AFCI-1.2 Covariance Library

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CSEWG Covariances, November 2009

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U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY

Outline:

- Goals of Advanced Fuel Cycle (AFCI) Data Adjustment
- Overview of the AFCI-v1.2 library
- Key Materials
- Quality Assurance

Developed for Data Adjustment:

- Overall goal: use integral experiments to adjust covariances and cross sections, create improved library
  - select integral experiment, calculate sensitivity S_R of experiment to nuclear data

$$(\Delta R)^2 = \mathrm{S}_R^{\mathrm{T}} \mathrm{D} \mathrm{S}_R$$

  - adjust nuclear data within bounds of covariances to improve C/E
- Requires good covariance estimates!

AFCI covariance library

- 110 materials (20 Actinides, 12 Light materials, 78 structural + FP)
- Important materials treated individually at several institutions.
- Bulk of library (approximately 70 of 110 files, FPs and structural) based on the ‘low-fidelity’ covariance estimates from LANL,ORNL,BNL
  - Experimental uncertainties in thermal, resonance regions, model-based covariances from EMPIRE +KALMAN in fast region

AFCI covariance library

- Initial version (GNEP 1.0) released October 2008
- GNEP 1.1 April 2009, mainly fixes for structural materials
- AFCI 1.2 August 2009, many fixes for minor actinides, structural and fission products

AFCI covariance library

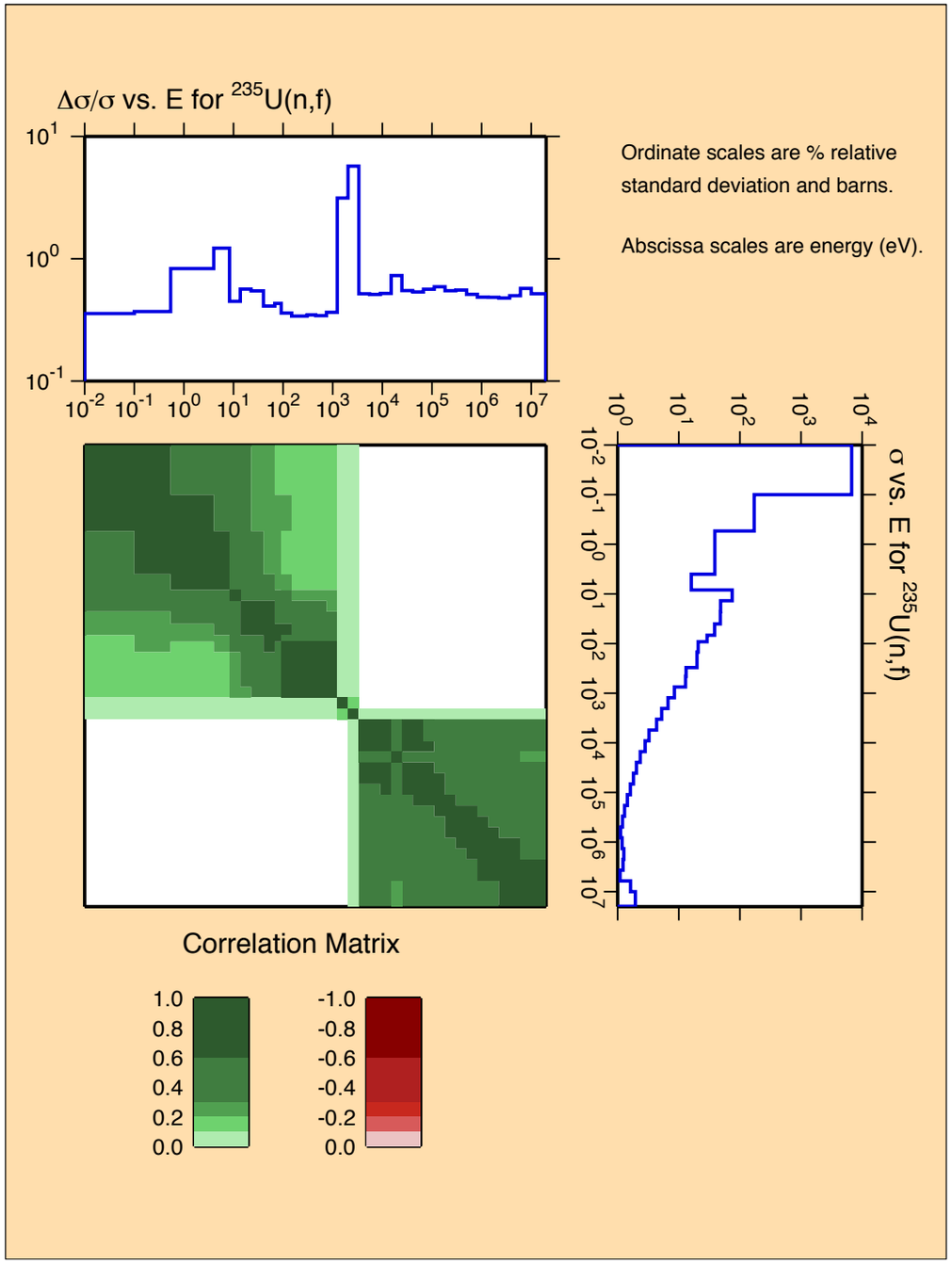
- Active user community (INL and ANL) are providing valuable feedback
- Library is currently available for testing and development. As the project evolves, a future version could become available for general use

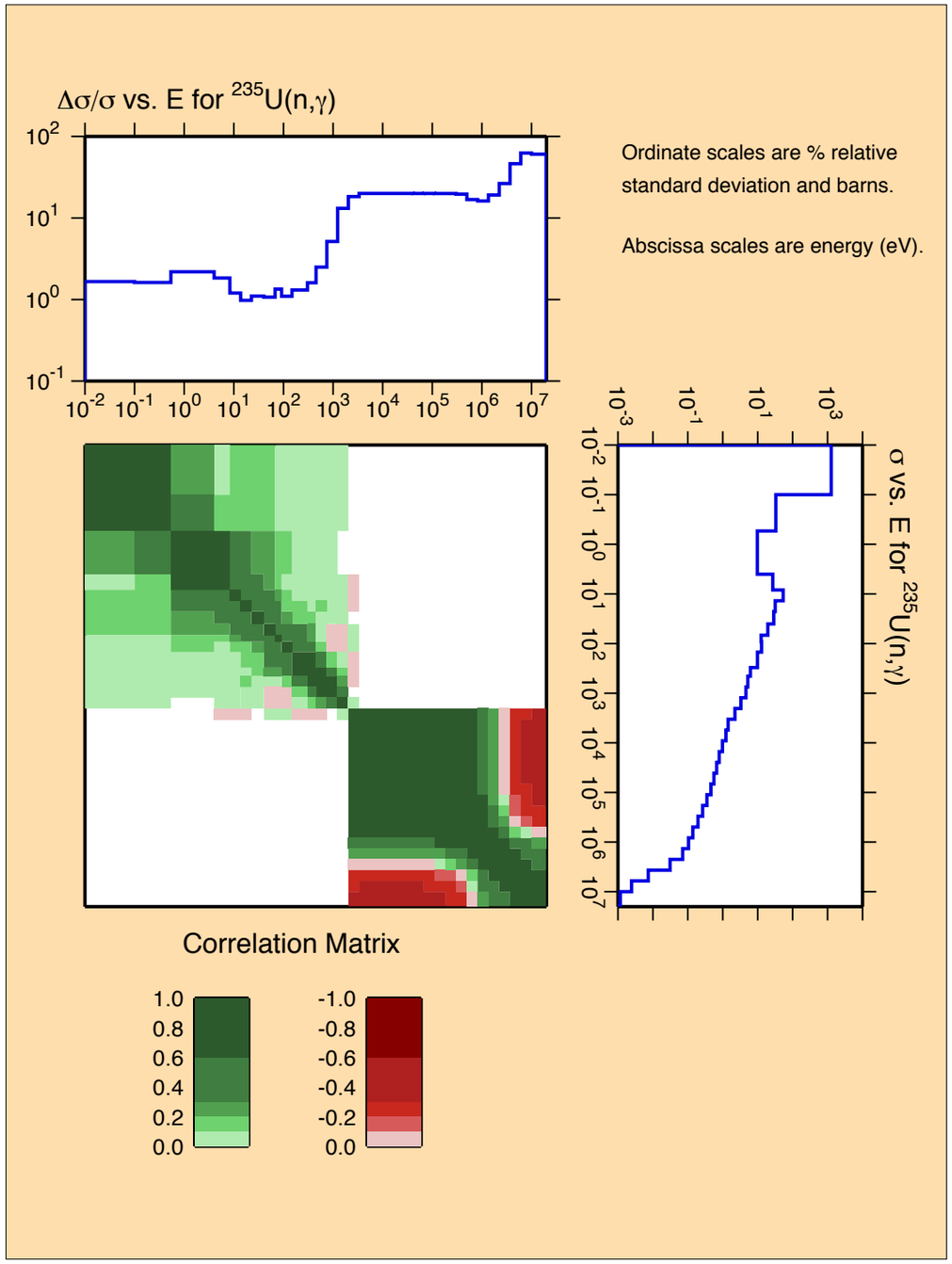
Major Actinides

- Produced by LANL and ORNL, using GNASH +KALMAN methodology in fast region, SAMMY for resonances

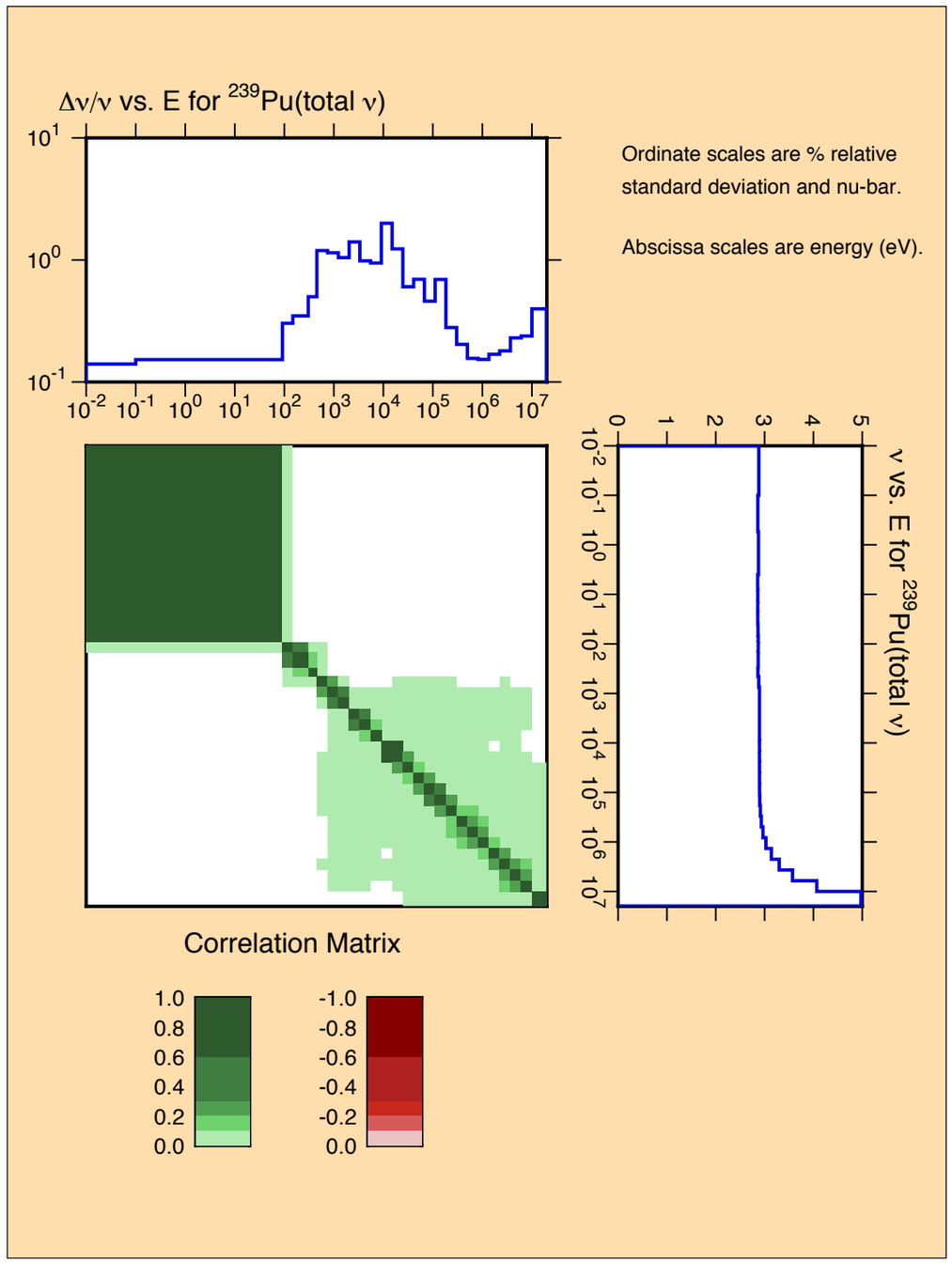
1	90-Th-232	ENDF/B-VII
2	92-U-233	ENDF/A, LANL/ORNL 2008
3	92-U-235	ENDF/A, LANL/ORNL 08/09
4	92-U-238	ENDF/A, LANL/ORNL 2008
5	94-Pu-239	ENDF/A, LANL/ORNL 08/09

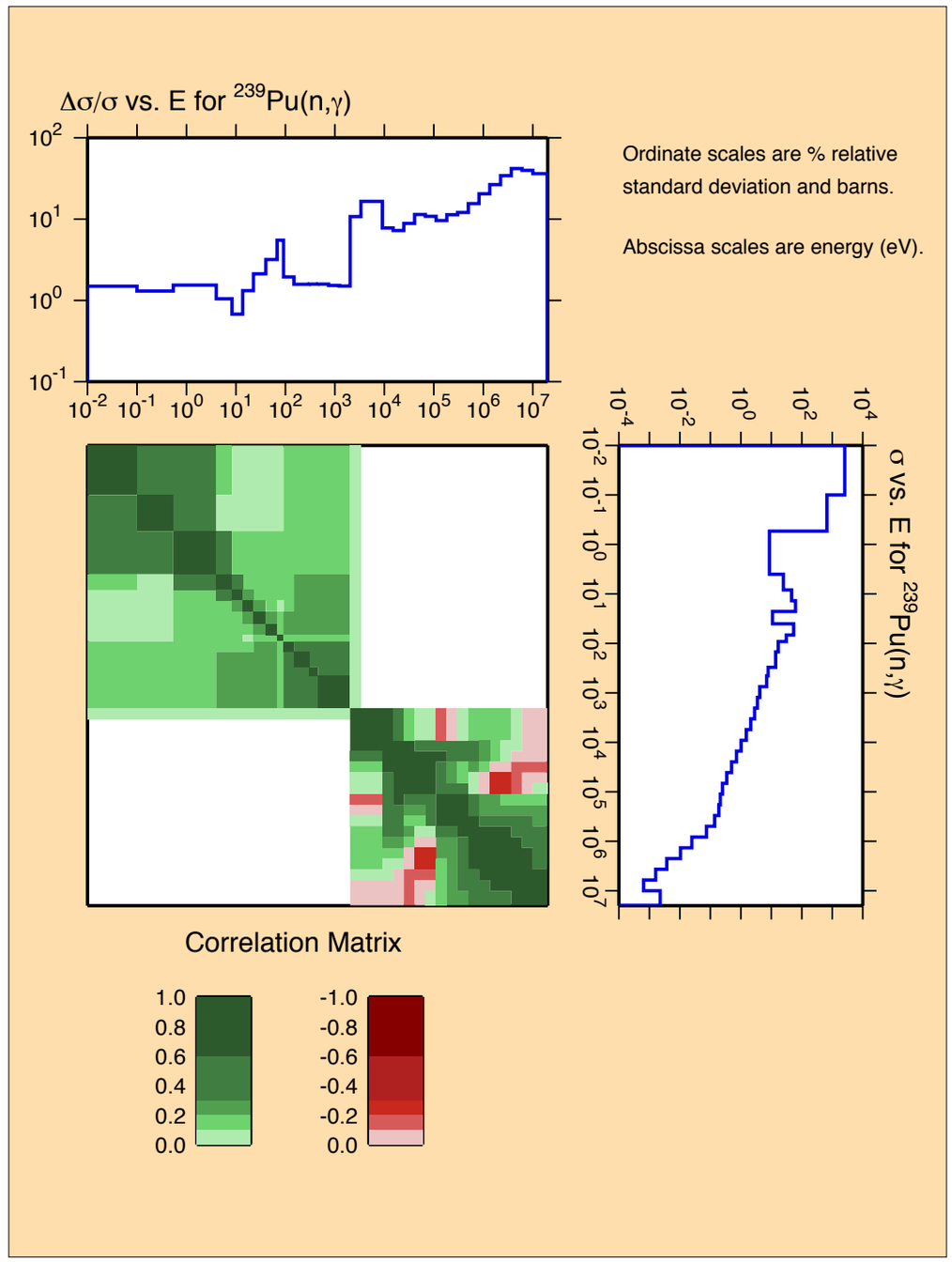
^{235}U


Δσ/σ vs. E for 235U(n,f)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 235U(n,f)
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

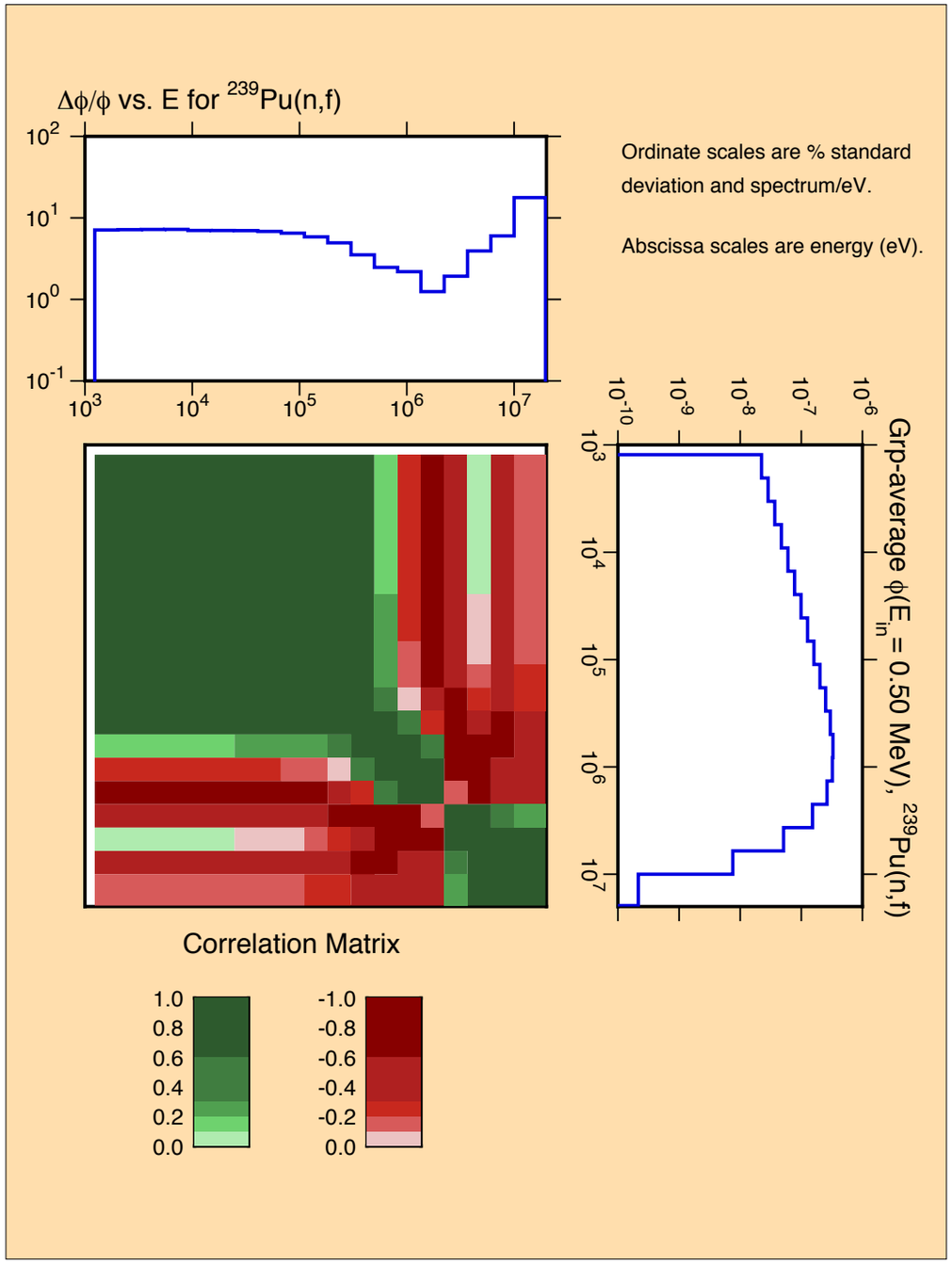

Δσ/σ vs. E for 235U(n,γ)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 235U(n,γ)
Correlation Matrix
1.0
0.8
0.6
0.4
0.2
0.0
-1.0
-0.8
-0.6
-0.4
-0.2
0.0

^{239}Pu


Δν/ν vs. E for 239Pu(total ν)
Ordinate scales are % relative standard deviation and nu-bar.
Abscissa scales are energy (eV).
ν vs. E for 239Pu(total ν)
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


Δσ/σ vs. E for 239Pu(n,γ)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 239Pu(n,γ)
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

^{239}Pu PFNS



Problem: covariance matrix should obey the sum-to-zero rule:

$$\sum_{i \ or \ j} M_{i,j} = 0$$

but processed 33-group file does not sum to zero now. Discuss further in later session?

Minor Actinides:

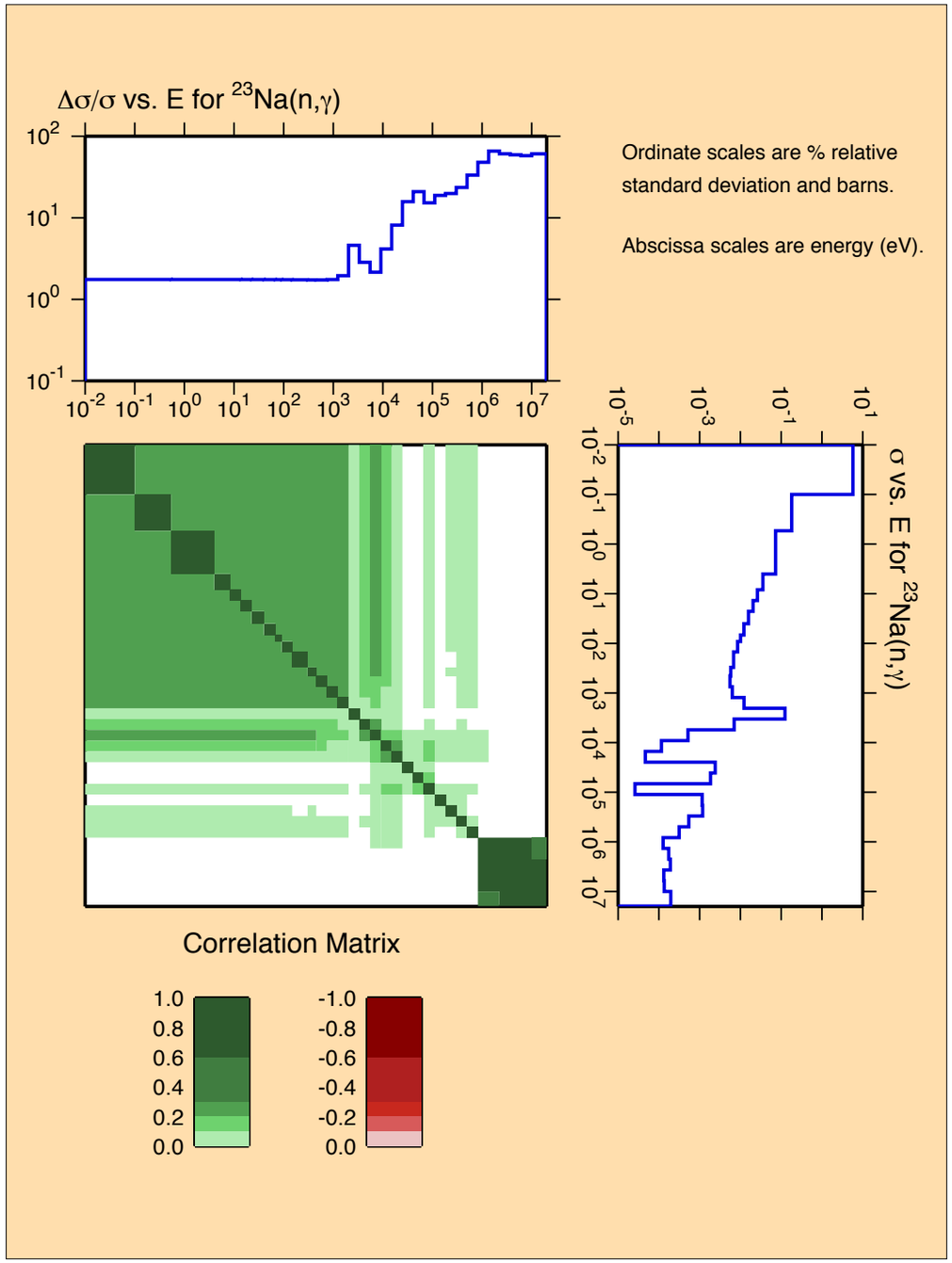
- For 1 Minor Actinide (^{246}Cm) covariances came from ENDF/B-VII
- Covariances for 14 MA previously produced using EMPIRE+KALMAN approach for SG26, adapted to current work
  - *Do not* correspond to processable ENDF files! Needs improvement

Structural Materials

- From several sources, include:
  - 23Na from M.Pigni (BNL), produced for Data Assimilation project
  - 56Fe adopted from JEFF-3.1 / BROND (Tagesen, Pronyaev, Vonach, 1995)
  - 52Cr, 53Cr and 58Ni, produced at BNL using EMPIRE+KALMAN in fast region, Atlas for resonance region.

^{23}Na:

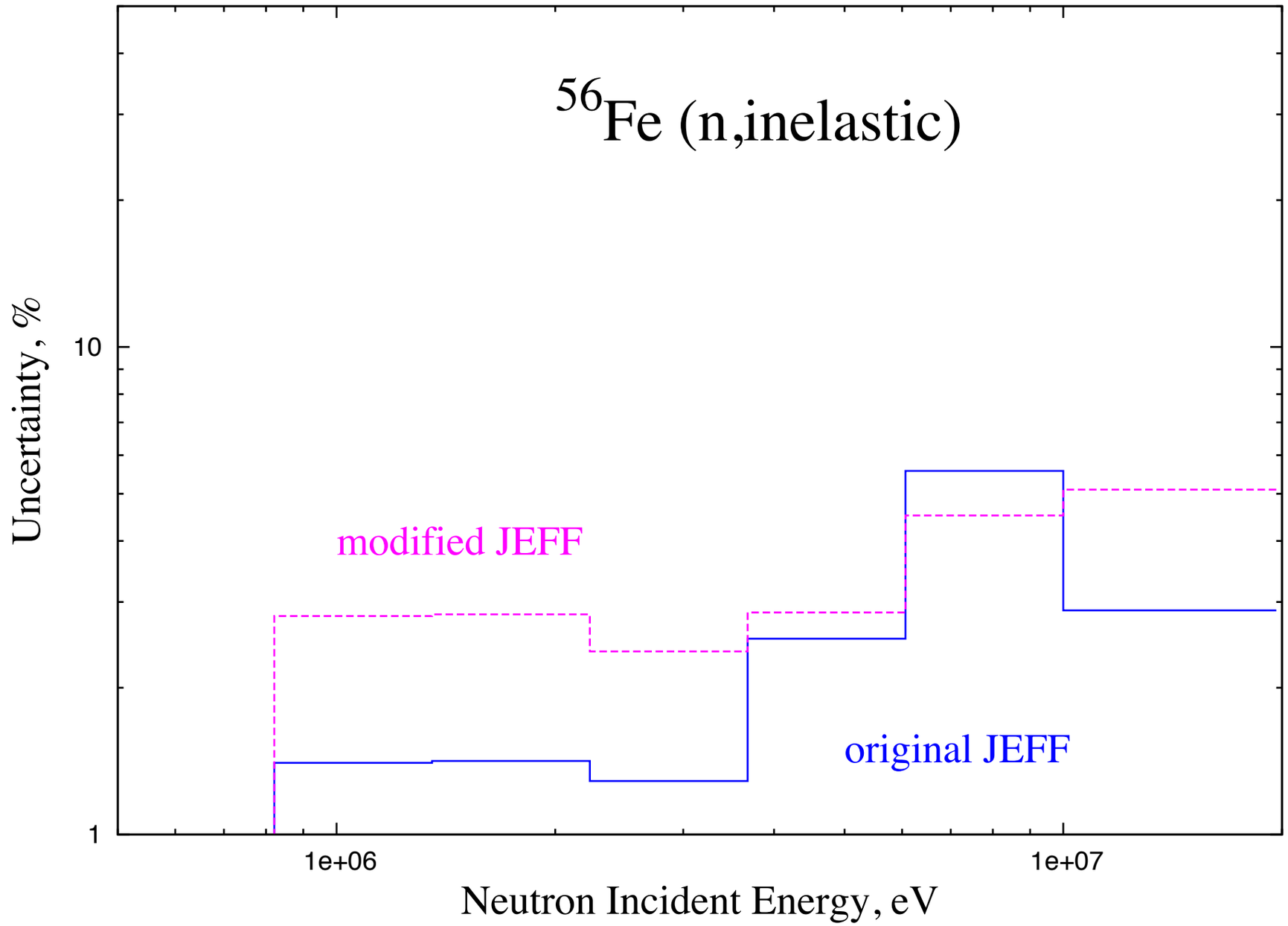
- Using new BNL evaluation by M. Pigni, created for AFCI Data Assimilation effort



^{56}Fe:

- Two ‘recent’ (mid-nineties) evaluations contain covariances: Shibata et al. in JENDL3.3 and Pronyaev/Vonach in JEFF3.1 (also adopted by BROND)
- Trouble in both: surprisingly low values for elastic uncertainties in JENDL, inelastic in JEFF
- Currently using JEFF/BROND version, some changes introduced

^{56}Fe cont.


56Fe (n,inelastic)
Uncertainty, %
10
1
1e+06
1e+07
Neutron Incident Energy, eV
modified JEFF
original JEFF

Low-fidelity

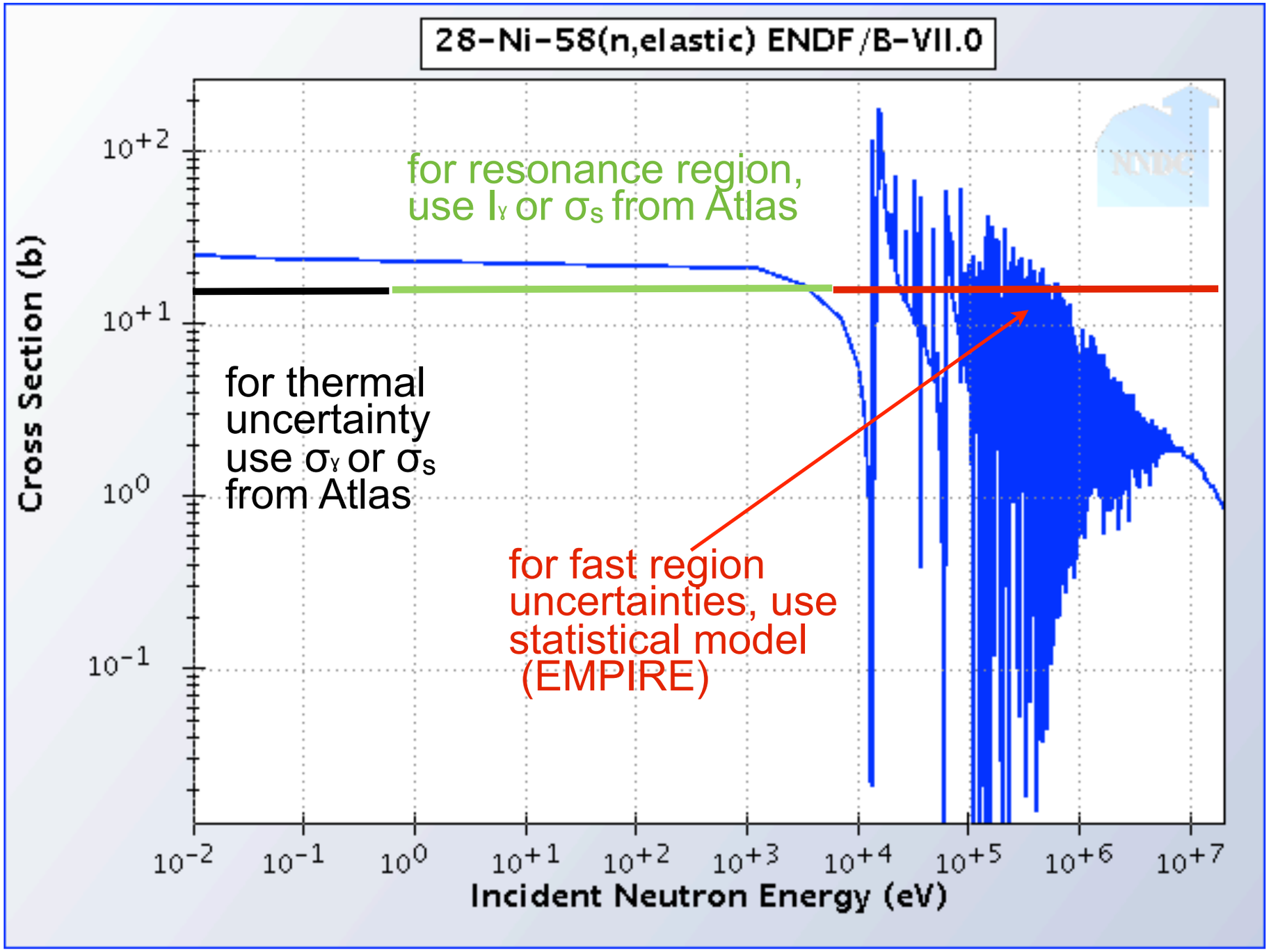
- Low-fidelity project [1] tries to address growing need for covariances. Takes uniform approach:
  - experimental basis in thermal, resonance regions (Atlas of Neutron Resonances)
  - EMPIRE+KALMAN approach in fast region
- Covariance estimates for >300 isotopes generated

[1] R.Little et al, Nuclear Data Sheets vol.**109**, 2008

Low-fidelity cont.

- Low fidelity project was the basis for many materials in library
- Some issues with low fidelity:
  - missing low-energy uncertainties if no values could be found. Especially for (n,elastic) in thermal, RR
  - Resolved region assumed to always end at 5 keV! Appropriate (perhaps) for actinides, not elsewhere

Trouble with Low-fidelity:



BUT, statistical model doesn't work well when the cross section is fluctuating! Produces large, unphysical uncertainties

Thus, we need to change treatment of resonance region

Quality Assurance:

- Early versions of library had trouble with
  - large uncertainties (> 100%)
  - small uncertainties (<< 1%)
  - uncertainty=0 for non-threshold reactions
  - ‘peaks’, ^{239}Pu nubar for example
  - and so on
- Library is all in uniform (33-group) format, so may automatically check for these problems

Quality Assurance (continued):

- program ‘unCor’ checks output of PUFF/NJOY for problems in ‘uncertainties’ and ‘correlations’
- Small uncertainties still appear in v1.2 of library

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Uncertainties too large: 19 total

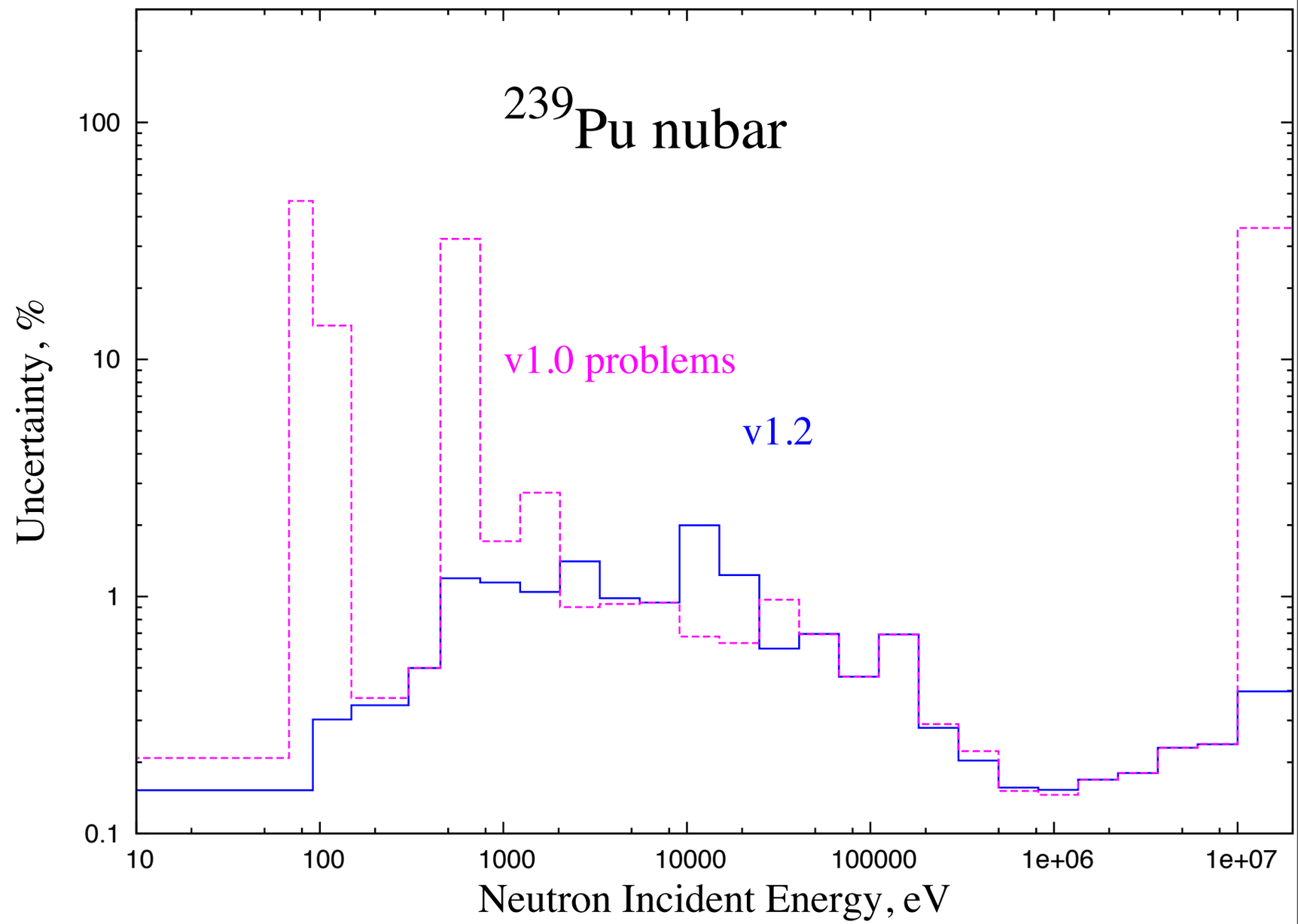
MT16  in  001_H_002, max = 100.00%
MT102 in 003_Li_007, max = 100.00%
MT4   in  005_B_010, max = 100.00%
MT102 in 040_Zr_090, max = 100.00%
MT102 in 040_Zr_095, max = 100.00%
MT2   in 040_Zr_095, max = 100.00%
MT51  in 090_Th_232, max = 100.00%
MT852 in 090_Th_232, max = 100.00%
MT18  in  092_U_238, 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

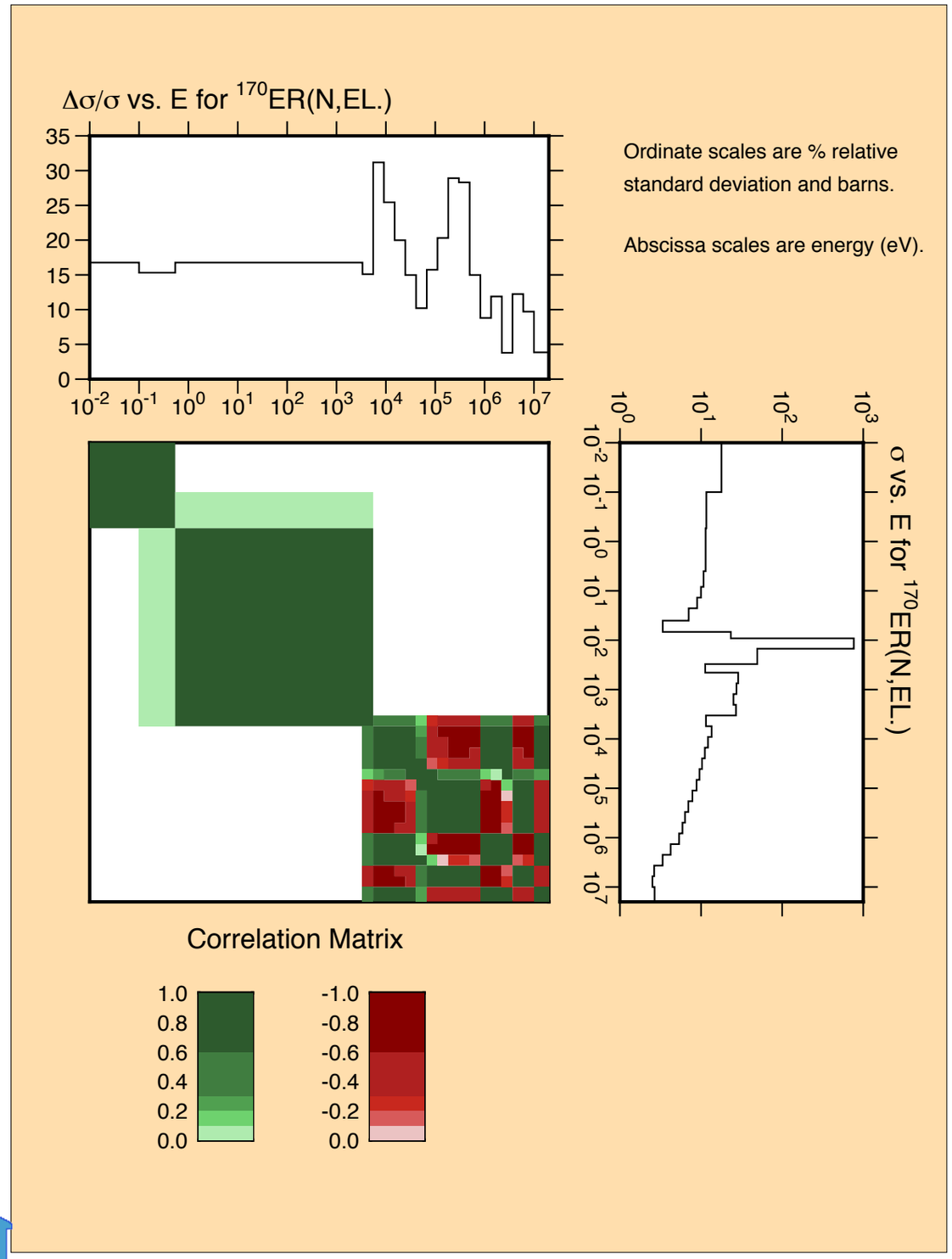
MT1   in  001_H_001, min = 0.29% in bin 33 (27 bins < 1%)
MT2   in  001_H_001, min = 0.30% in bin 12 (27 bins < 1%)
MT1   in 002_He_004, min = 0.50% in bin 11 (28 bins < 1%)
MT2   in 002_He_004, min = 0.50% in bin 11 (28 bins < 1%)
MT1   in 003_Li_006, min = 0.20% in bin 30 (21 bins < 1%)
MT105 in 003_Li_006,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

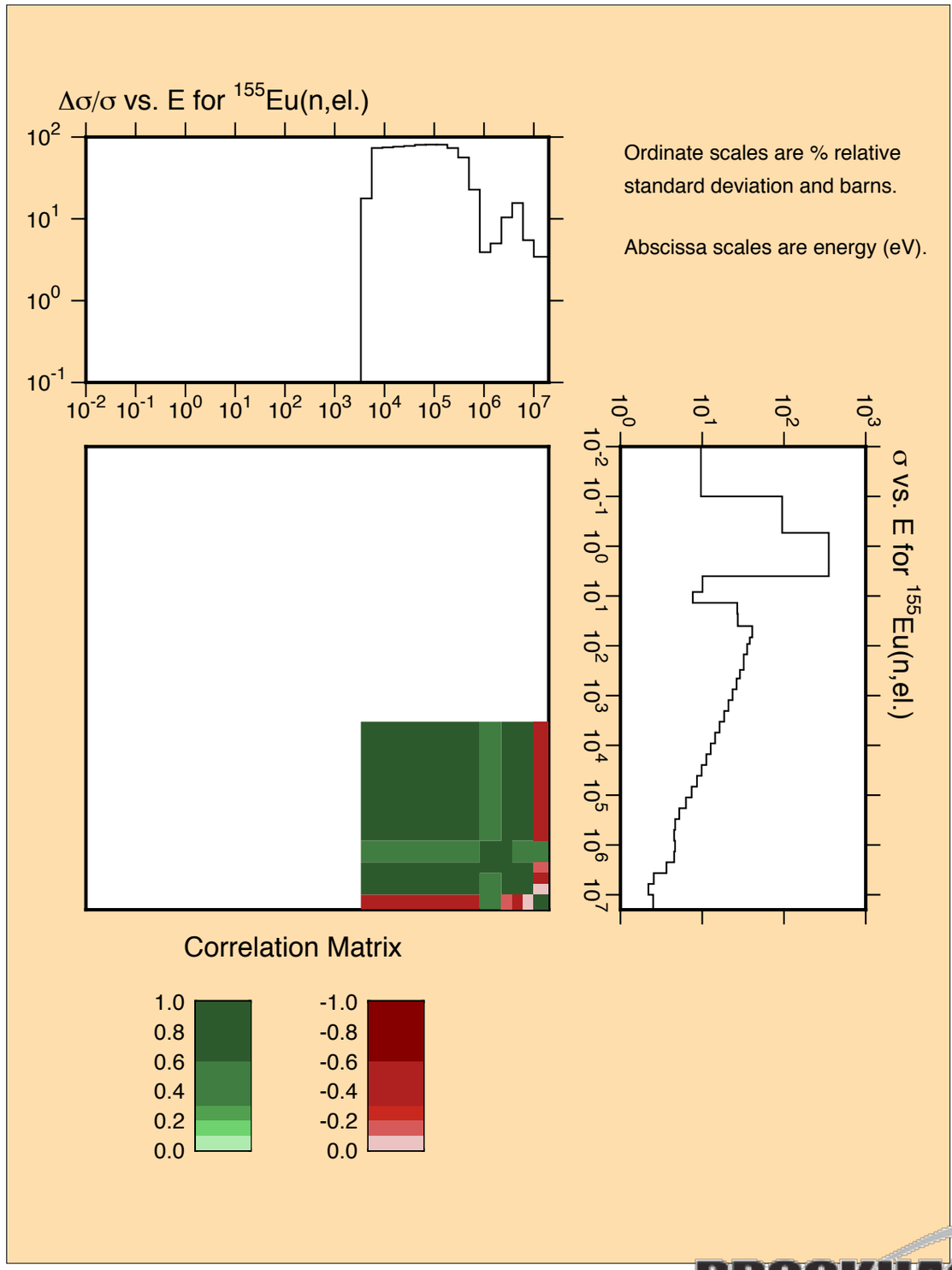
^{239}Pu nubar:

- 'Peaks' in v1.0 from uncertainty fluctuations are smoothed:



(n,elastic) OM peaks:





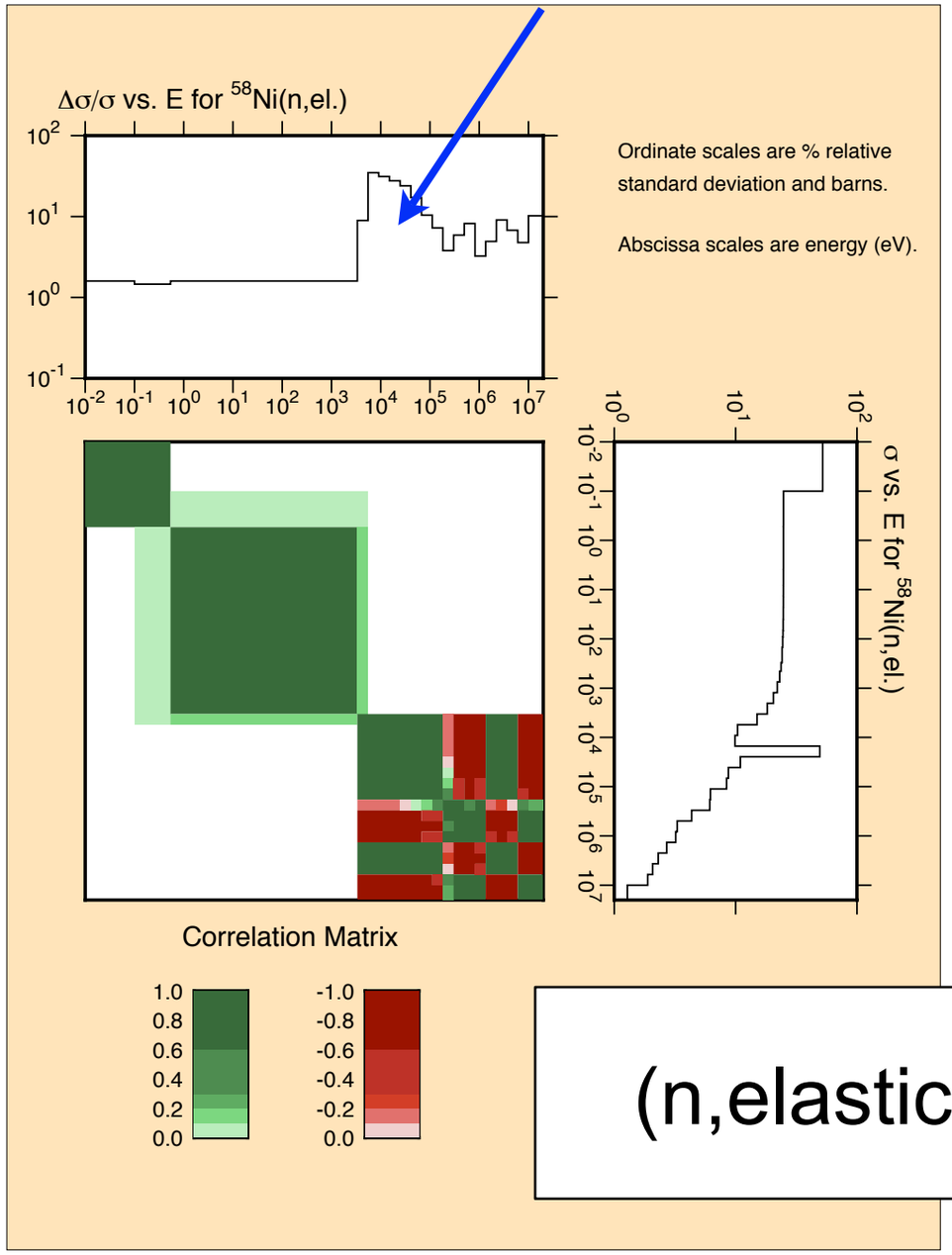
Summary

- New version (v1.2) of AFCI covariance library released August 2009
- Active user community (mainly ANL,INL) are providing valuable feedback towards improving the library
- Files are being tested visually and using automatic procedure for quality assurance

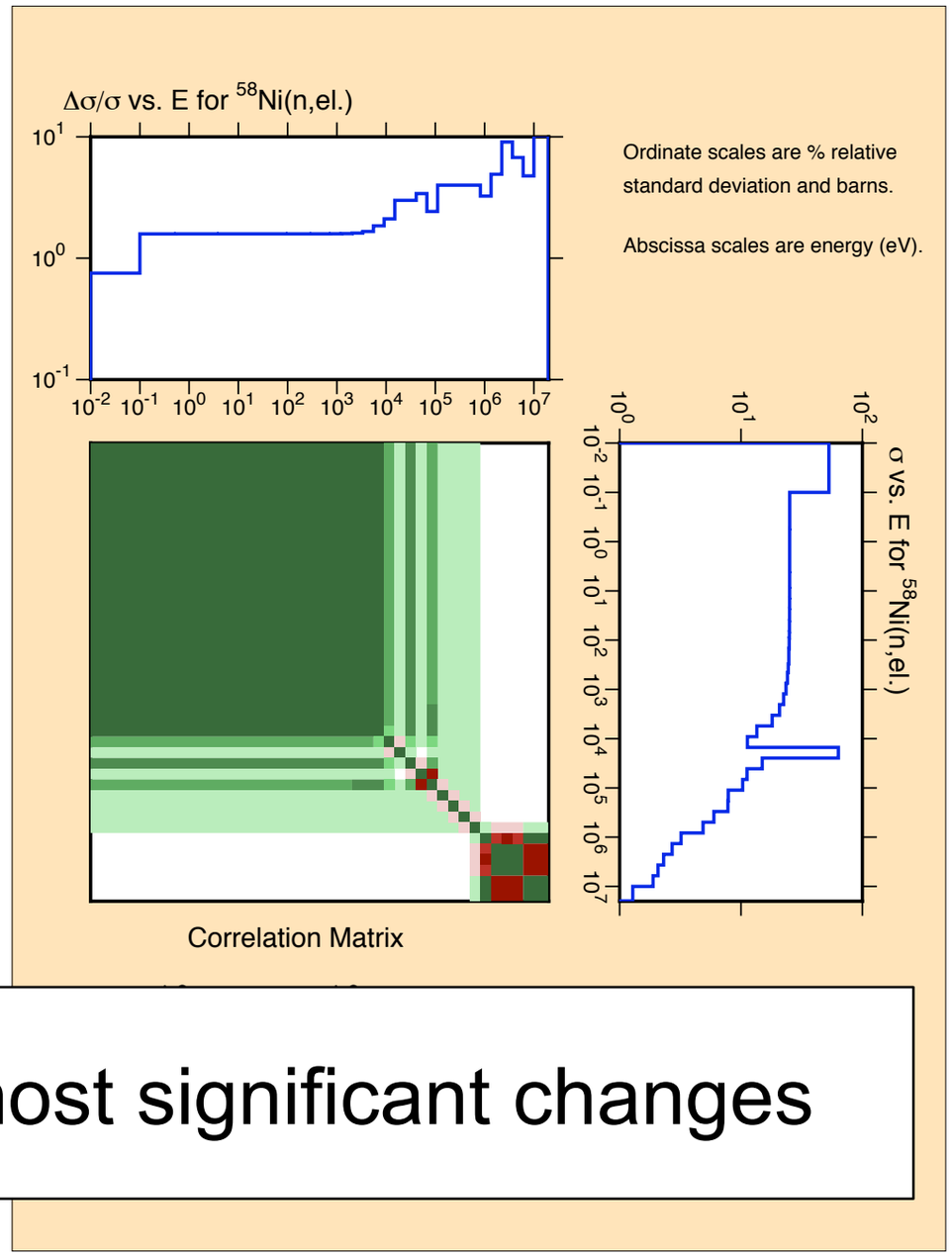
Extras

^{58}Ni:

GNEP v1.0 problem



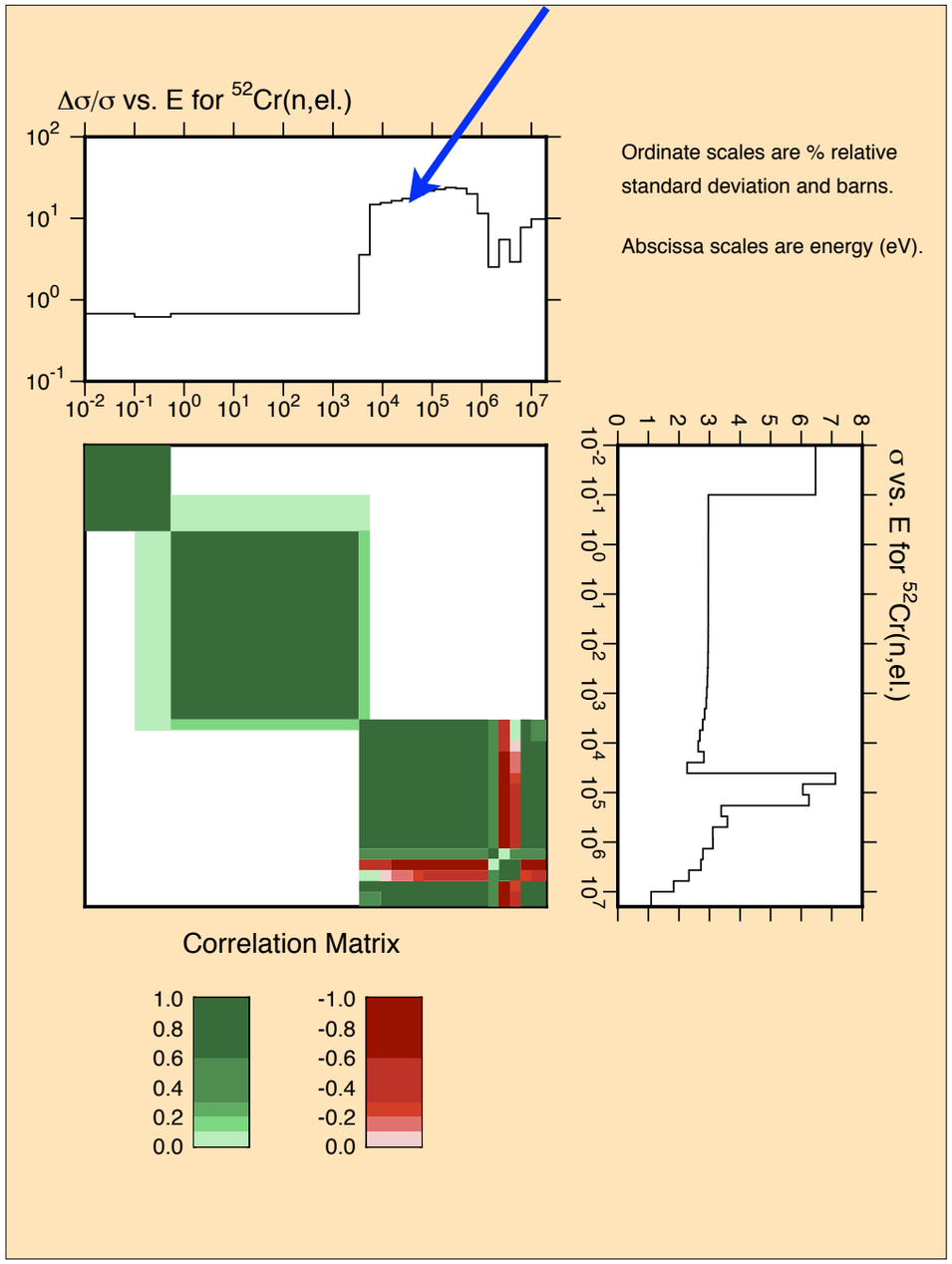
GNEP v1.1:



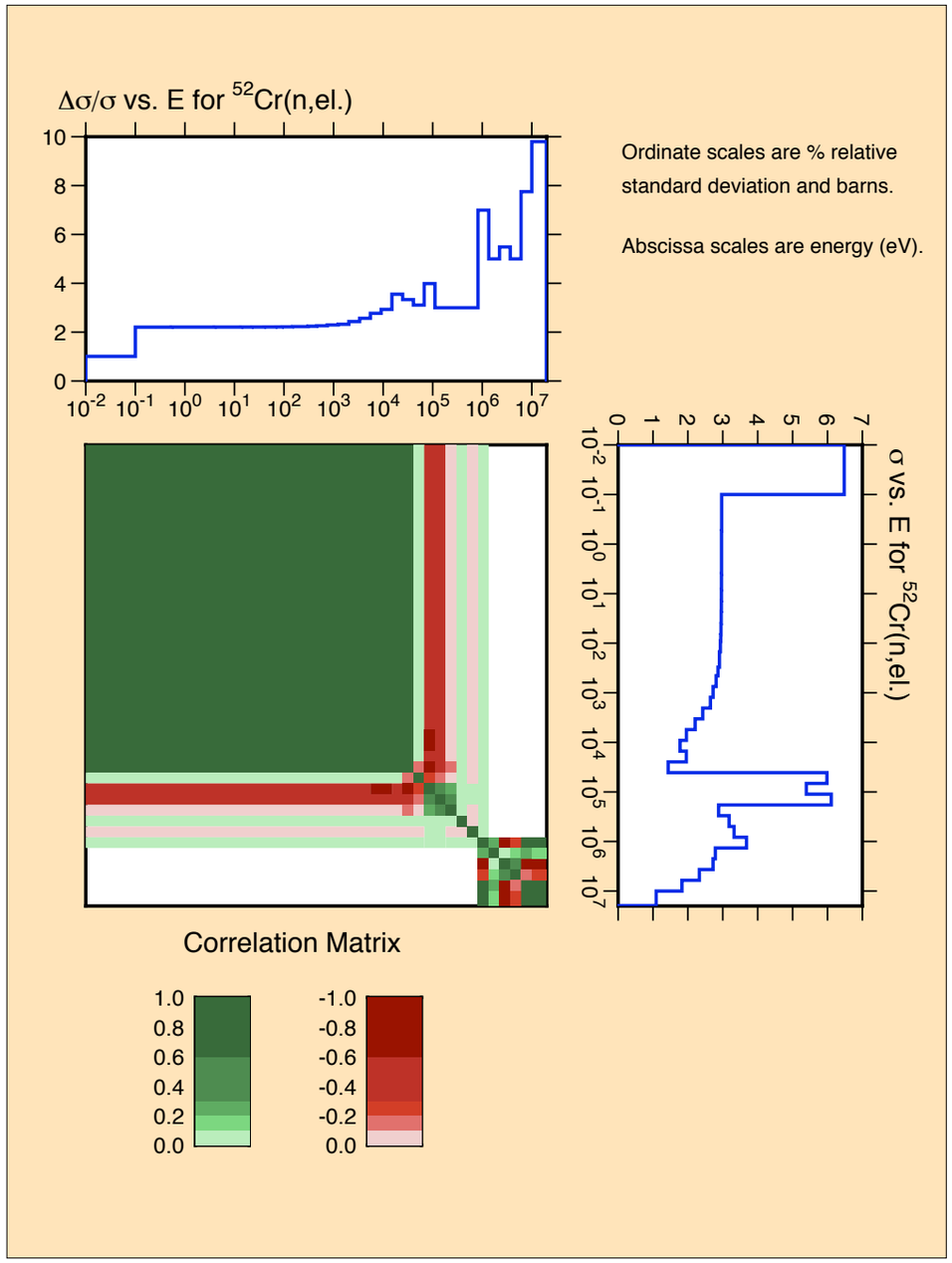
(n,elastic) sees most significant changes

^{52}Cr:

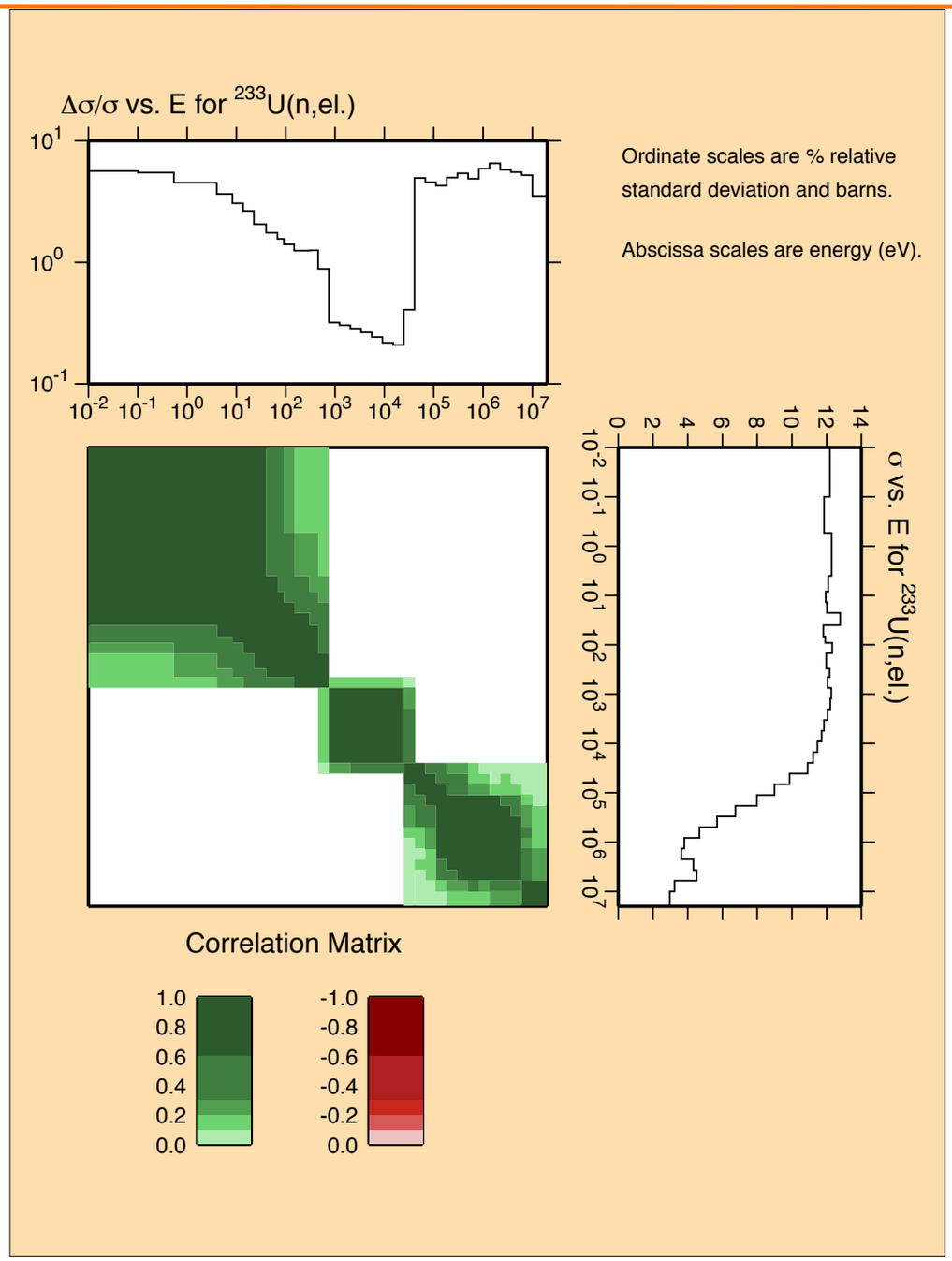
GNEP v1.0 problem



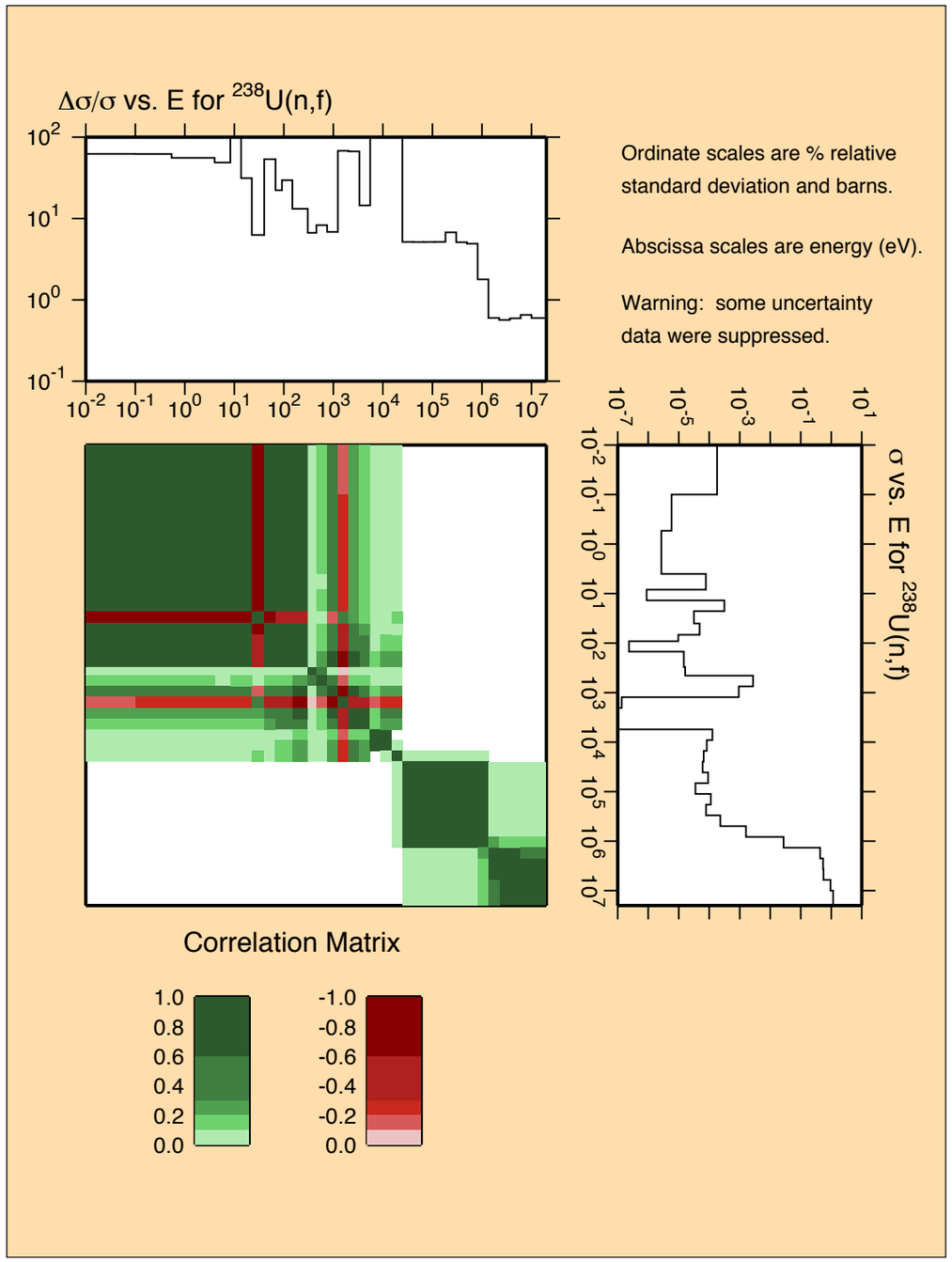
GNEP v1.1:



^{233}U elastic (and fission):



^{238}U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Warning: some uncertainty data were suppressed.
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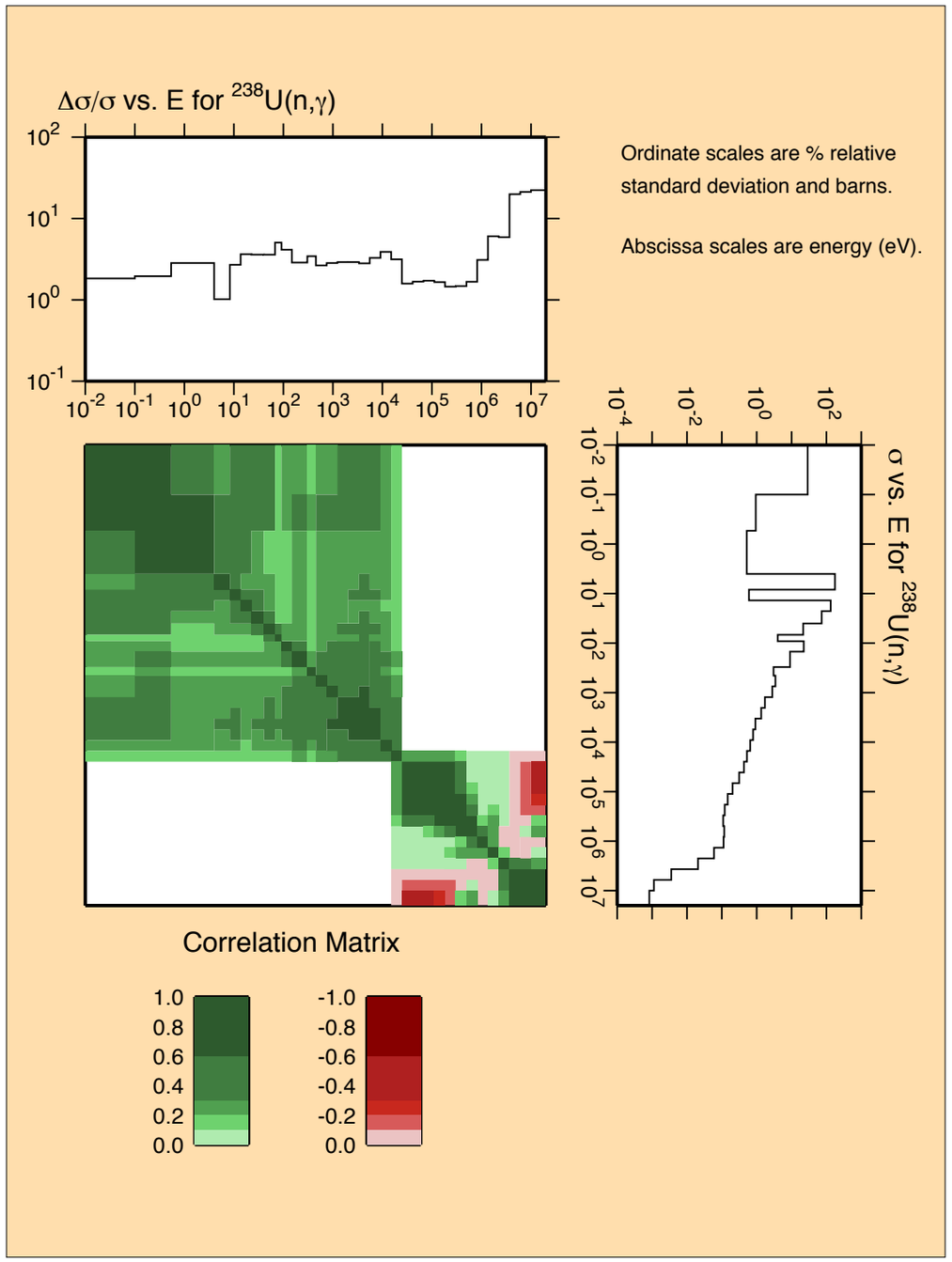
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