

AFCI-2.0 β Covariance Library

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Outline

- Purpose of library: Data Adjustment
- Overview of AFCI 2.0 β library
- Additions and changes
- Quality Assurance (QA)

1: Purpose

- Provide neutron cross-section covariances for 110 materials relevant to fast reactor R&D:
 - 12 light nuclei (LANL)
 - 78 structural materials (BNL)
 - 20 (major and minor) actinides (LANL + BNL)
- Library coupled to ENDF/B-VII.0 central values for cross sections
- AFCI covariances to be adopted for ENDF/B-VII.1

AFCI Data Adjustment Requirements

- Requires neutron cross sections (ENDF/B-VII.0 based) with associated covariances
- Prefer multigroup (processed) covariances with uniform lethargy energy groups (33 group, 1/E flux)
- Reaction channels of interest: (n,el), (n,inl), (n,2n), (n, γ), (n,f), nubar. Also some mubar and prompt fission neutron spectra.

AFCI Methodology

Covariance evaluation methodology determined by priorities:

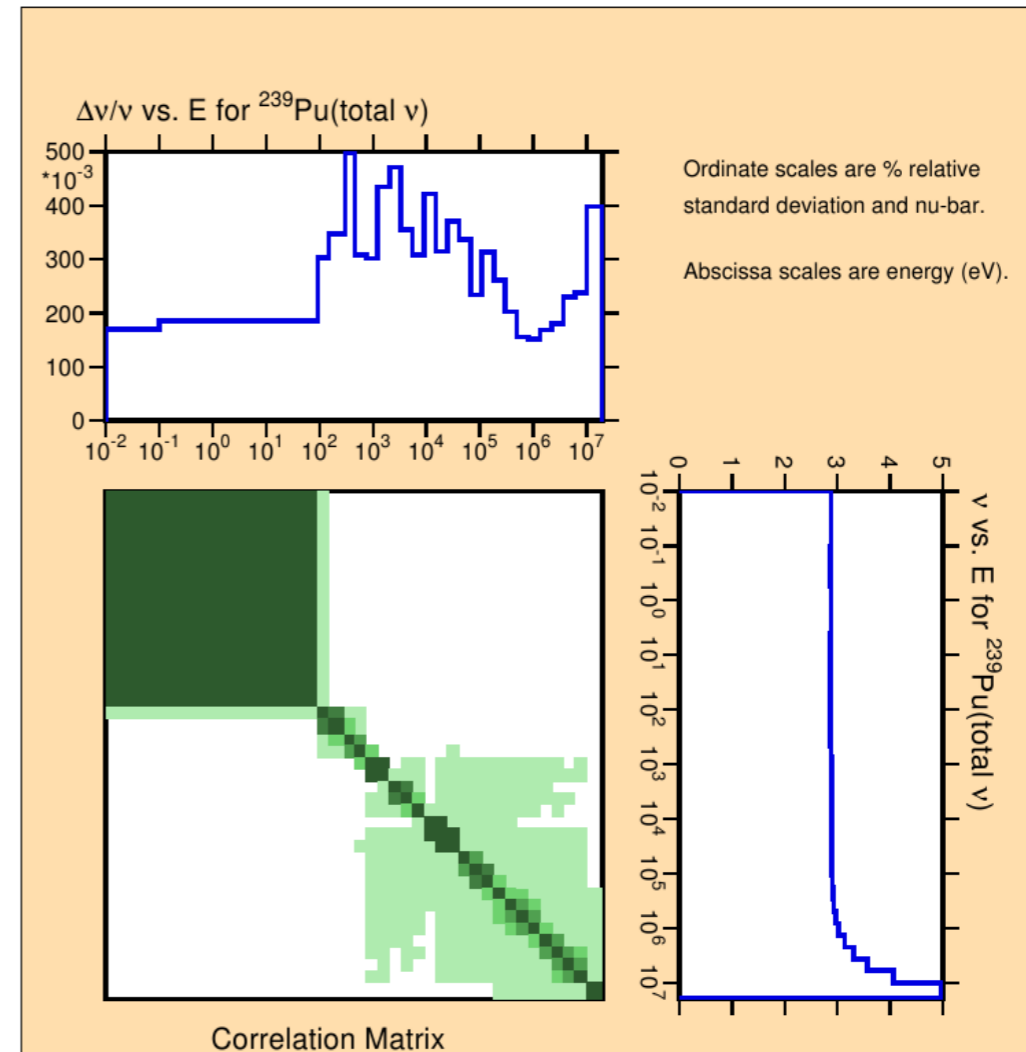
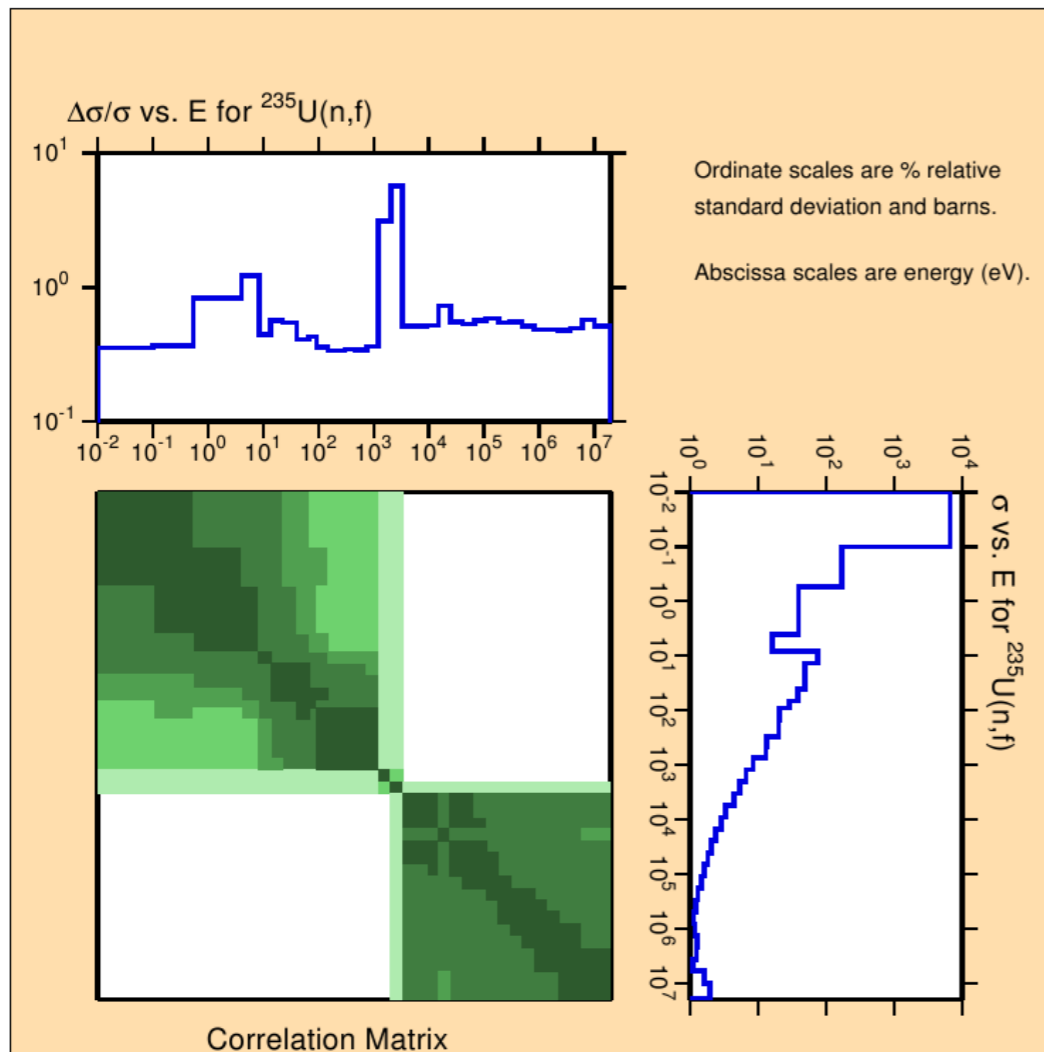
- Most important materials (~30) treated with sophisticated methods
- Medium importance materials (~40) treated with simplified methods
- Low priority materials (~40, mostly fission products) treated with low-fidelity type approach

Contents of Library

- Major Actinides produced by LANL/ORNL
 - $^{233,235,238}\text{U}$, ^{239}Pu – simultaneous evaluation
- Structural materials produced by BNL
 - ^{23}Na , ^{52}Cr , ^{56}Fe , ^{58}Ni , Pb, Bi, ...
- Light nuclei from LANL/ORNL (R-matrix, also low-fi)
- Minor Actinides partly based on V. Maslov estimates, partly on BNL and LANL efforts
- Fission products most based on low-fidelity covariances
- Mubar covariances for ^{23}Na , ^{56}Fe
- Prompt fission neutron spectra for $^{238,239,240}\text{Pu}$

33-group structure

- AFCI is a processed covariance library, using 33 energy bins.
- Group boundaries chosen so that in most cases, $\ln(E_2/E_1)=0.5$



AFCI library timeline

- Initial version under Global Nuclear Energy Partnership (GNEP) released Oct 2008
- Name changed to Advanced Fuel Cycle Initiative (AFCI) at version 1.2
- Ver. 1.3 release in Apr 2010 included many improved structural & actinide evaluations
- AFCI 2.0 β released Oct 2010, final release scheduled for Dec 2010

Key changes for AFCI-2.0 beta

- Many structural materials updated at NNDC using Kernel approach in RRR and Empire/Kalman approach in fast region
- New minor actinide evaluations from LANL ($^{238,239,240}\text{Pu}$, ^{241}Am)
- new evaluations for minor actinides from BNL (^{242}Pu , ^{237}Np)

New structural materials (BNL)

- 23-Na
- 24-Mg, 27-Al
- 28,29,30-Si
- 50,52,53-Cr
- 55-Mn
- 54,56,57-Fe
- 58,60-Ni
- 90,91,92,94-Zr
- 92-Mo
- 109-Ag
- 143,145,146,148-Nd
- 141-Pr
- 204,206,207,208-Pb
- 209-Bi

Changes: Structural Materials

- Kernel approximation (Y.S. Cho and P. Oblozinsky, et. al.) used in resonance region:

capture: $\langle \sigma \rangle \propto \Gamma_n \Gamma_\gamma / \Gamma_{\text{tot}}$

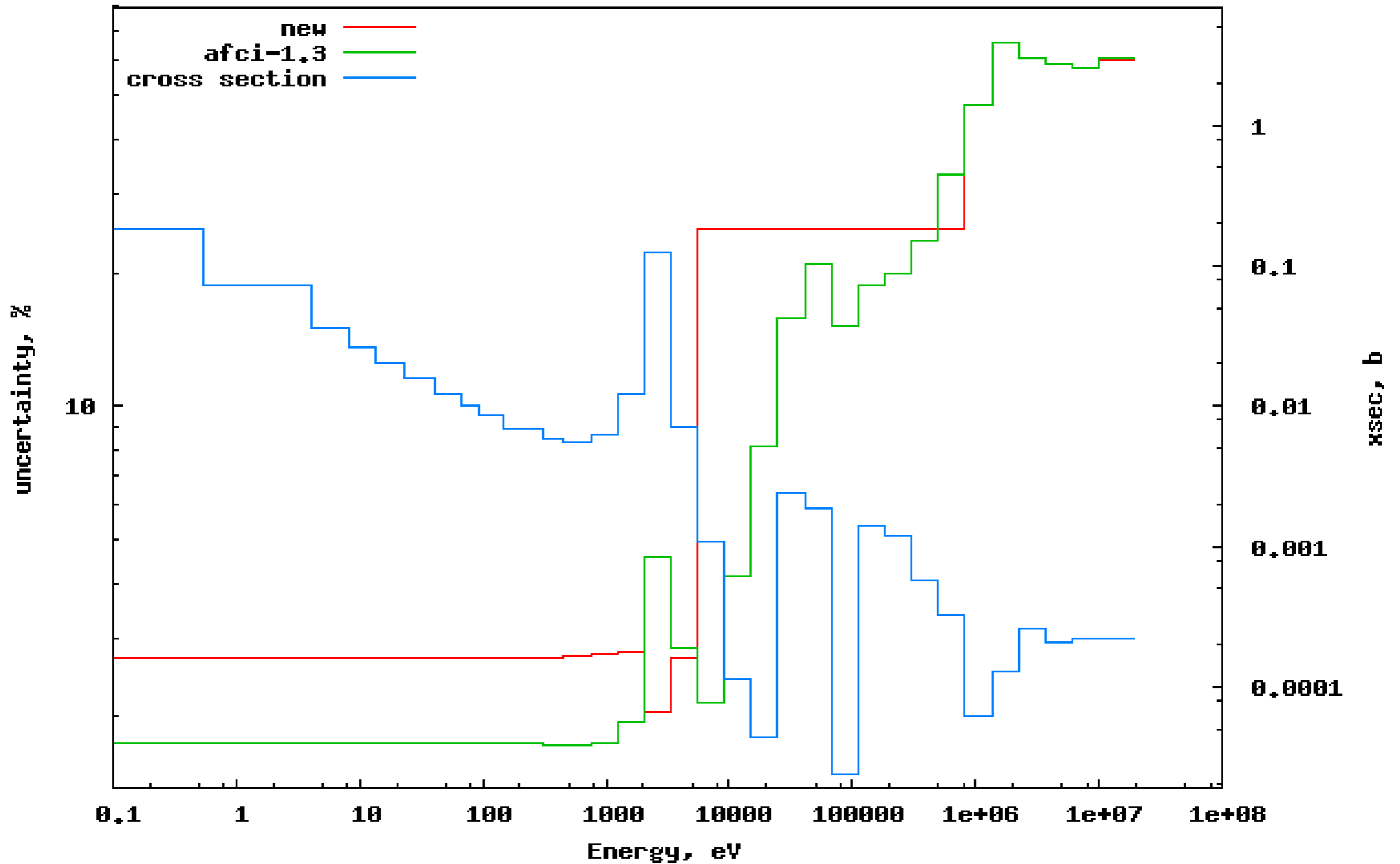
elastic: $\langle \sigma \rangle \propto \Gamma_n^2 / \Gamma$

potential scattering ($\sim 4\pi R'^2$) included in elastic

- Fast region calculated with Empire/Kalman or taken from ENDF/B-VI.8

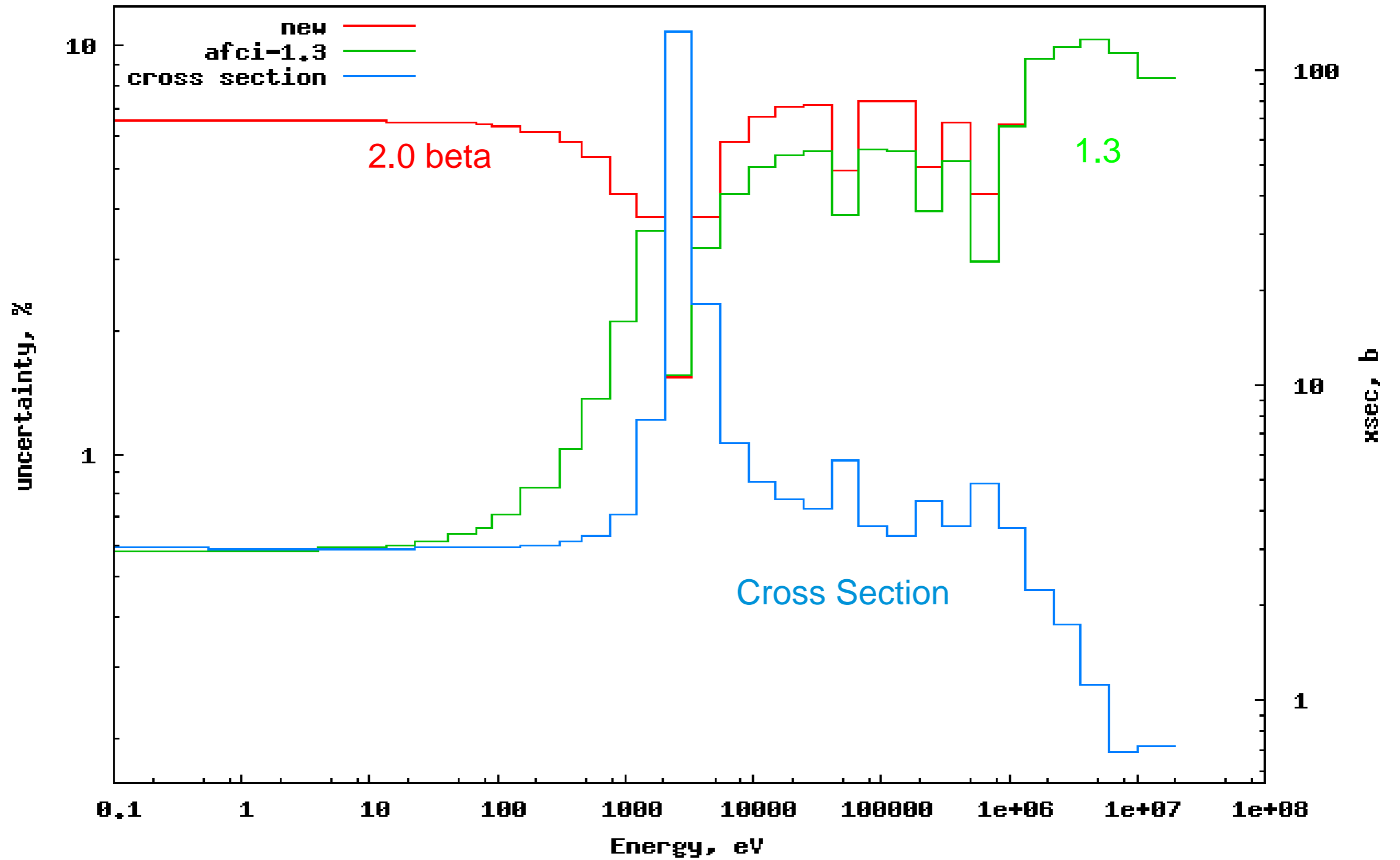
23-Na capture (M. Pigni)

011_Na_023 - HT102

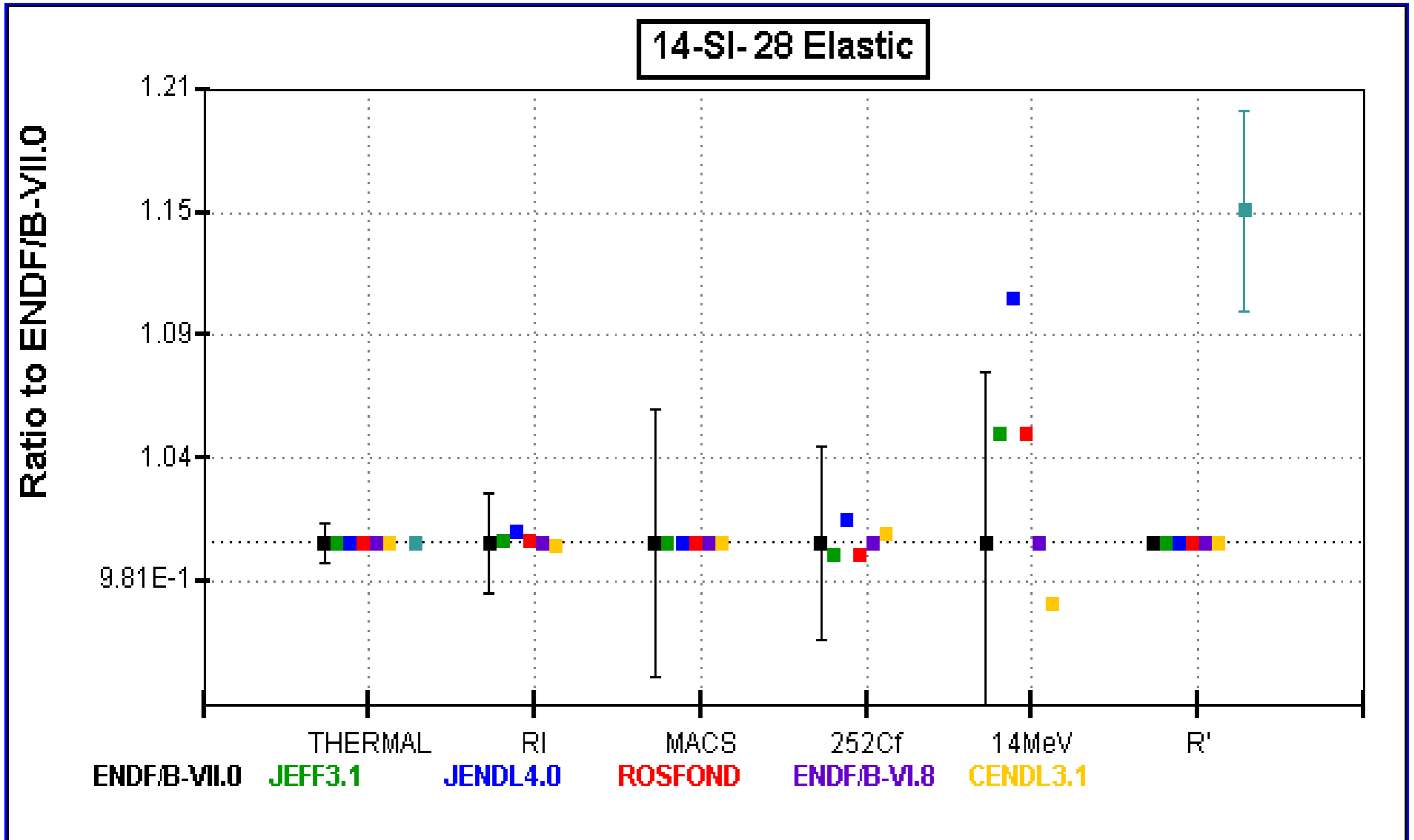


23-Na elastic

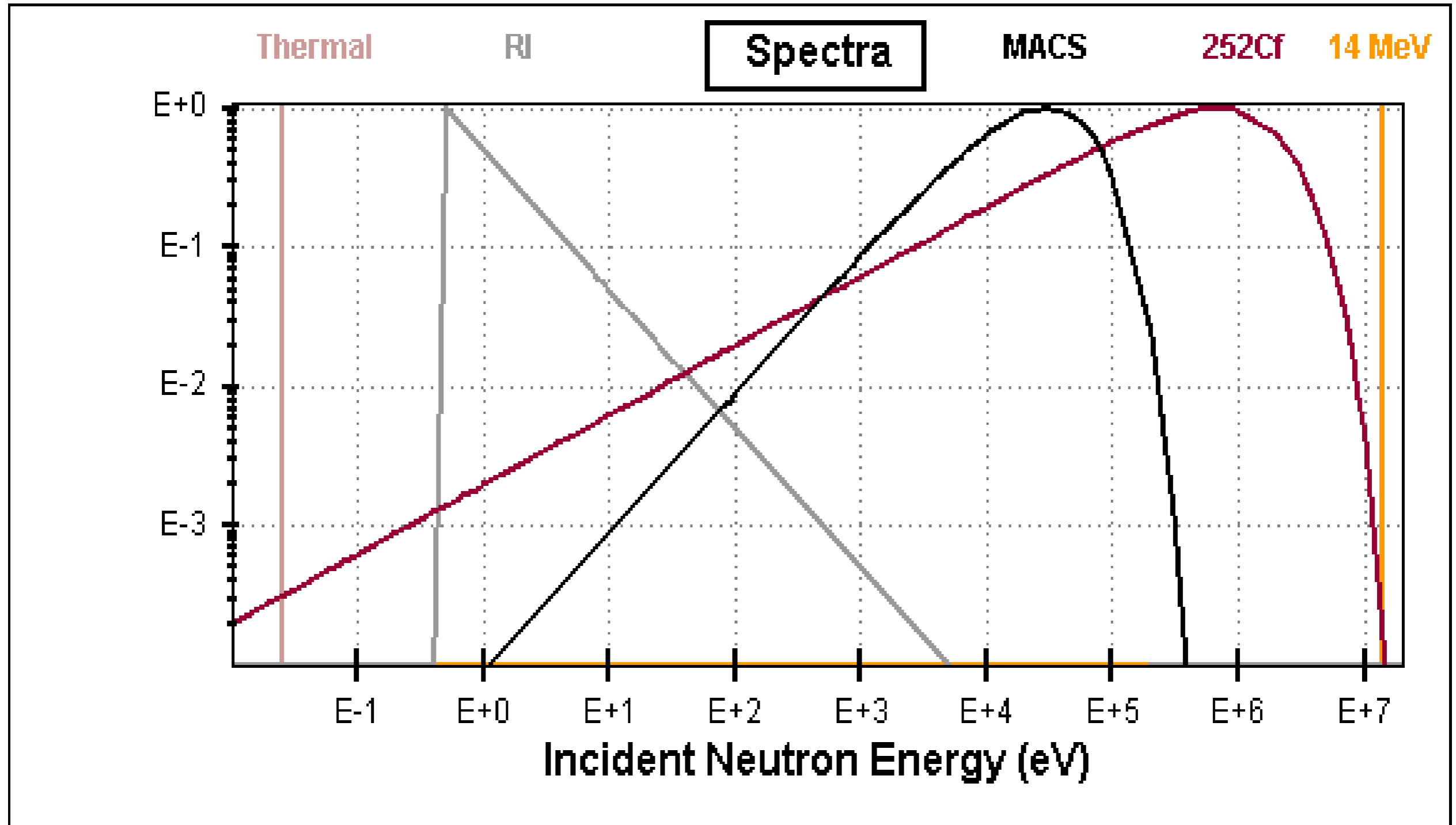
011_Na_023 - MT2



^{28}Si integral quantities from Sigma-QA (A. Sonzogni)



Integral Weightings

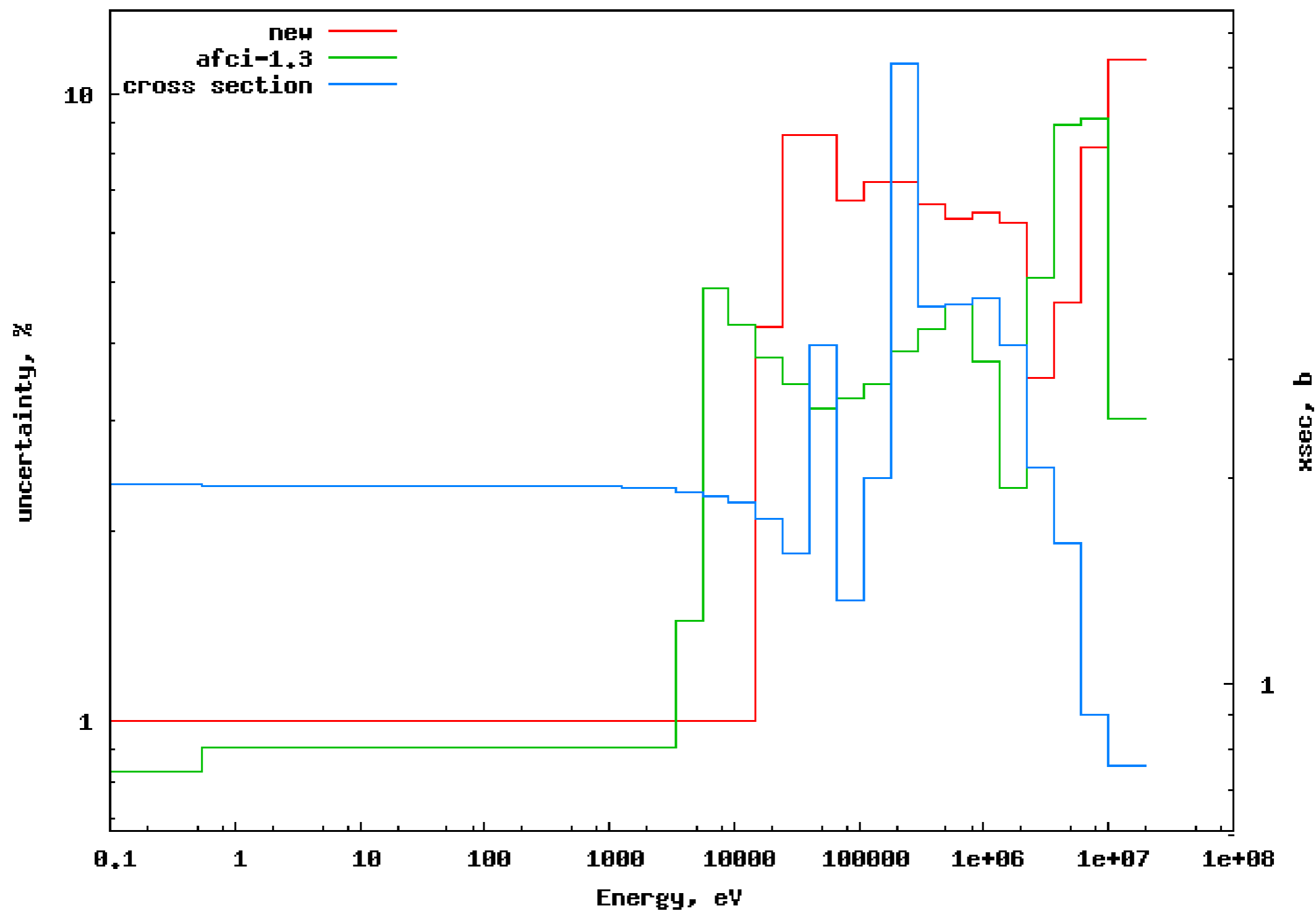


^{28}Si elastic integral quantities from Sigma-QA

Elastic						
Library	THERMAL	RI 0.5-2E+7 eV	MACS 30 keV	^{252}Cf	14 MeV	R' (fm)
ENDF/B-VII.0	1.992	3.882E+1	2.382	2.871	6.620E-1	4.136
JEFF3.1	1.992	3.885E+1	2.382	2.854	6.969E-1	4.136
JENDL4.0	1.992	3.904E+1	2.382	2.902	7.400E-1	4.136
ROSFOND	1.992	3.885E+1	2.382	2.854	6.969E-1	4.136
ENDF/B-VI.8	1.992	3.882E+1	2.382	2.871	6.620E-1	4.136
CENDL3.1	1.992	3.879E+1	2.382	2.884	6.424E-1	4.136
Atlas	1.992					4.800
Atlas Δ	6.000E-3 3.01E-1%					2.000E-1 4.16%
AFCI2.0 Δ	1.992E-2 1.00%	9.587E-1 2.46%	1.540E-1 6.46%	1.351E-1 4.70%	5.435E-2 8.20%	
Recommended Δ	6.000E-3 3.01E-1%					3.073E-1 7.43%

^{28}Si elastic

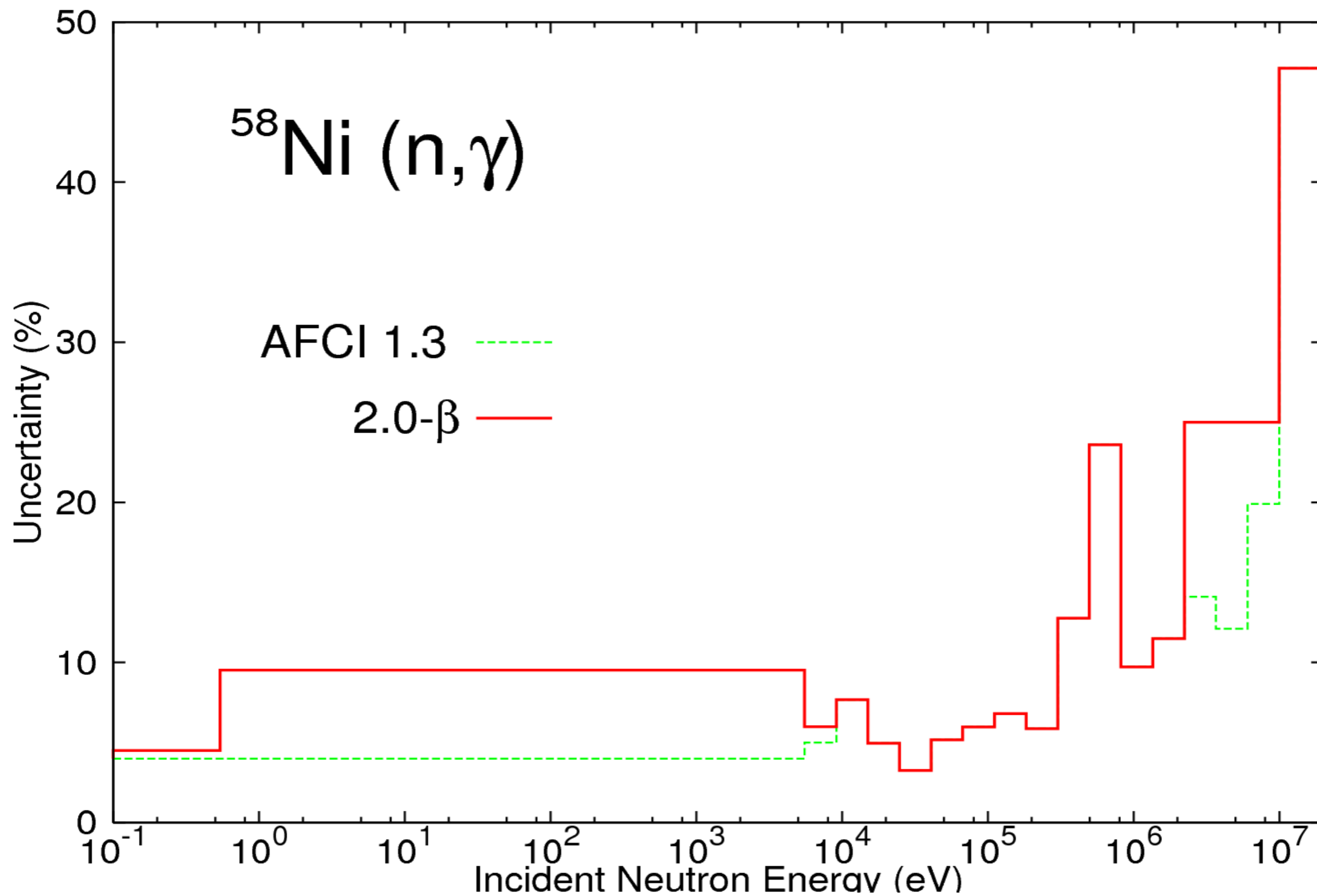
014_Si_028 - NT2



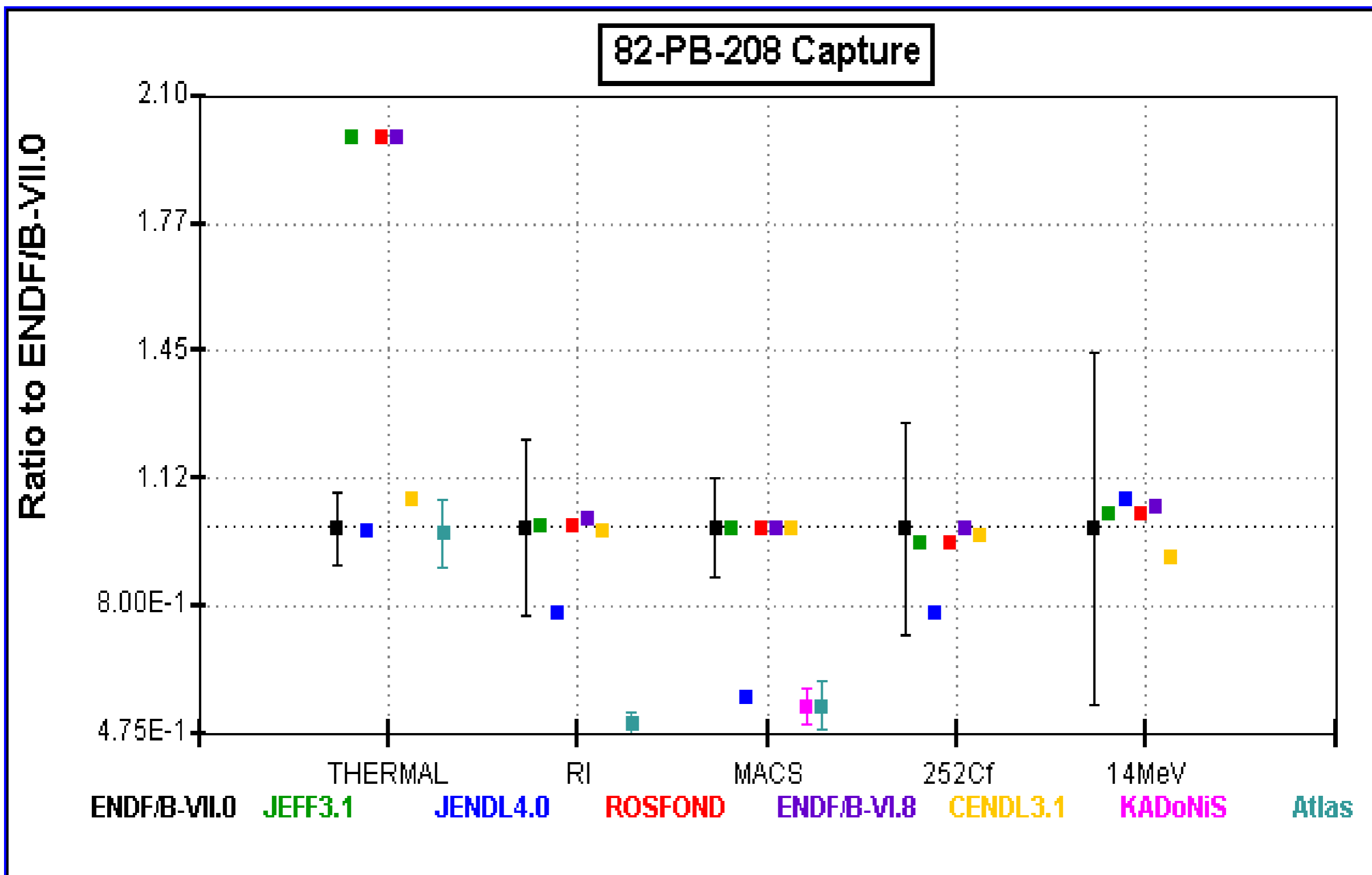
^{58}Ni capture integral quantities from Sigma-QA

Library	Capture				
	THERMAL	RI 0.5-2E+7 eV	MACS 30 keV	^{252}Cf	14 MeV
ENDF/B-VII.0	4.633	2.231	4.000E-2	6.242E-3	4.791E-4
JEFF3.1	4.633	2.225	3.999E-2	7.482E-3	5.044E-4
JENDL4.0	4.633	2.228	4.000E-2	8.442E-3	5.412E-5
ROSFOND	4.633	2.225	3.999E-2	7.482E-3	5.044E-4
ENDF/B-VI.8	4.633	2.222	3.999E-2	6.242E-3	4.791E-4
CENDL3.1	4.633	2.222	3.999E-2	6.189E-3	1.190E-3
KADONIS			3.870E-2		
Atlas	4.370	2.100	4.020E-2		
Kadonis Δ			1.500E-3 3.87%		
Atlas Δ	1.000E-1 2.28%	2.000E-1 9.52%	2.500E-3 6.21%		
AFCI2.0 Δ	1.853E-1 3.99%	1.921E-1 8.61%	1.763E-3 4.40%	4.361E-4 6.98%	9.536E-5 1.99E+1%
Recommended Δ	1.353E-1 2.92%	2.124E-1 9.52%	2.487E-3 6.21%		

^{58}Ni capture

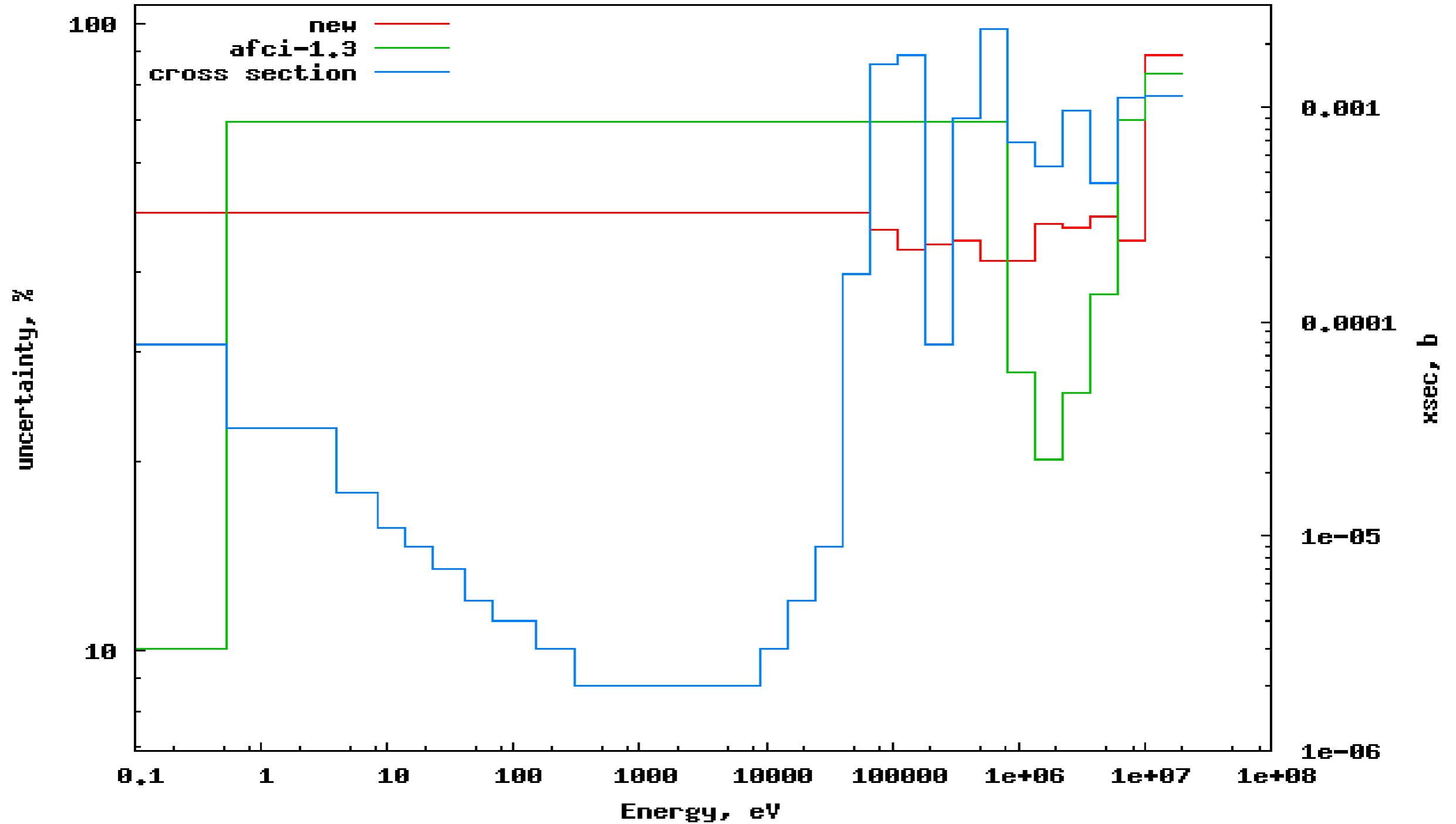


208-Pb capture integral QA



208-Pb capture

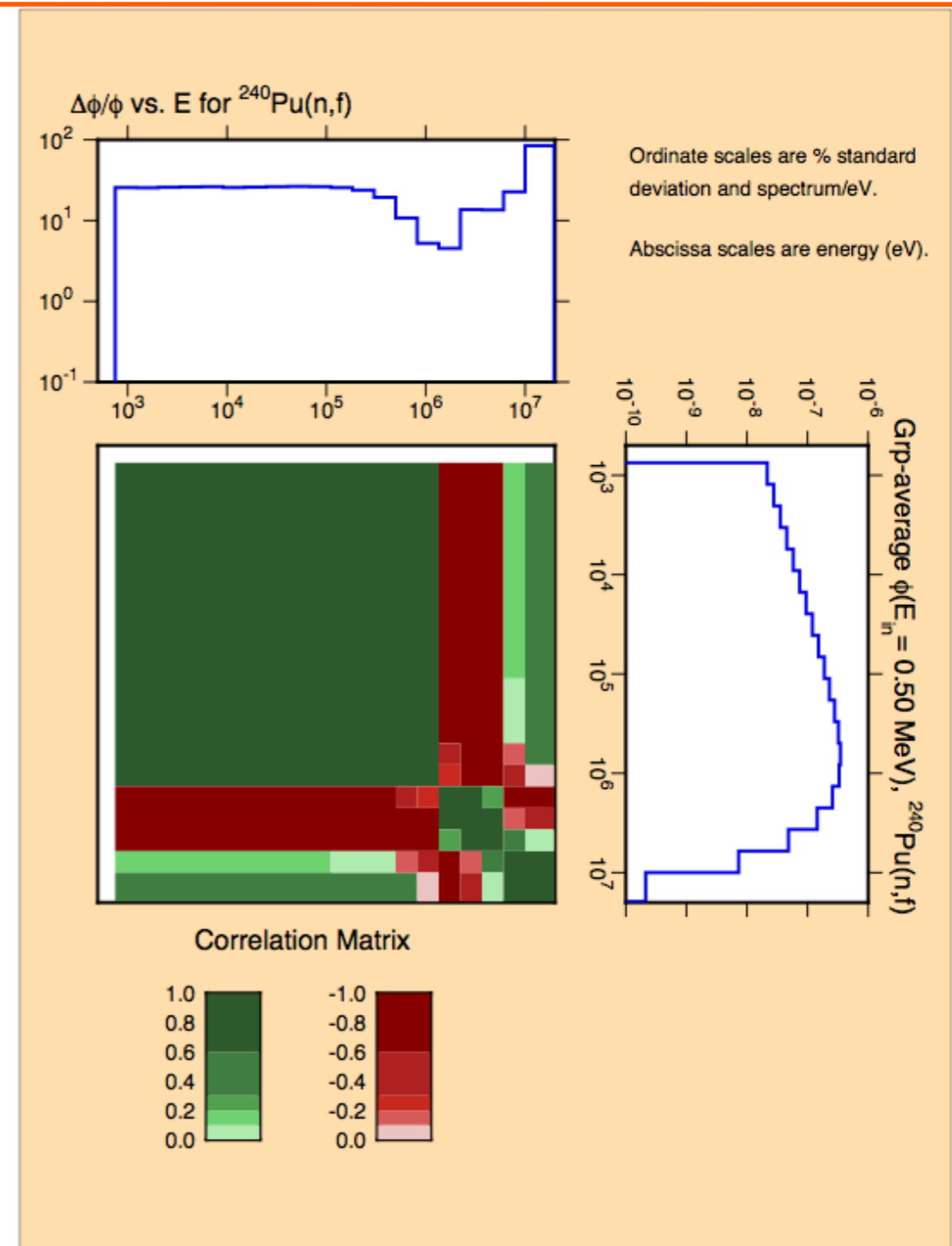
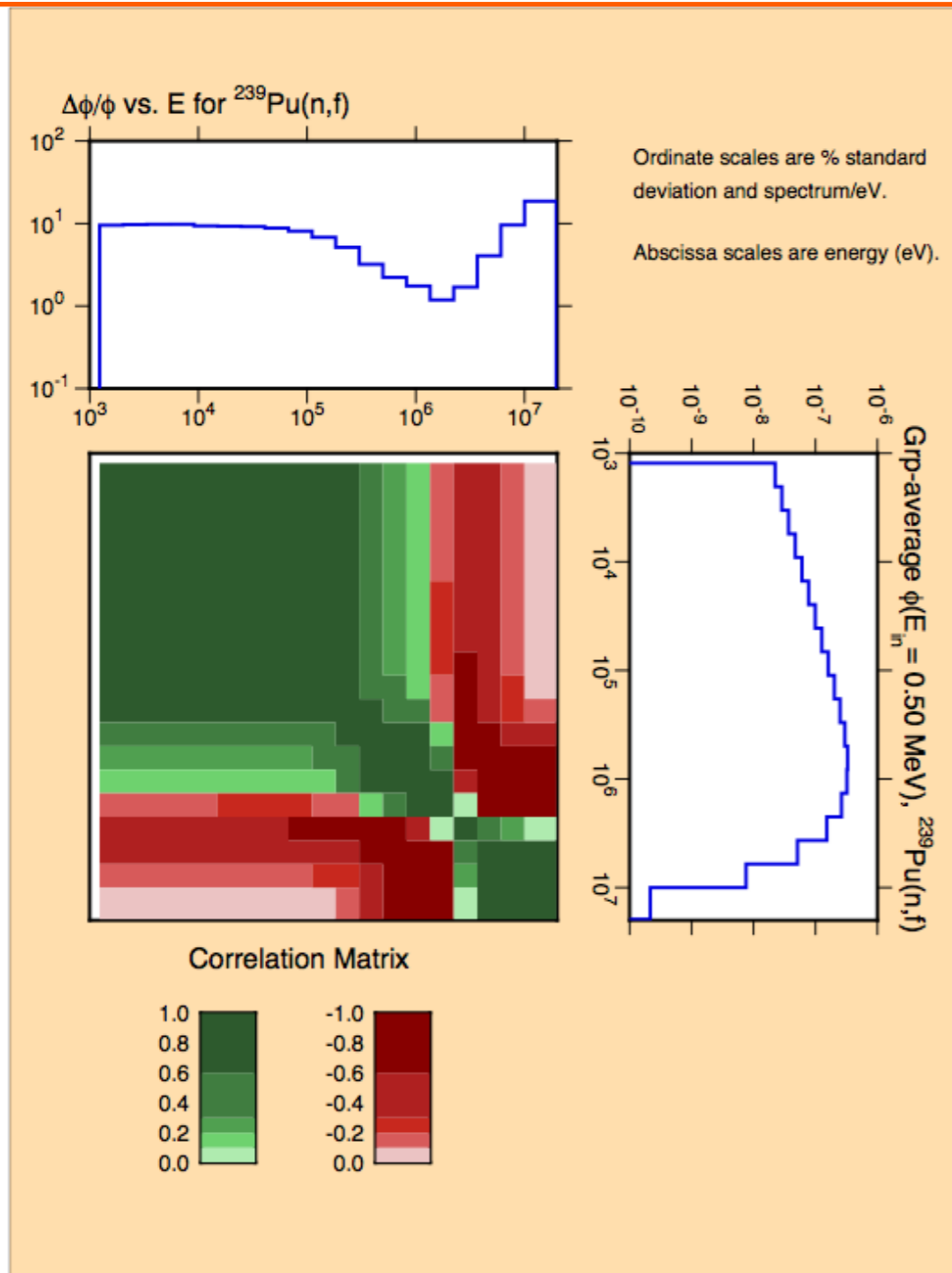
082_Pb_208 - HT102



Fission Spectra (LANL)

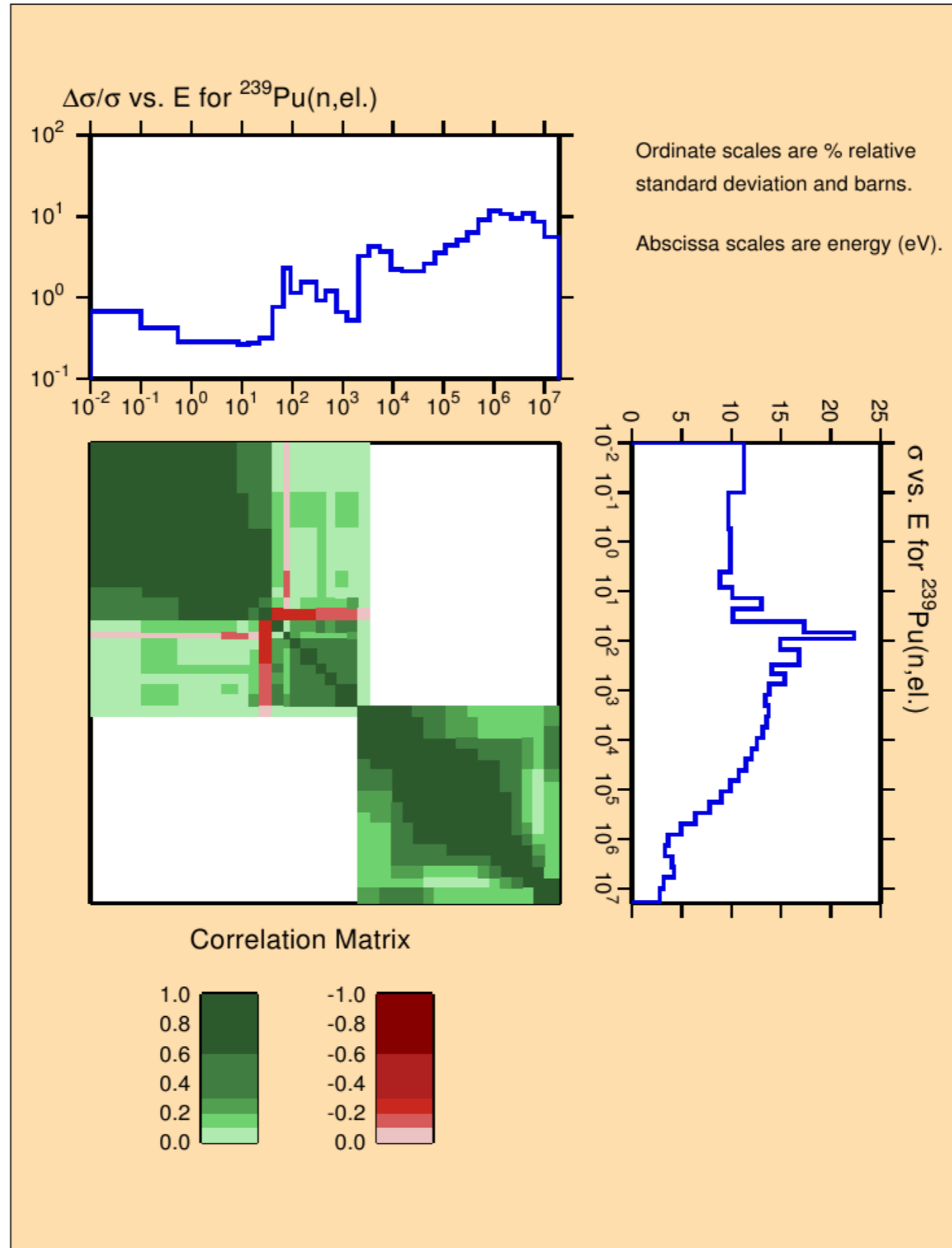
- $^{238,239,240}\text{Pu}$ PFNS contained in library
- Problem in AFCI-v1.2: rows/columns of PFNS did not sum to zero as expected for MF35 covariance matrix of normalized distribution
- All PFNS matrices now obey sum-to-zero condition

239,240Pu PFNS (LANL)

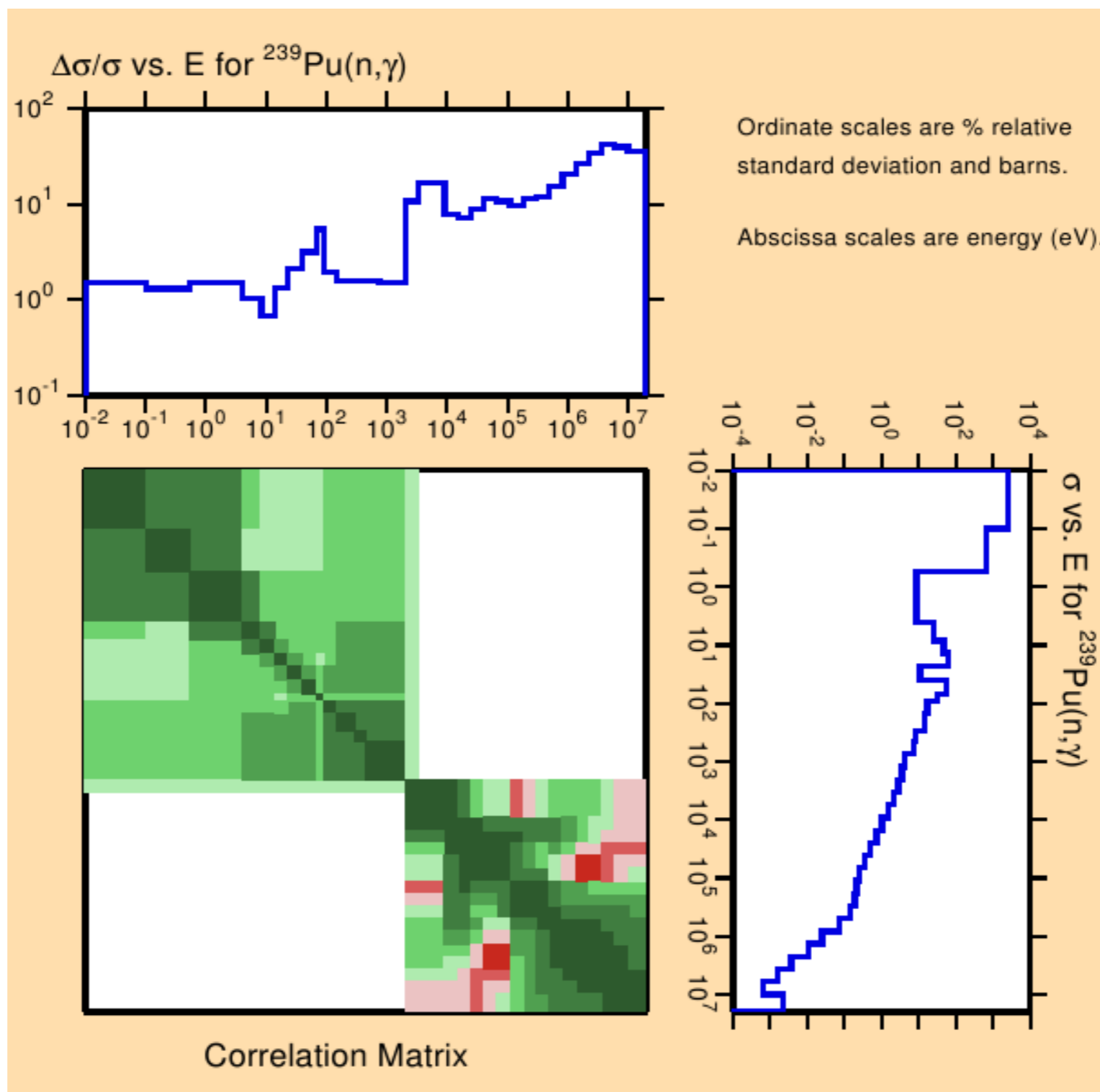


Fix: PFNS covariance matrices now obey sum-to-zero condition

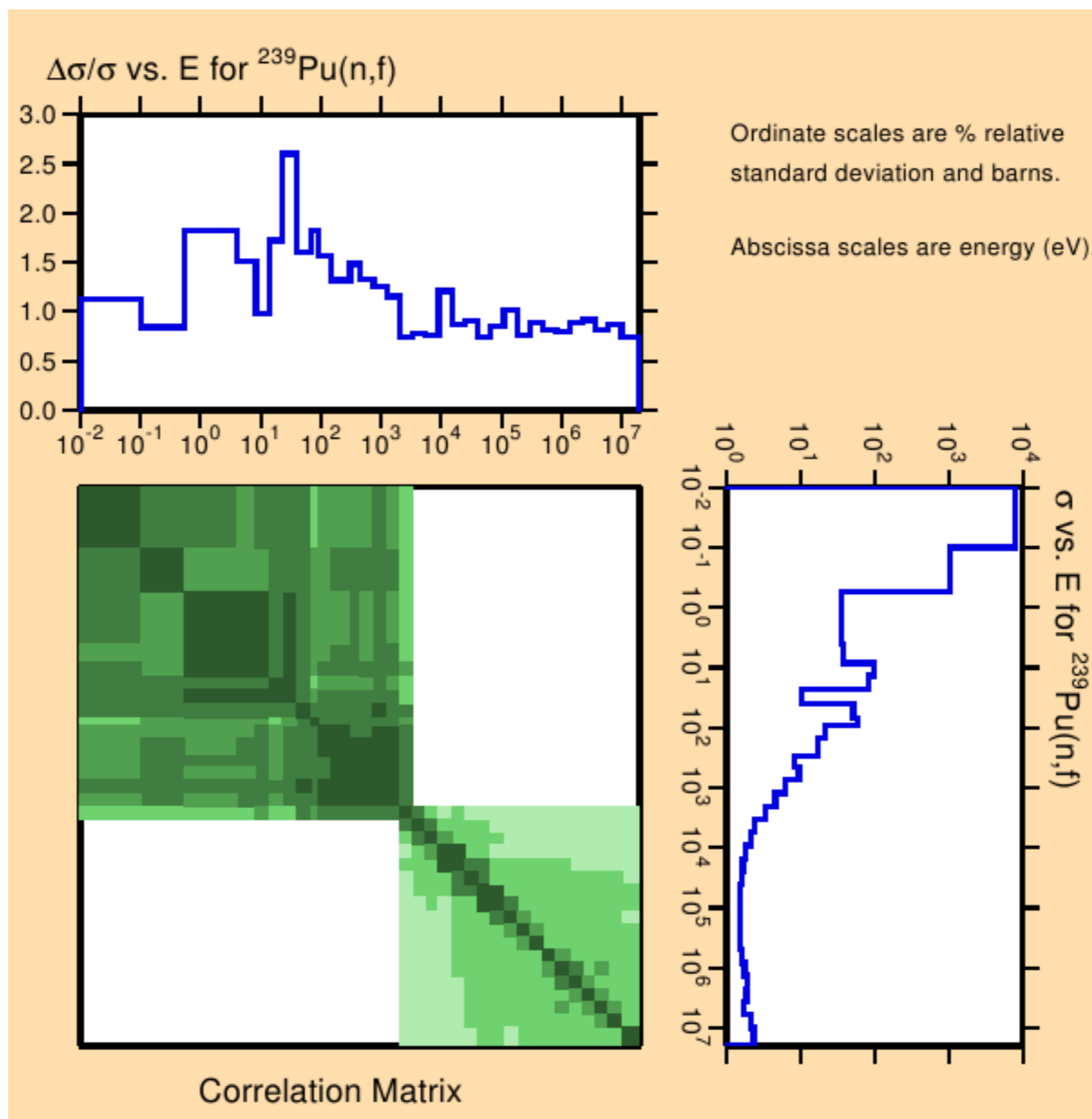
239-Pu elastic (LANL)



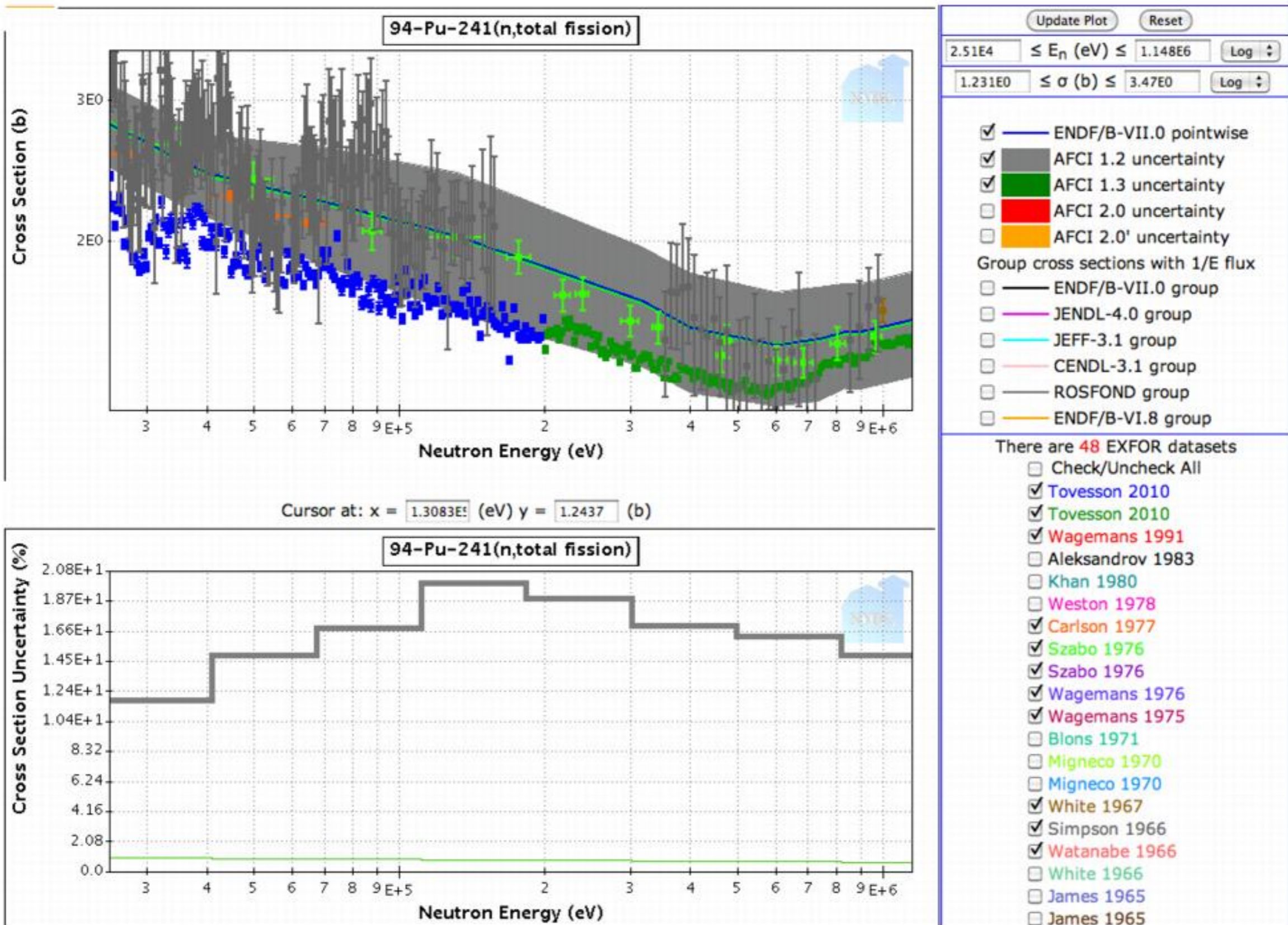
239-Pu capture (LANL)



^{239}Pu fission (LANL)



241-Pu fission (LANL)



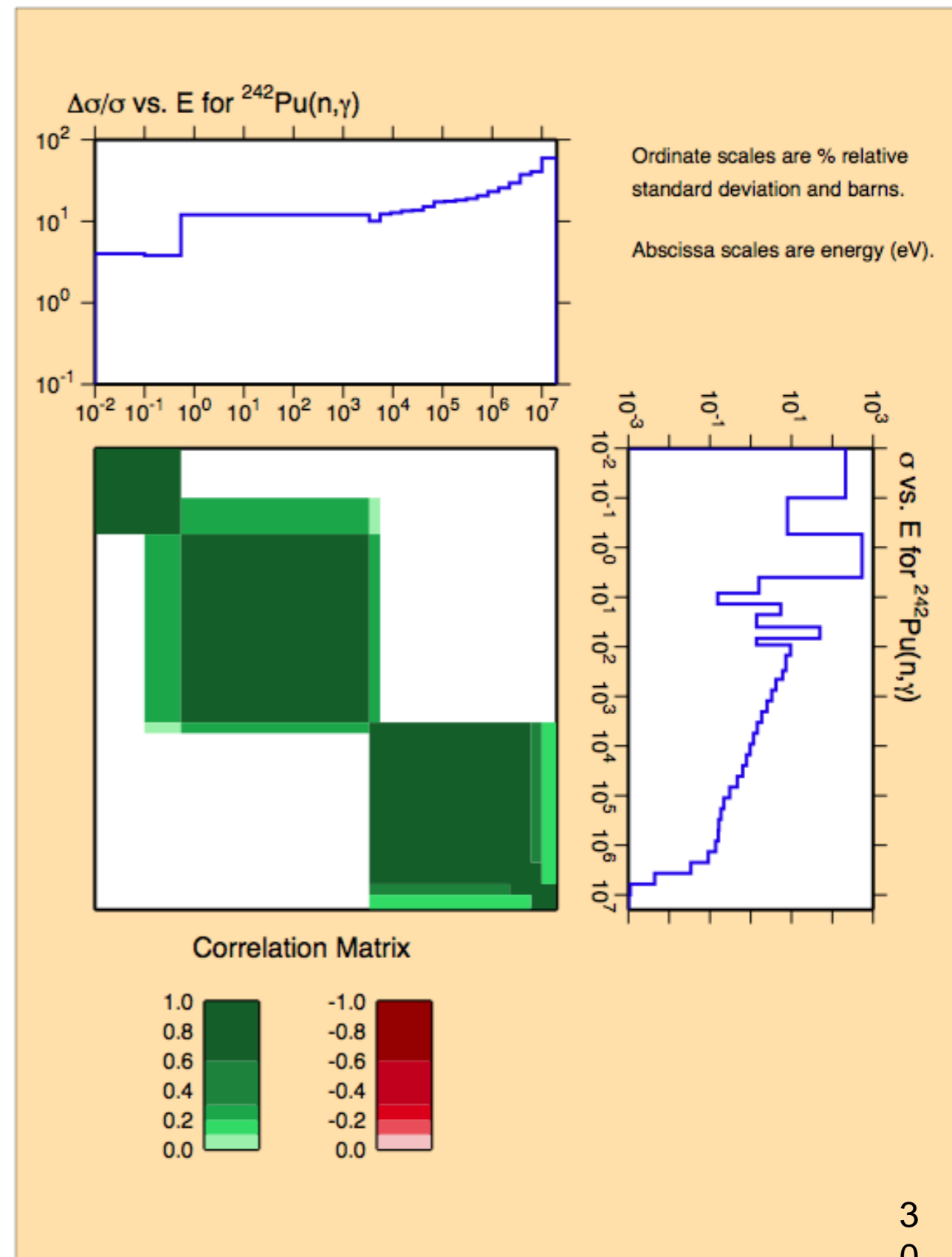
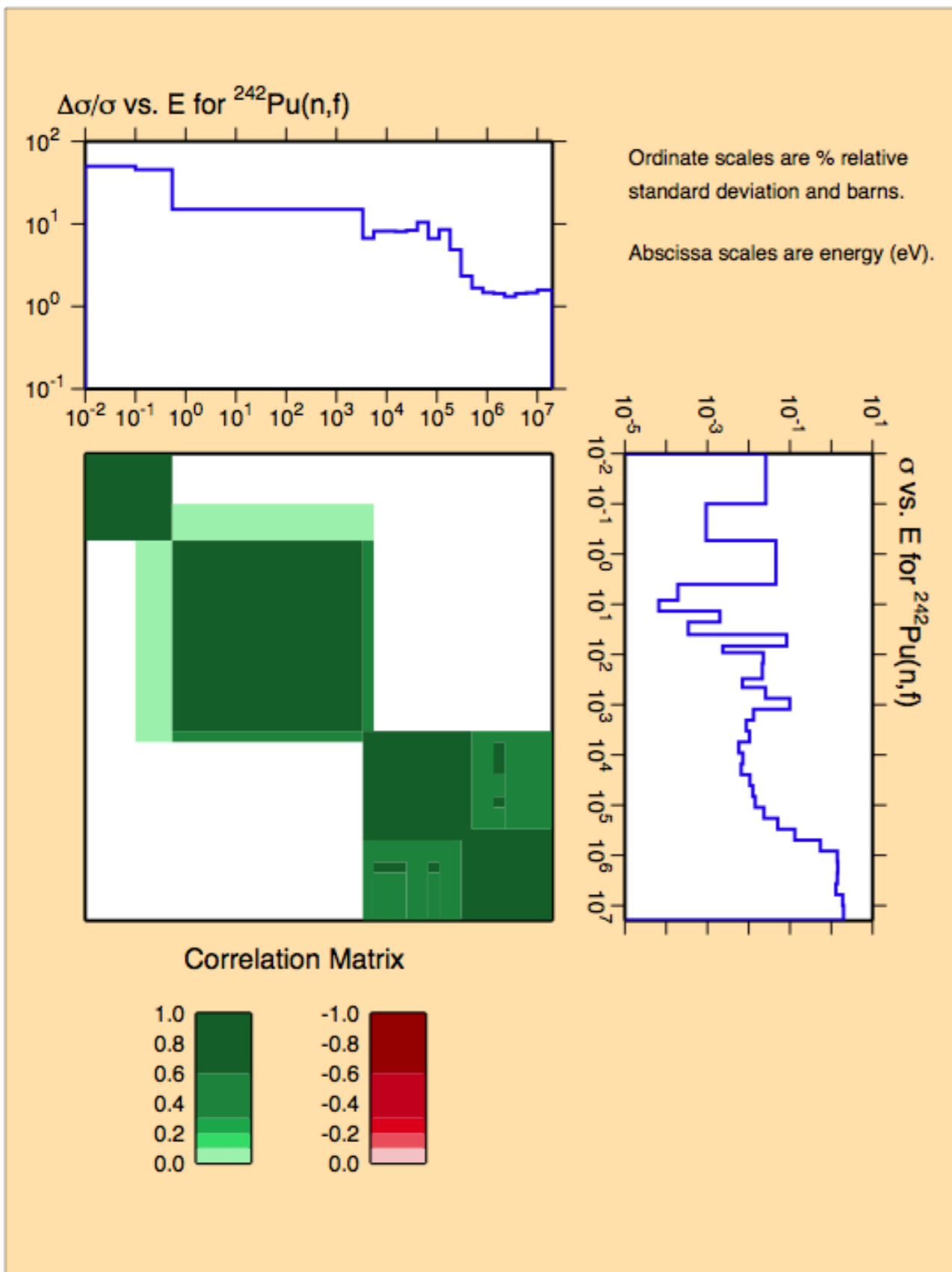
Minor Actinides

- $^{238,240,241}\text{Pu}$, ^{241}Am - new files from LANL
- ^{237}Np , ^{242}Pu - new covariances from BNL (M.T. Pigni, C. Mattoon)
- These replace older estimates based on V.Maslov recommendations

^{242}Pu (C. Mattoon)

- Using new input for EMPIRE (M.Sin, Bucharest), varying fission barrier and optical model parameters
- Experimental data for (n,tot) , (n,el) , (n,f)
 - For fission, new data, Tovesson, et al (2009)
- Covariances produced with KALMAN code
- At lower energies, using low-fidelity estimates

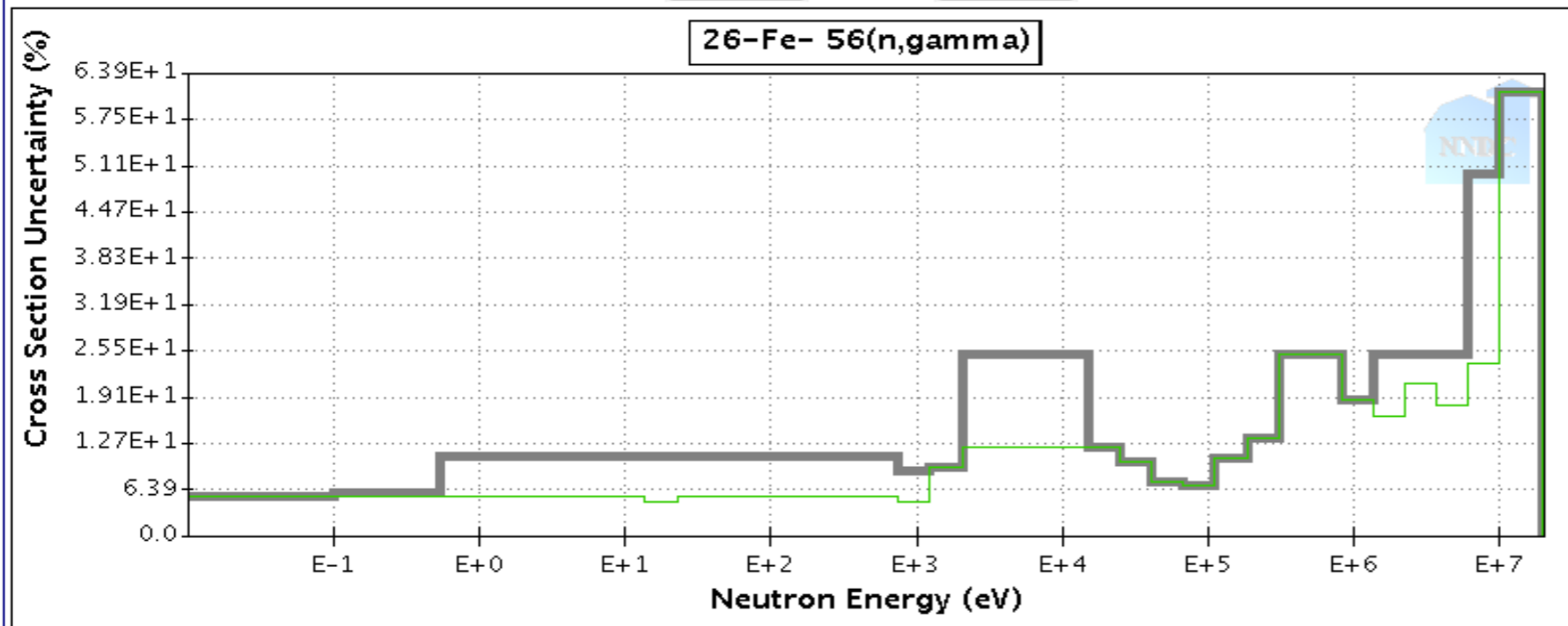
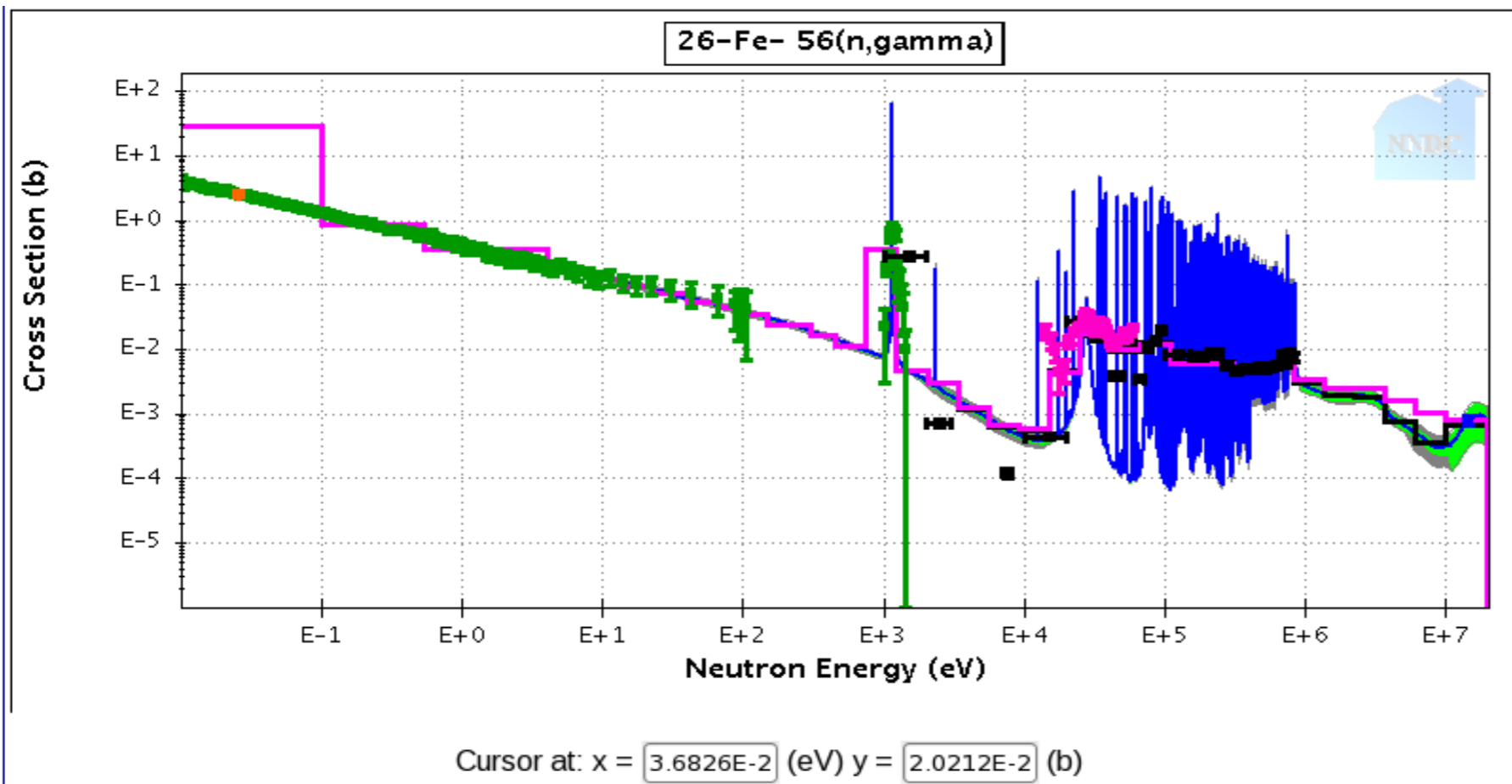
^{242}Pu continued



Quality Assurance

- New web-based Sigma-QA (A. Sonzogni) allows visual and also quantitative inspection of:
 - Differential uncertainties (dynamic)
 - Integral uncertainties (static)
- UnCor applied to full library, performs 8 tests, warnings for possible problems including:
 - small uncertainties: $(n,tot) < 1\%$, (n,el) and $(n,\gamma) < 2\%$,...
 - non-positive-definite matrices
 - PFNS covariance not summing to zero
- non-positive-definite matrices are usually fixable by slightly reducing the off-diagonal elements.

Example of Sigma-QA AFCI plot



Update Plot Reset

1E-2 ≤ E_n (eV) ≤ 2E7 Log

1E-6 ≤ σ (b) ≤ 1.924E2 Log

- ENDF/B-VII.0 pointwise
- AFCI 1.2 uncertainty
- AFCI 1.3 uncertainty
- AFCI 2.0 uncertainty
- AFCI 2.0' uncertainty

Group cross sections with 1/E flux

- ENDF/B-VII.0 group
- JENDL-4.0 group
- JEFF-3.1 group
- CENDL-3.1 group
- ROSFOND group
- ENDF/B-VI.8 group

There are 7 EXFOR datasets

- Check/Uncheck All
- Huang Zheng-De 1980
- Shcherbakov 1977
- Shcherbakov 1977
- Allen 1982
- Allen 1976
- Macklin 1964
- Pomerance 1952

Remove EXFOR

[Download plot for your article](#)

Quality Assurance (continued):

- Code 'unCor', (Mattoon, Oblozinsky) checks the library for possible problems in uncertainties and/or correlations
- Some small uncertainties still appear in v2.0-beta of library

```
Uncertainties too large: 19 total
```

```
MT16 in 001_H_002, max = 100.00%  
MT102 in 003_Li_007, max = 100.00%  
MT4 in 005_B_010, max = 100.00%  
MT102 in 040_Zr_090, max = 100.00%  
MT102 in 040_Zr_095, max = 100.00%  
MT2 in 040_Zr_095, max = 100.00%  
MT51 in 090_Th_232, max = 100.00%  
MT852 in 090_Th_232, max = 100.00%  
MT18 in 092_U_238, max = 100.00%  
MT102 in 094_Pu_238, max = 100.00%  
MT4 in 094_Pu_238, max = 100.00%  
MT102 in 094_Pu_240, max = 100.00%  
MT102 in 094_Pu_241, max = 100.00%  
MT102 in 094_Pu_242, max = 100.00%  
MT102 in 095_Am_242m, max = 100.00%  
MT102 in 096_Cm_242, max = 100.00%  
MT18 in 096_Cm_242, max = 100.00%  
MT4 in 096_Cm_242, max = 100.00%  
MT102 in 096_Cm_244, max = 100.00%
```

```
Uncertainties too small: 55 total
```

```
MT1 in 001_H_001, min = 0.29% in bin 33 (27 bins < 1%)  
MT2 in 001_H_001, min = 0.30% in bin 12 (27 bins < 1%)  
MT1 in 002_He_004, min = 0.50% in bin 11 (28 bins < 1%)  
MT2 in 002_He_004, min = 0.50% in bin 11 (28 bins < 1%)  
MT1 in 003_Li_006, min = 0.20% in bin 30 (21 bins < 1%)  
MT105 in 003_Li_006, min = 0.20% in bin 18 (25 bins < 1%)  
MT1 in 003_Li_007, min = 0.27% in bin 3 (7 bins < 1%)  
MT2 in 003_Li_007, min = 0.42% in bin 4 (6 bins < 1%)  
MT1 in 004_Be_009, min = 0.50% in bin 24 (14 bins < 1%)  
MT2 in 004_Be_009, min = 0.50% in bin 24 (14 bins < 1%)
```

Summary

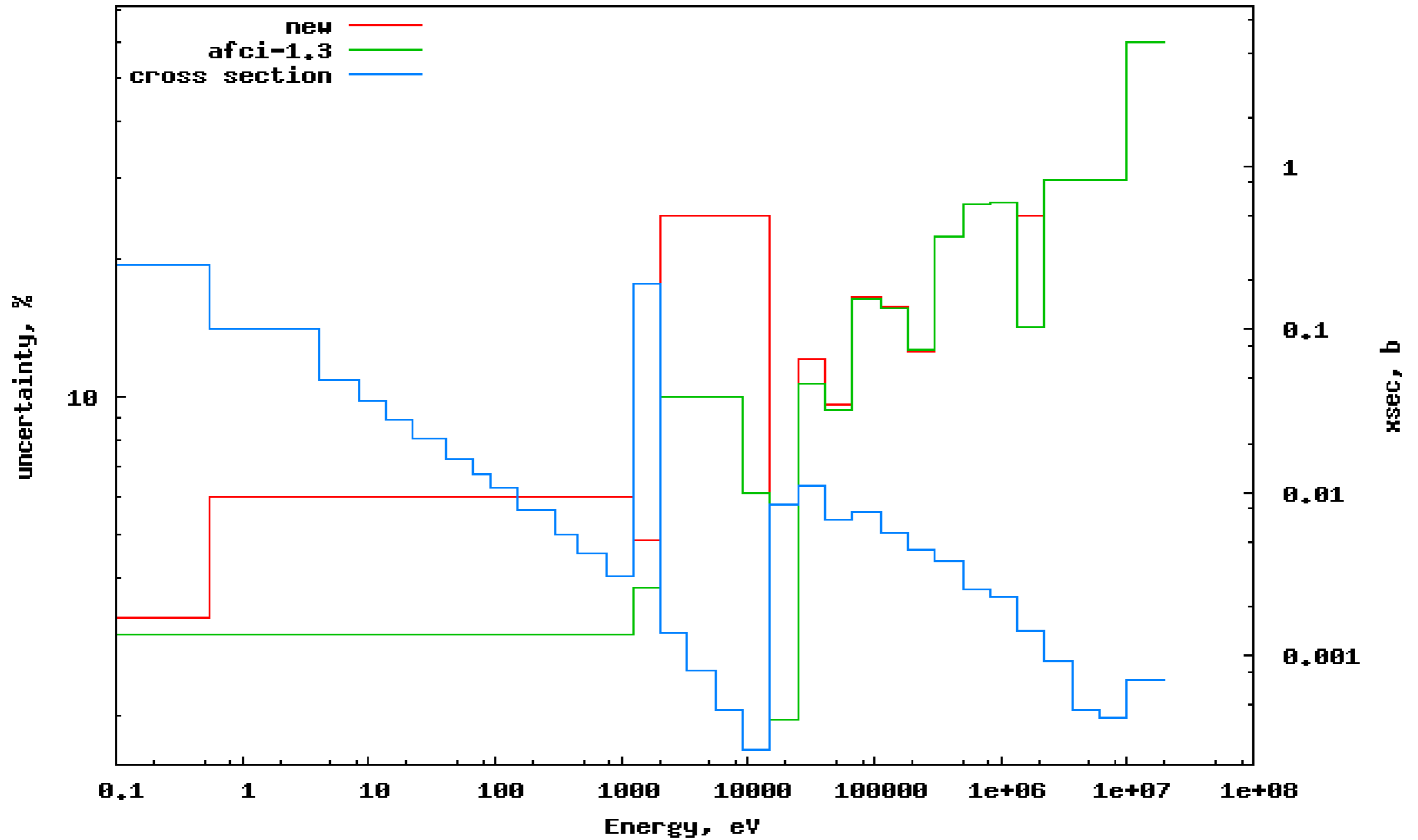
- AFCI-2.0 β covariance library released Oct 2010. Final release planned for Dec 2010.
- Files being tested using Sigma-QA and UnCor procedures for quality assurance
- Active user community (mainly ANL,INL) provides valuable feedback; feedback also expected from WPEC-SG33 international data adjustment
- Many AFCI covariance files expected to make it into ENDF/B-VII.1 library

EXTRAS

- Extra slides

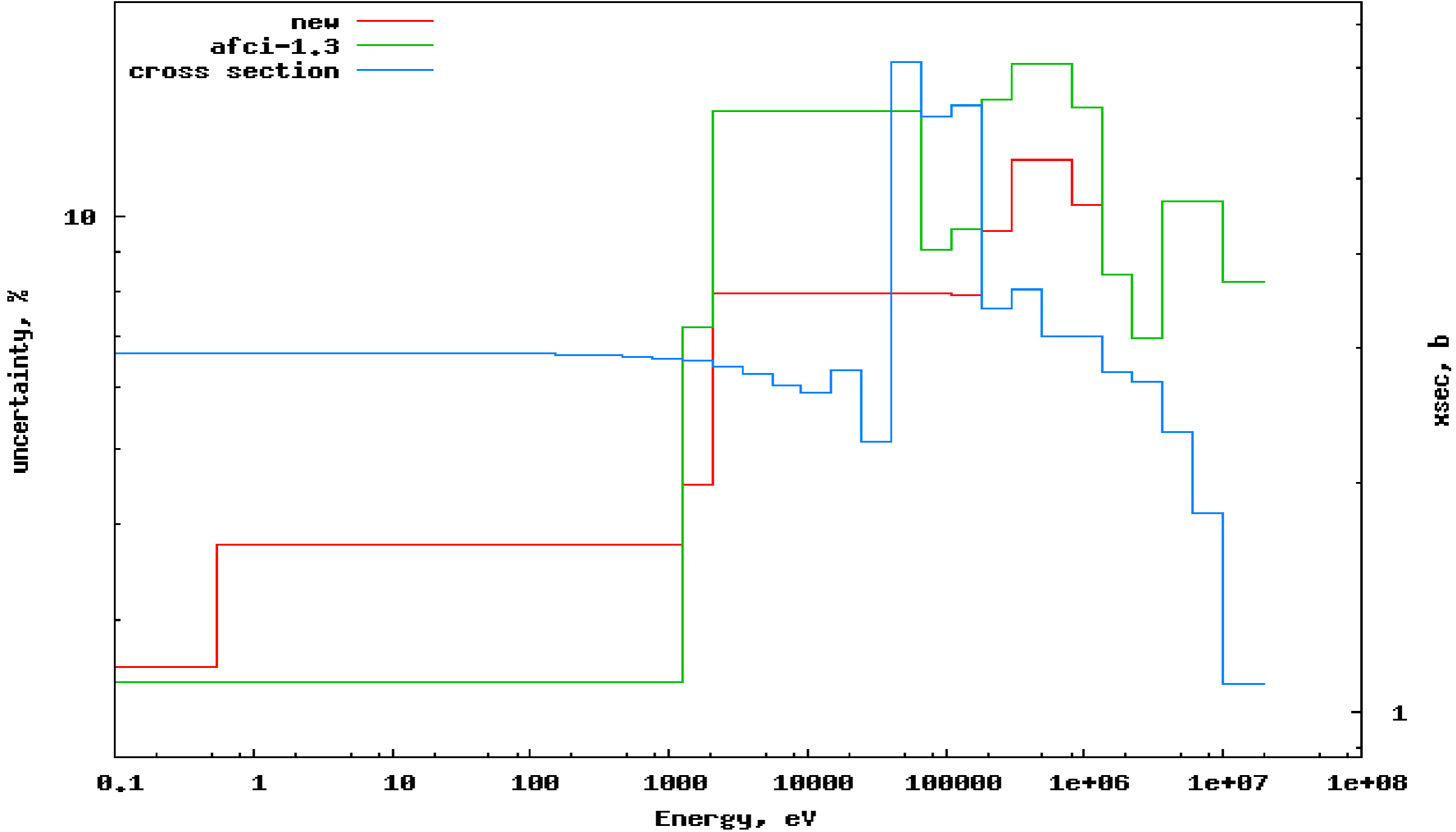
52-Cr capture

024_Cr_052 - HT102

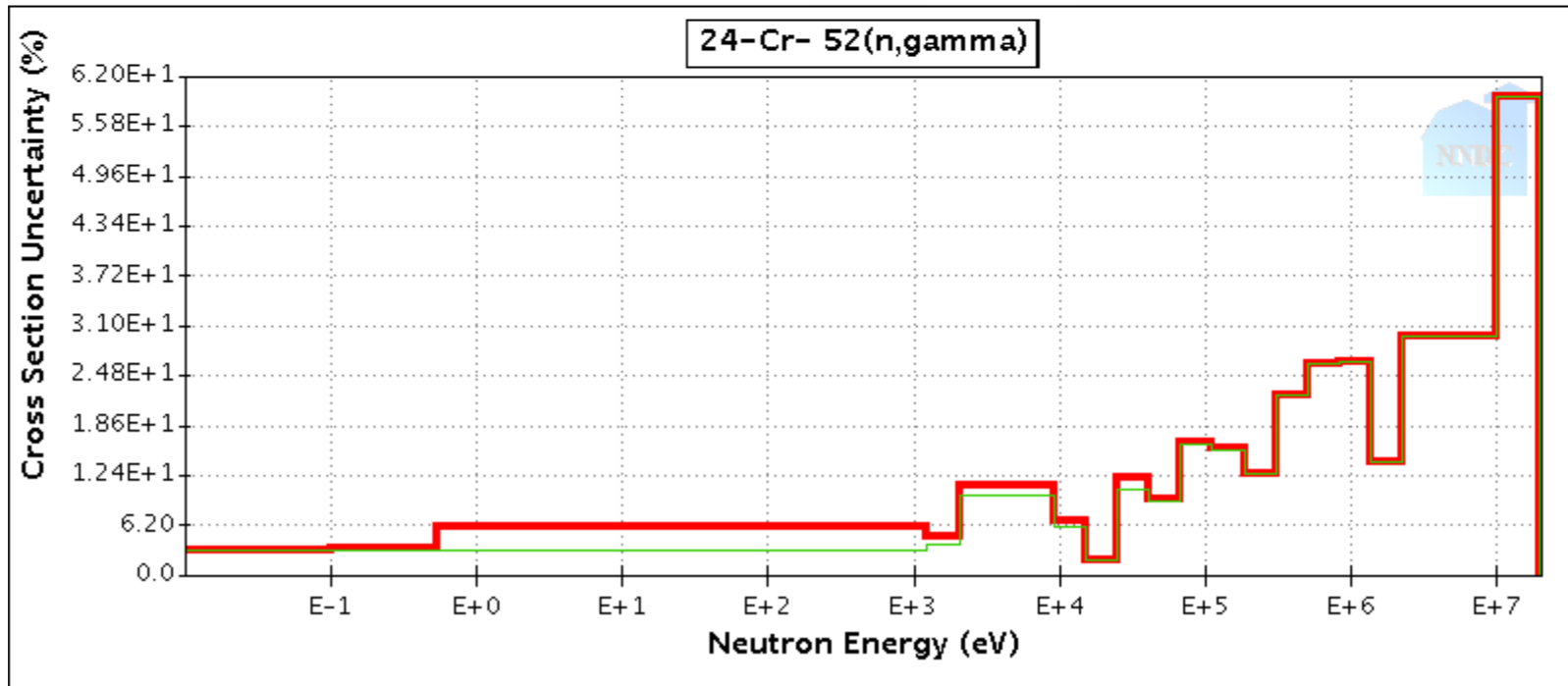
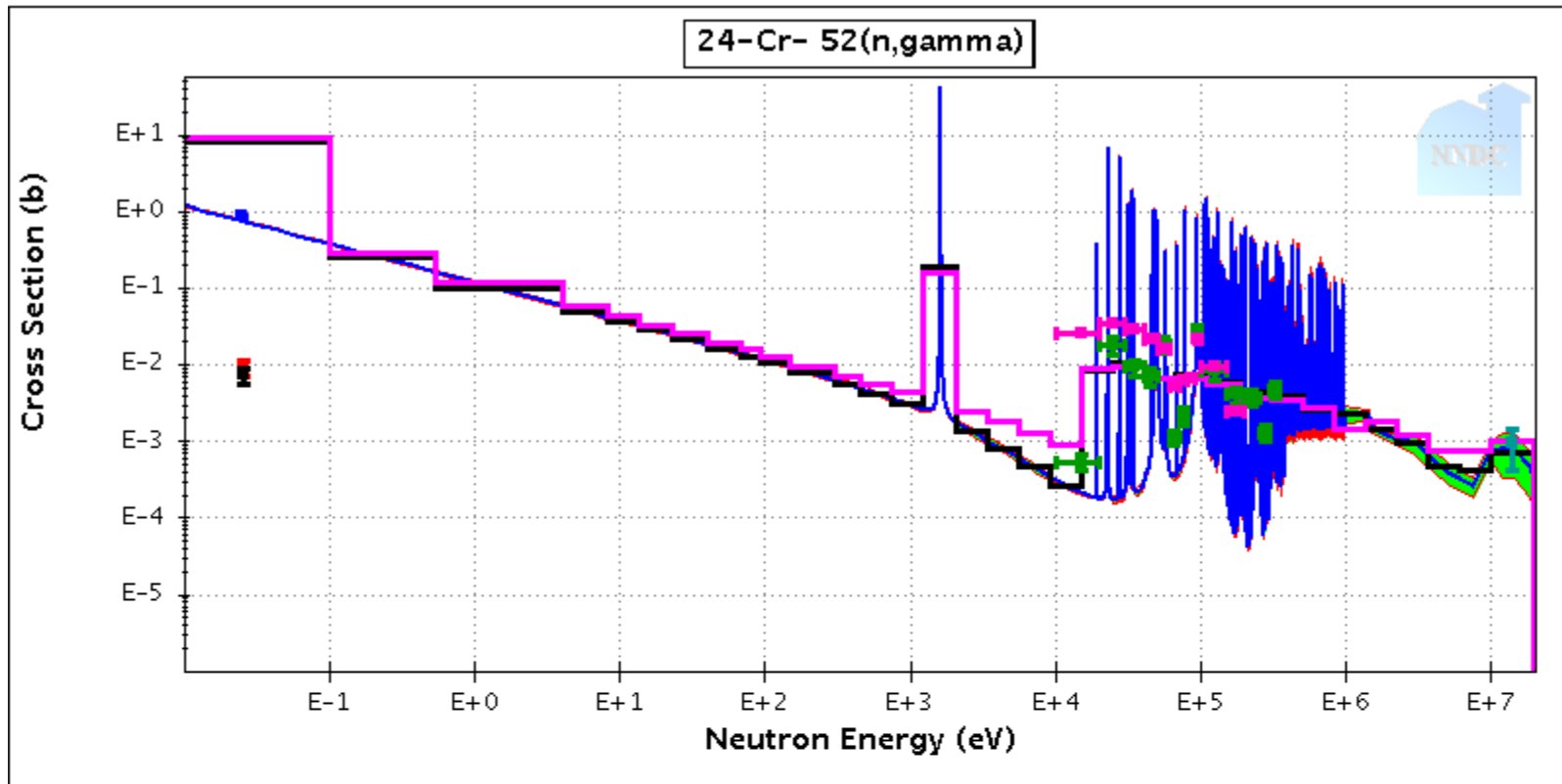


52-Cr elastic

024_Cr_052 - HT2



52-Cr QA



Update Plot Reset

≤ E_n (eV) ≤ Log

≤ σ (b) ≤ Log

- ENDF/B-VII.0 pointwise
- AFCI 1.2 uncertainty
- AFCI 1.3 uncertainty
- AFCI 2.0 uncertainty
- AFCI 2.0' uncertainty

Group cross sections with 1/E flux

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- JENDL-4.0 group
- JEFF-3.1 group
- CENDL-3.1 group
- ROSFOND group
- ENDF/B-VI.8 group

There are 8 EXFOR datasets

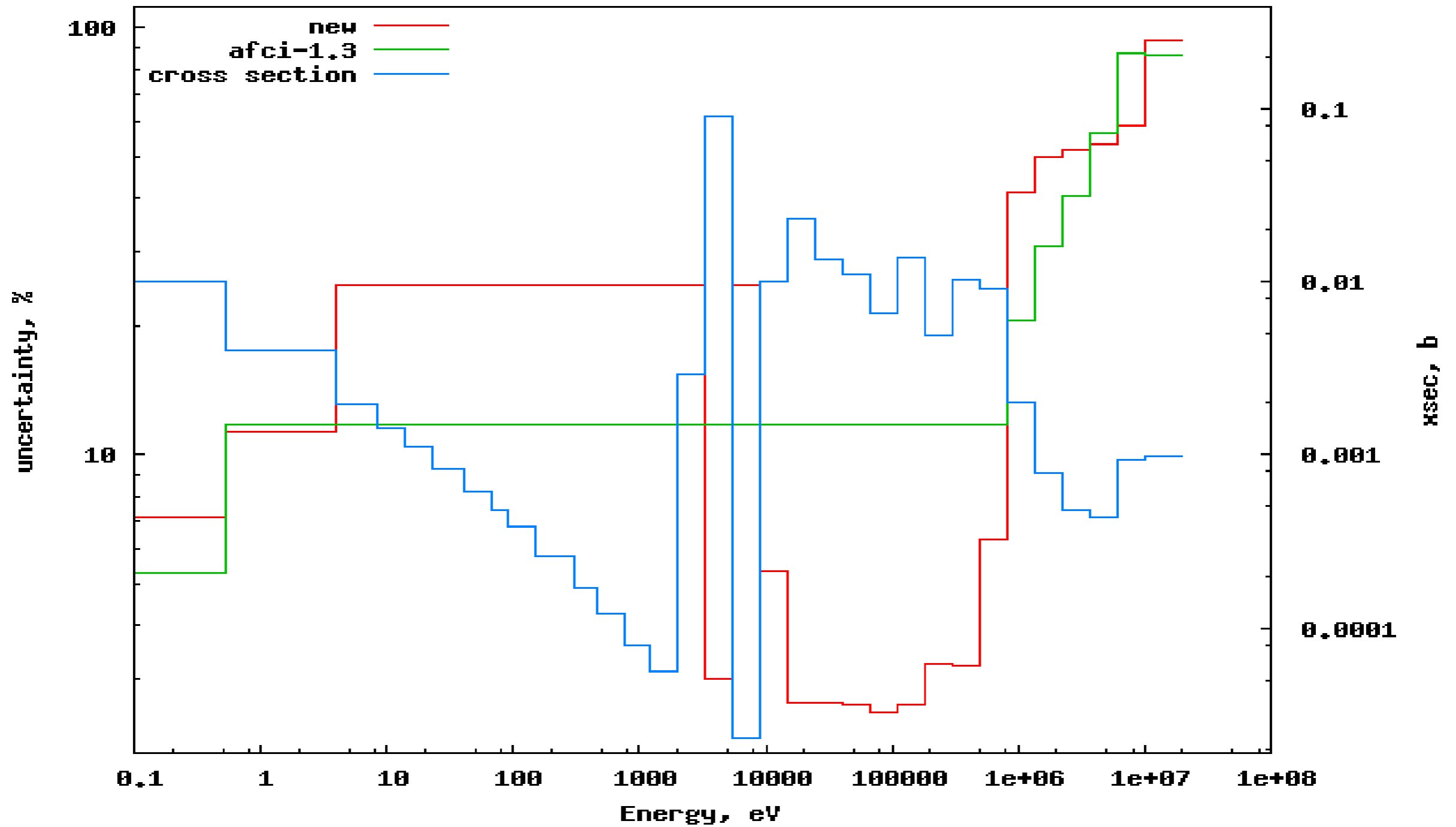
- Check/Uncheck All
- Venturini 1997
- Kenny 1977
- Kenny 1977
- Allen 1975
- Frenes 1974
- Stieglitz 1971
- Kapchigashev 1964
- Pomerance 1952

Remove EXFOR

[Download plot for your article](#)

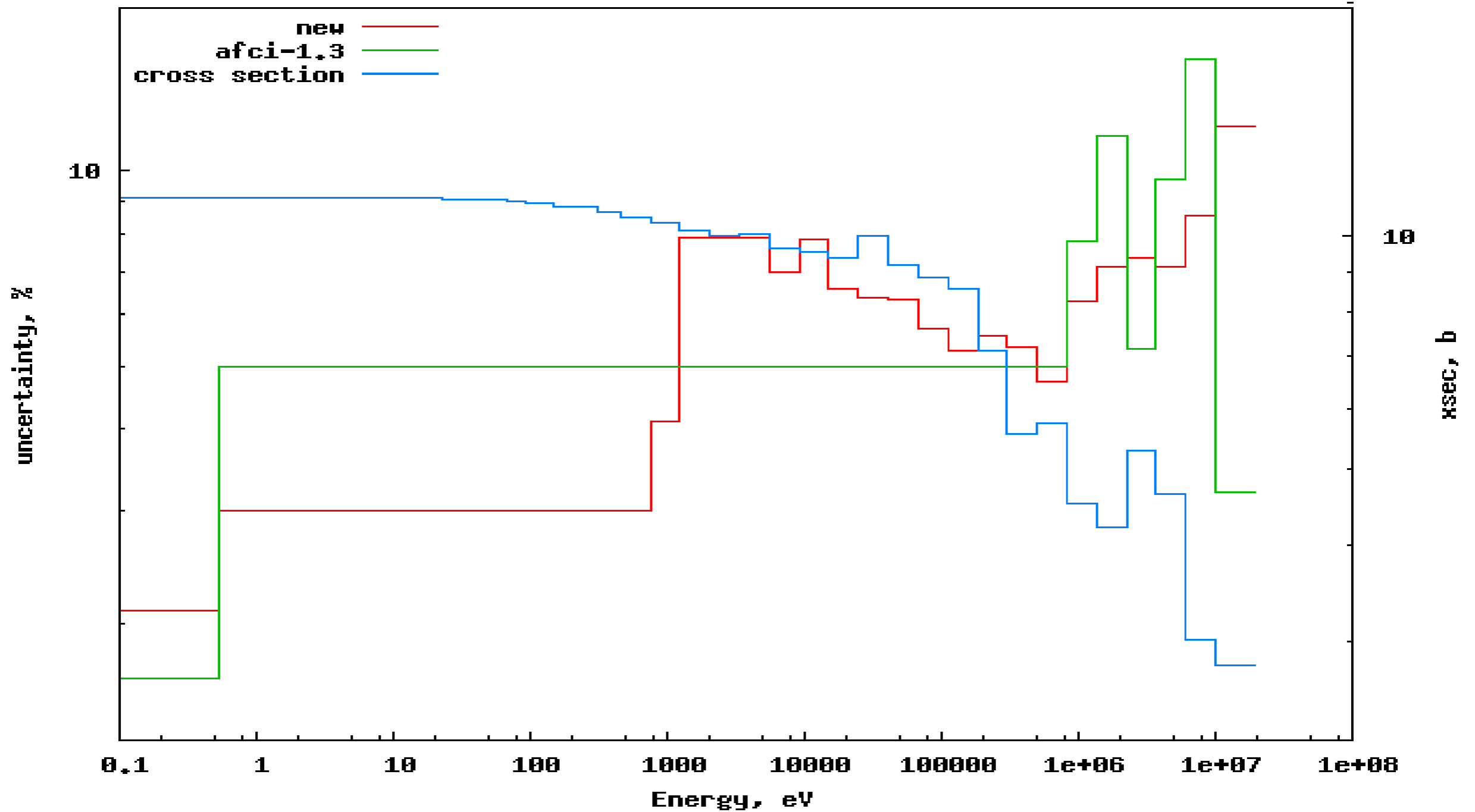
206-Pb capture

082_Pb_206 - HT102



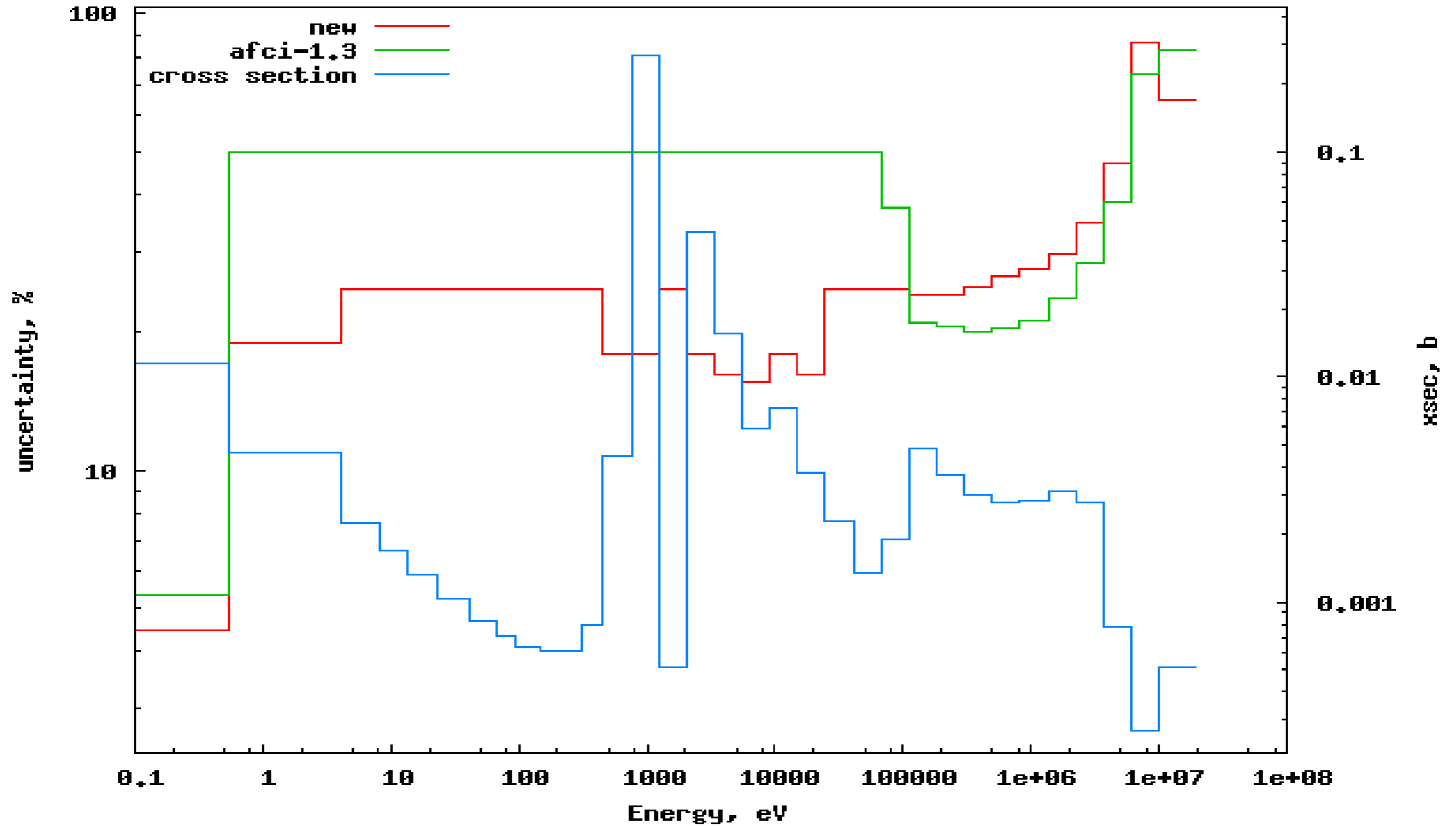
206-Pb elastic

082_Pb_206 - MT2



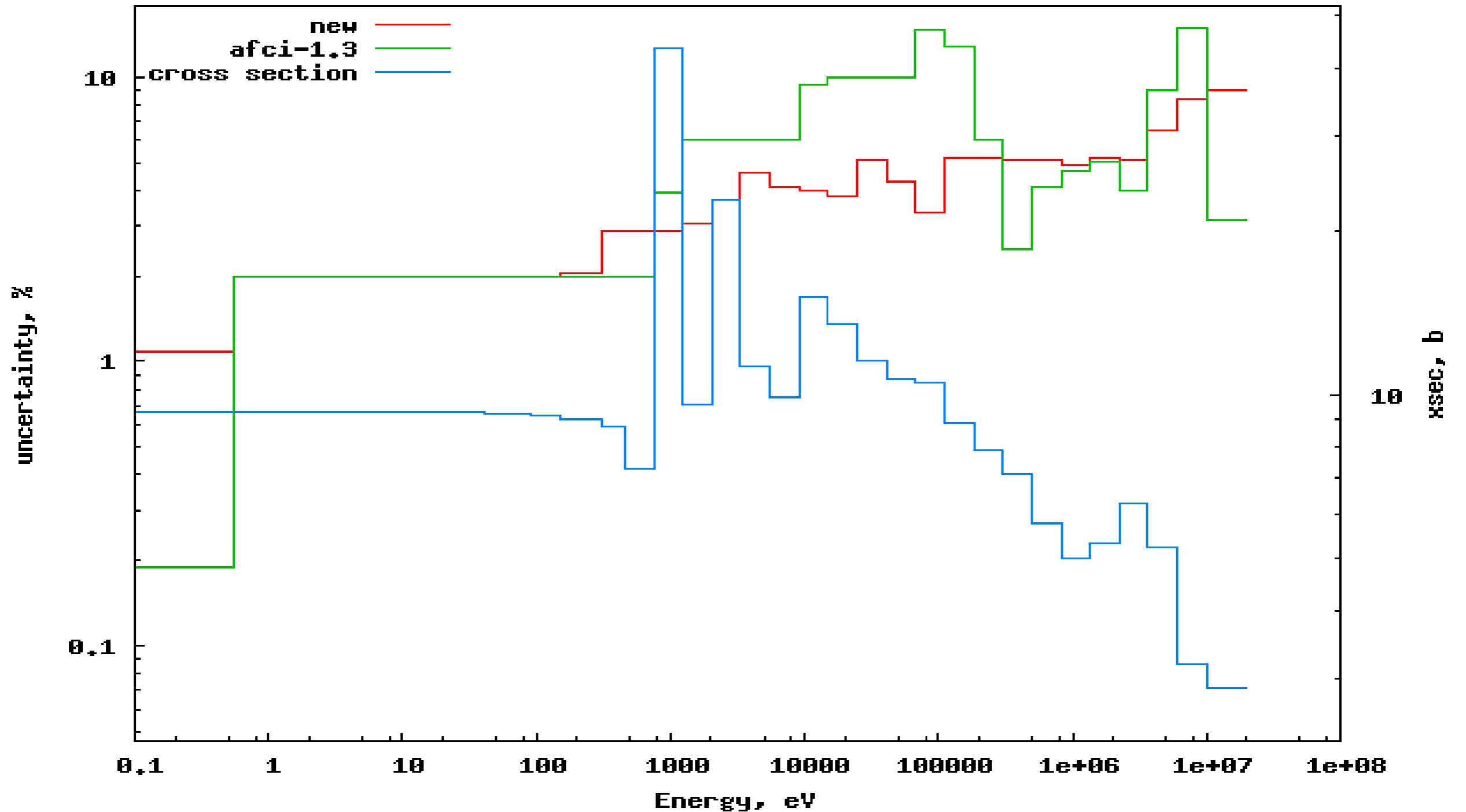
209-Bi capture

083_Bi_209 - HT102

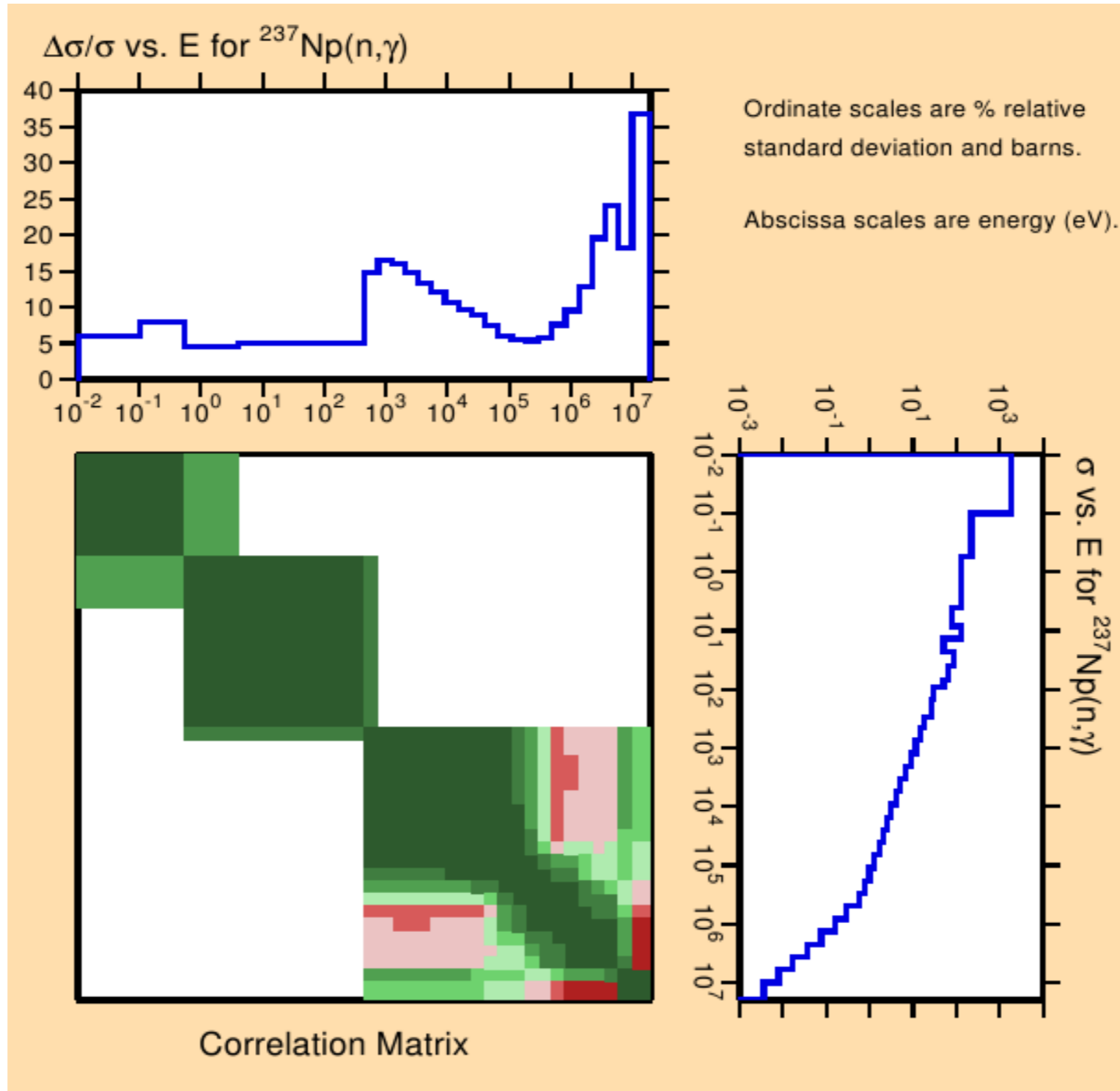


209-Bi elastic

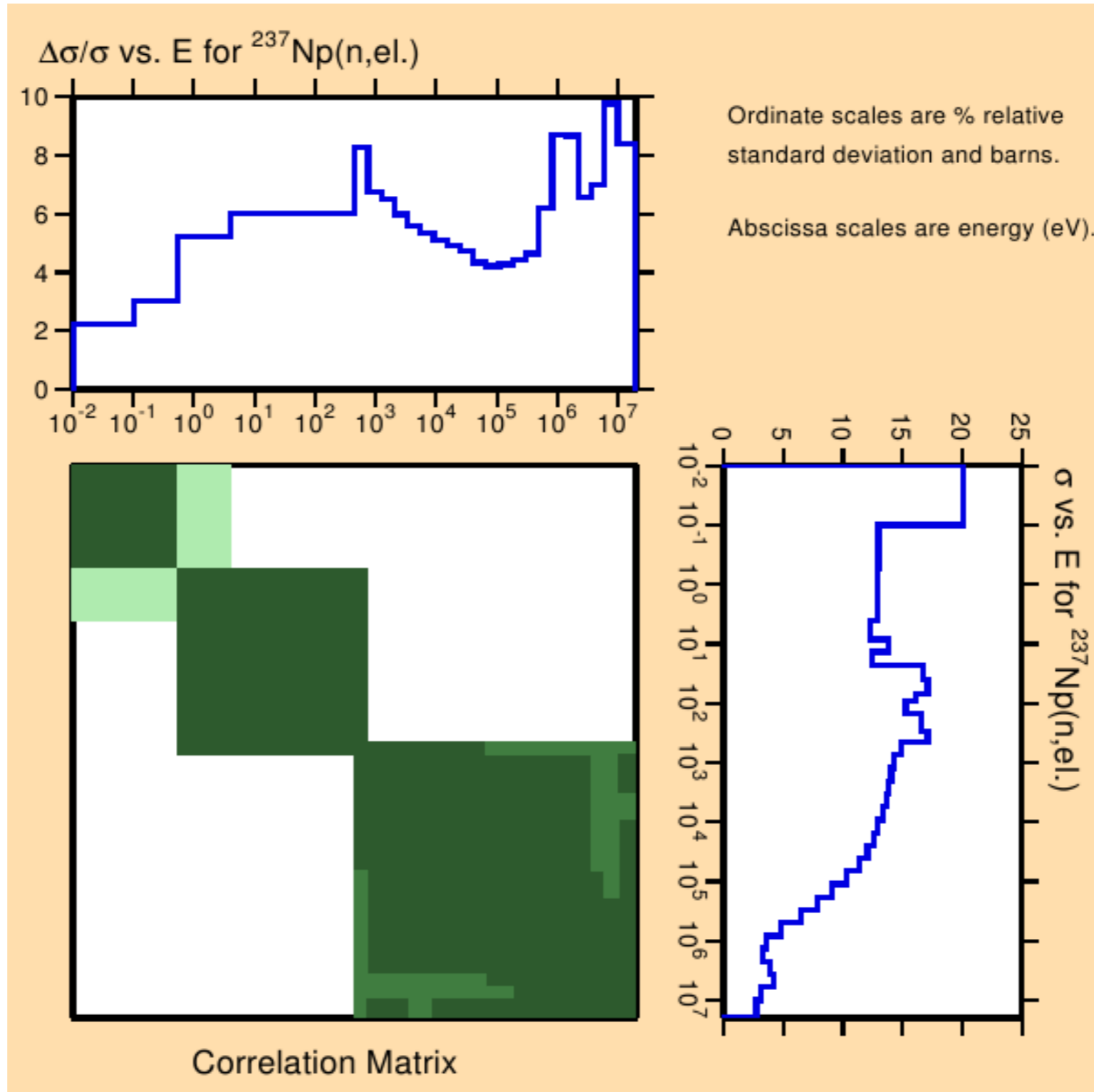
083_Bi_209 - HT2



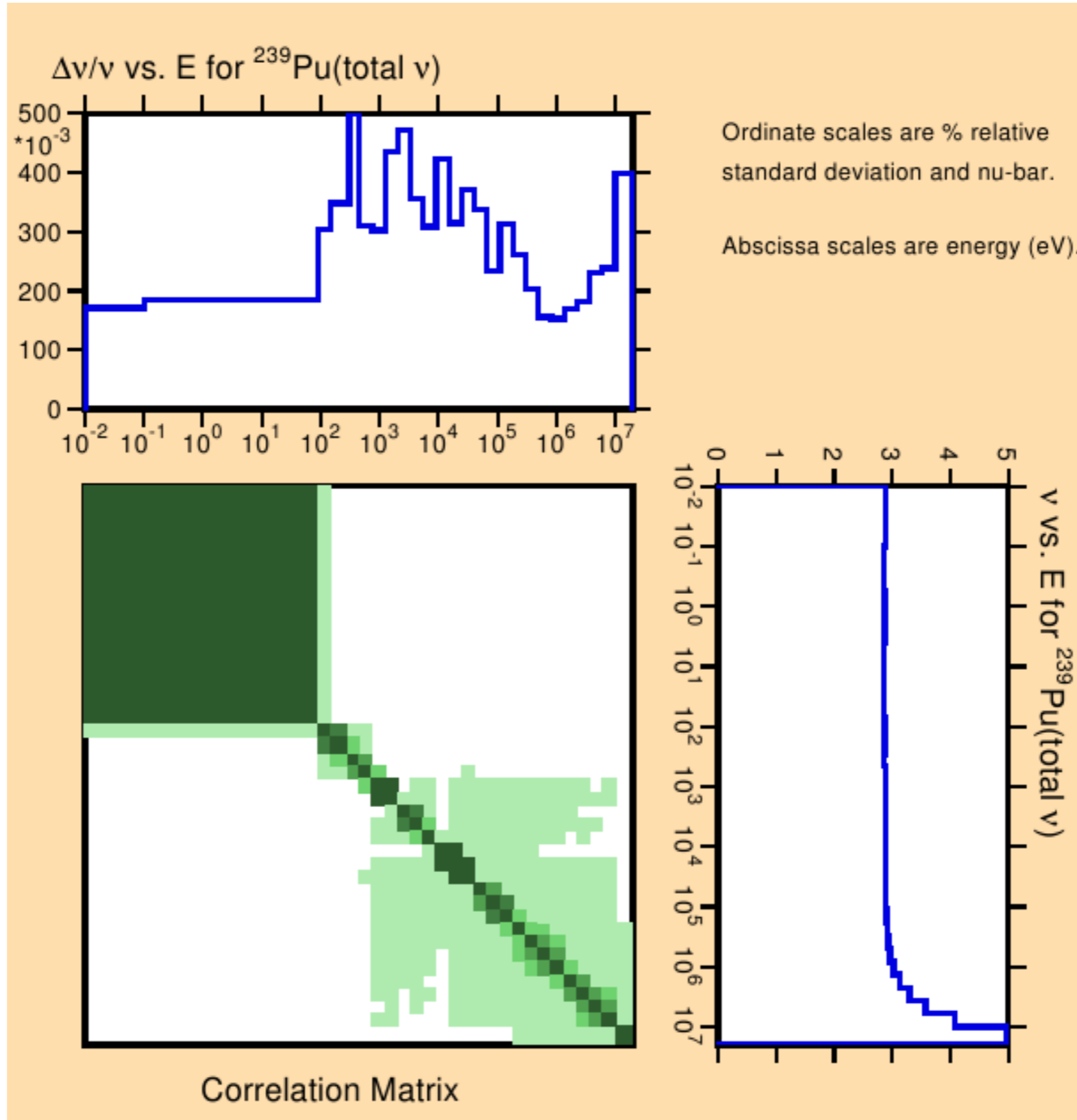
237-Np capture



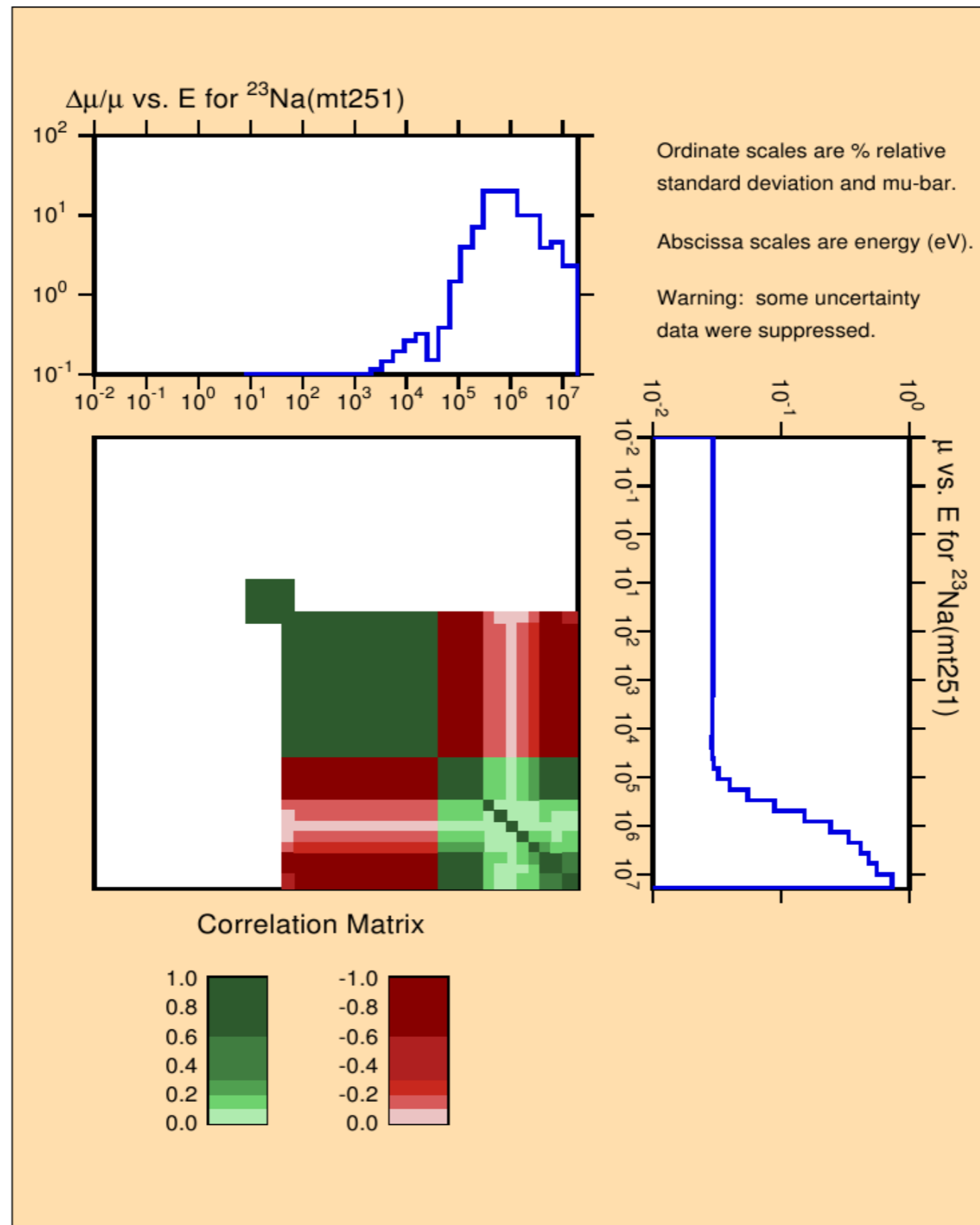
237-Np elastic



239-Pu nubar (LANL)



^{23}Na mubar (BNL)



^{56}Fe mubar

