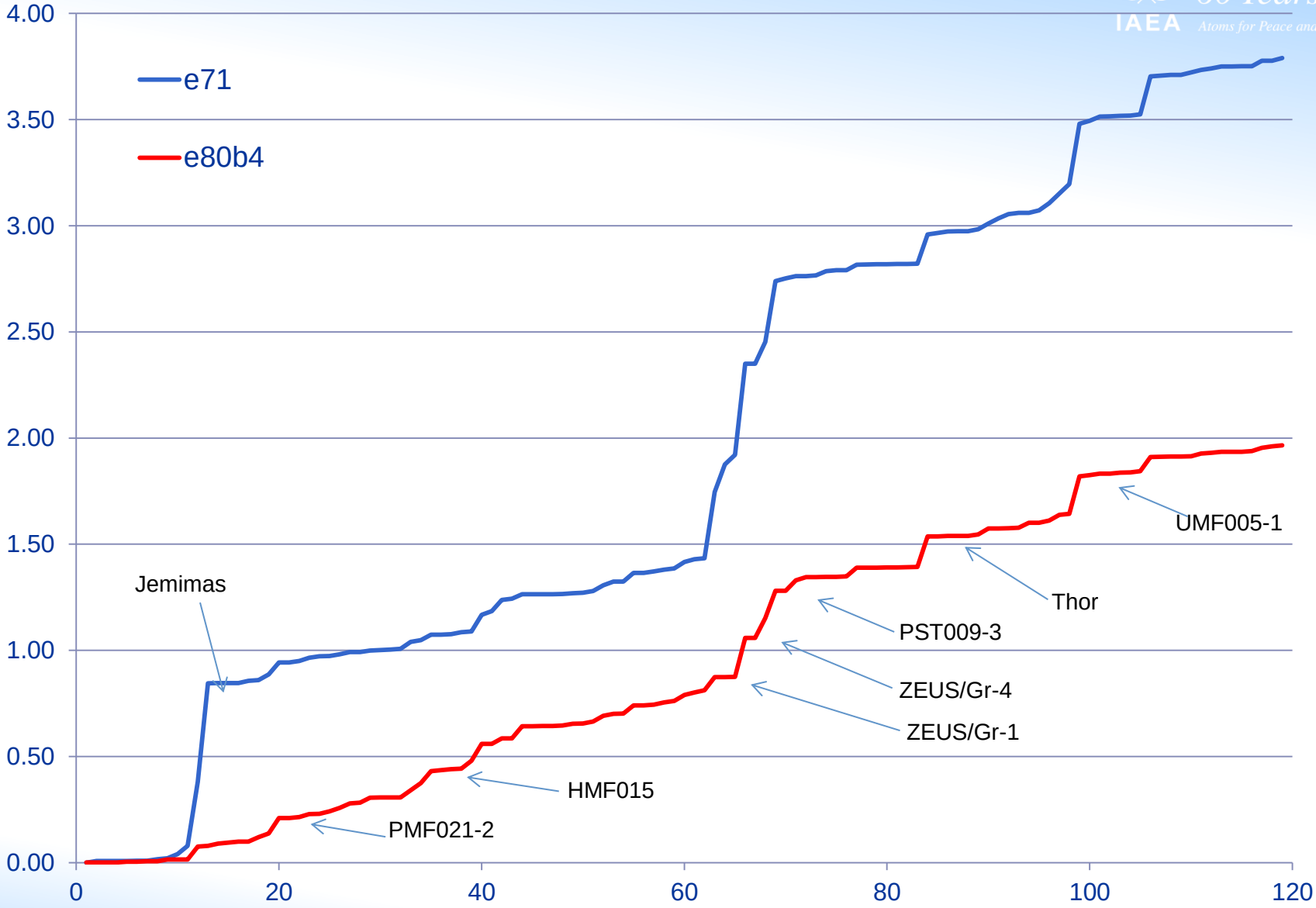
- ICSBEP – example of bare spheres:
  - Sensitivity mainly to U-235
  - Sensitivity profiles practically equal
  - Benchmark uncertainty ~200 pcm
  - Spread in results ~1500 pcm

No response so far from France, Russia, ORNL ?


ICSBEP HEU-MET-Fast Benchmarks (bare)
Integral Parameter Intercomparison
e71
e80b4
1 Godiva
2 VNIITF-CTF-bare
3 VNIITF-CTF-UnrCy1
4 VNIITF-CTF-UnrCy2
5 VNIIEF_Sphere
6 ORCEF-01
7 ORCEF-02
8 ORCEF-03
9 ORCEF-15
10 ORCEF-16
11 ORCEF-17
12 ORSphere-1
13 ORSphere-2
14 Caliban
Delta k-eff (10^3 pcm)
1.0
0.5
0.0
-0.5
2
4
6
8
10
12
14
Benchmark

Nevertheless…

- Progress was made in library performance on criticality benchmarks
- Several compensating errors were identified and eliminated
- Practically no compromises were made regarding differential data, Standards were observed
- Significant improvement was made in the quality of covariance information


4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
0
20
40
60
80
100
120
e71
e80b4
Jemimas
PMF021-2
HMF015
ZEUS/Gr-1
ZEUS/Gr-4
PST009-3
Thor
UMF005-1

Conclusions

- Library performance is not easily quantifiable
- It depends on:
  - Evaluators' skills, modelling tools, availability of high-quality experimental data
  - Robust and reliable processing tools
  - Robust and reliable analysis tools
  - Reliable clean integral benchmarks.

In all of these there is room for improvement

https://www-nds.iaea.org/CIELO/QA_Summary.html
https://www-nds.iaea.org/CIELO/Heating_Summary.html
https://www-nds.iaea.org/CIELO/e80b5_list.html