ENDF/B-VII.1 Covariances

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Covariances circa ENDF/B-VII.0

- Total materials with covariance data : 26

Covariance	# materials
MF31	2
MF32	10
MF33	24
MF34	0
MF35	0

Covariances in ENDF/B-VII.1

- Total materials with covariance data : 190

Covariance	# materials
MF31	73
MF32	55
MF33	183
MF34	68
MF35	64

Covariances by material

- Light materials : 12
- Structural & fission products : 105
- Actinides : 20
- Minor actinides : 53

Source of covariances

- New ORNL, LANL, BNL evaluations
- IAEA/JSI evaluations
- COMMARA-2.0
- Neutron standards
- JENDL-4
- ENDF/VII.0 evaluations

Methodology

Thermal and Resonance Region

- Source of data
- Experiments
- ENDF file (retroactive method)
- Atlas of Neutron Resonances (ANR)
- SAMMY analysis
- full analysis (MF32, Exp. data)
- retroactive (MF32, ENDF file)
- EMPIRE Resonance Module (MF32, ANR, scattering radius and thermal point uncertainties reproduced through correlations (if possible)
- "Kernel Approximation" (MF33, ANR)
- MF32 with systematic uncertainties in MF33
- 'low-fidelity' (Mark Williams) solution
- Assimilation

Fast neutron range (MF33)

- EMPIRE/KALMAN considering experimental data
- Least Square fitting of experimental data (SOK code)
- EMPIRE/KALMAN without experimental data (Low-Fidelity)
- Dispersion analysis - differences among evaluations (and exp. data)
- Reconsider previous work (ENDF/B-VI.8, Low-Fidelity)
- Visual analysis of experimental data
- Assimilation

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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 in *processed* library, including:

  – small uncertainties: (n,tot) < 1%, (n,el) and (n,γ) < 2%, etc.

  – non-positive-definite matrices

  – ➫Substantial warnings still produced for β5!

  – Negative eigenvalues removed in ENDF files by Dave Brown with fudge

Quality Assurance

- Review of error messages from standard checking codes checkr, fizcon and psyche.

- Some remaining fizcon errors (probably ok):

  - large errors in MF1/MT458 for : ^{227}Ac, ^{237}U, ..

  - doubly-indirect NC-style covariances: ^{16}O, Pb isotopes

  - threshold reactions covariance not starting at 1.0E-05, (allowed in format): W isotopes and ^{232}Th

  - lower energy not 1.0E-05 for each for cross-correlation with threshold reaction: W isotopes and ^{232}Th

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BNL additions

Major focus at BNL has been the adoption of AFCI/COMMARA covariance data

Most materials in COMMARA library had no covariance data in VII.0 and the (mostly MF33) covariances were moved directly

A few materials contained new MF32 covariances which required special handling: ^{50,52,53}Cr and ^{58,60}Ni.

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Additional modifications...

- Zr isotopes: New BNL eval with total modulated following VI.8, JENDL-4 ang dist. for elastic. Modified thermal capture for Zr-90.

- Standards covariances adopted for ^{6}Li, ^{10}B, ^{197}Au, ^{237}U, ^{238}U, ^{239}Pu. Uncertainties increased to cover dispersion, where necessary.

- **Many** more minor fixes & updates.

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COMMARA-2.0 MF33 ⇨ ENDF/B-VII.1β3

- ^{1,2}H, ^{6}Li, ^{9}Be, ^{10,11}B, ^{12}C, ^{15}N, ^{16}O, ^{27}Al

- ^{24,25,26}Mg, ^{28,29,30}Si, ^{54,56,57}Fe

- ^{90,91,92,93,94,95,96}Zr, ^{92,94,95,96,97,98,100}Mo

- ^{155,156,157,158,160}Gd, ^{109}Ag, ^{141}Ce

- ^{101,102,103,104,105}Ru, ^{105,106,107,108}Pd

- ^{143,145,146,148}Nd, ^{149,151,152}Sm, ^{95}Nb, ^{127,129}I

- ^{131,132,134}Xe, ^{133,135}Cs, ^{166167,168,170}Er, ^{153,155}Eu

- ^{141}Pr, ^{139}La, ^{147}Pm, ^{204,206,207,208}Pb, ^{209}Bi

- ^{236}U, ^{237}Np, ^{241}Pu, ^{242m,243}Am

^{50,52,53}Cr & ^{60}Ni

- Here, we adopted COMMARA covariance data in the fast region.

- An addtional MF33 LB=1 section was added to elastic to account for the uncertainty in the scattering radius R'

- For ^{50,52}Cr and ^{58}Ni an addtional MF33 LB=1 sections were added to capture to match COMMARA uncertainties.
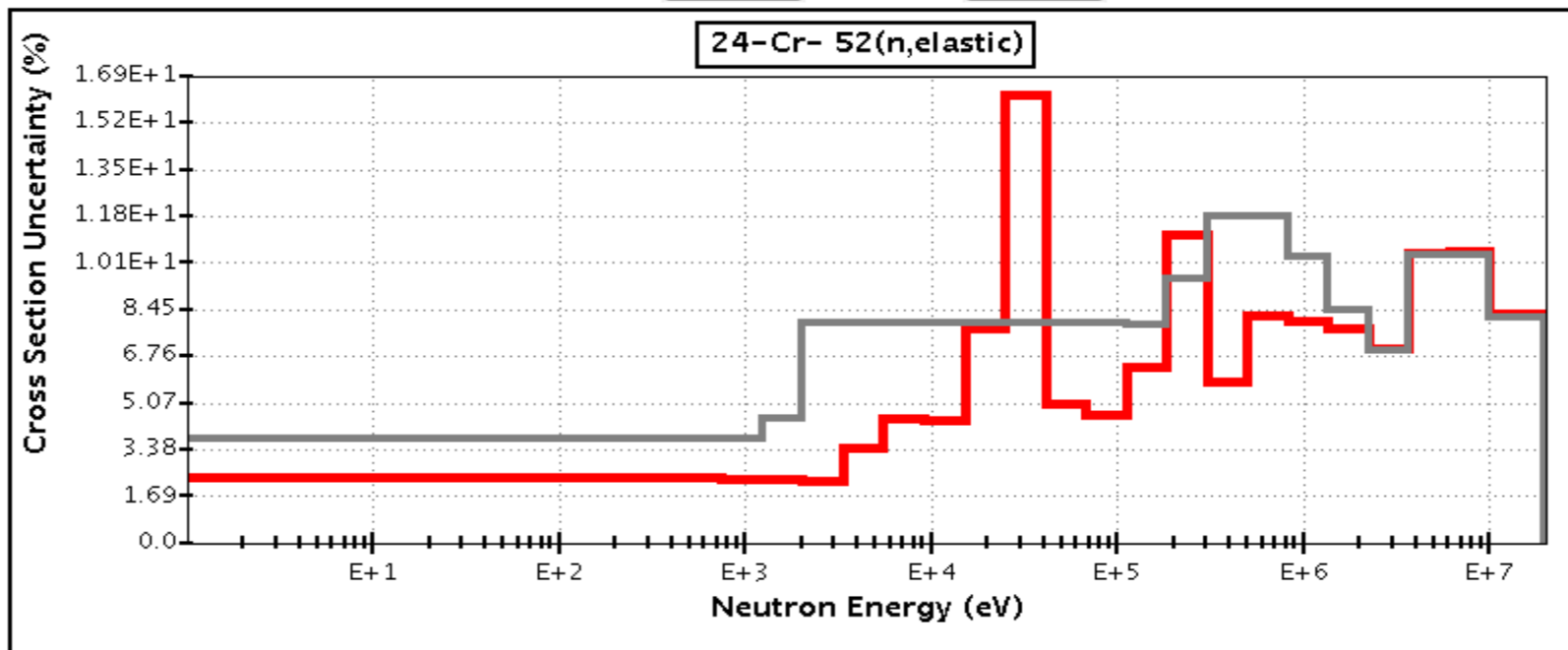
^{52}Cr

MF32 Resonance region only
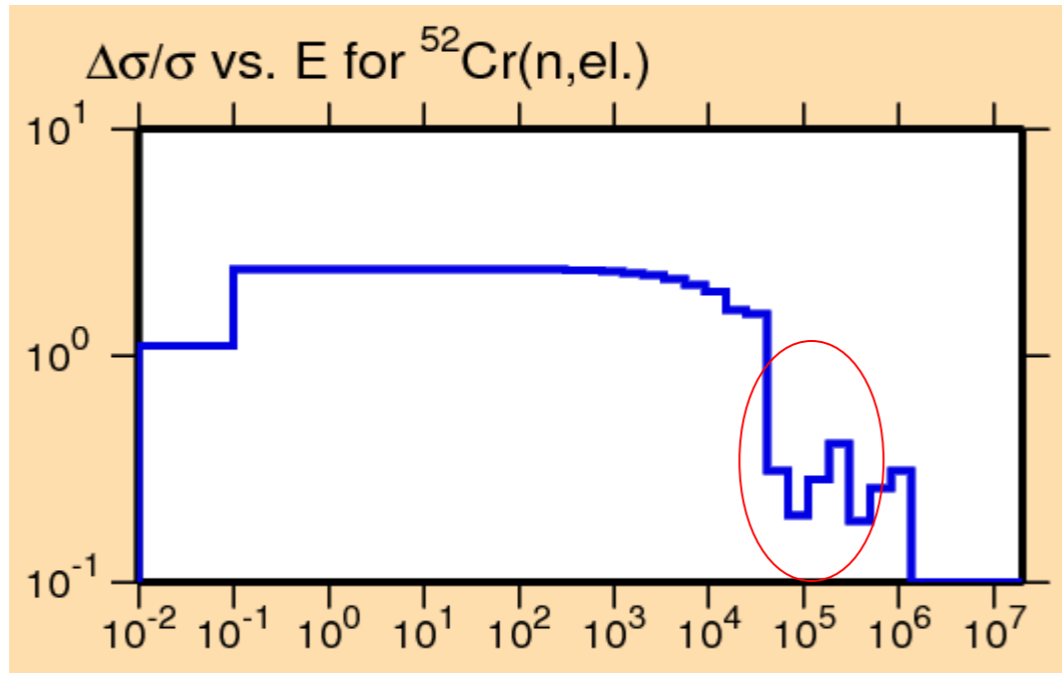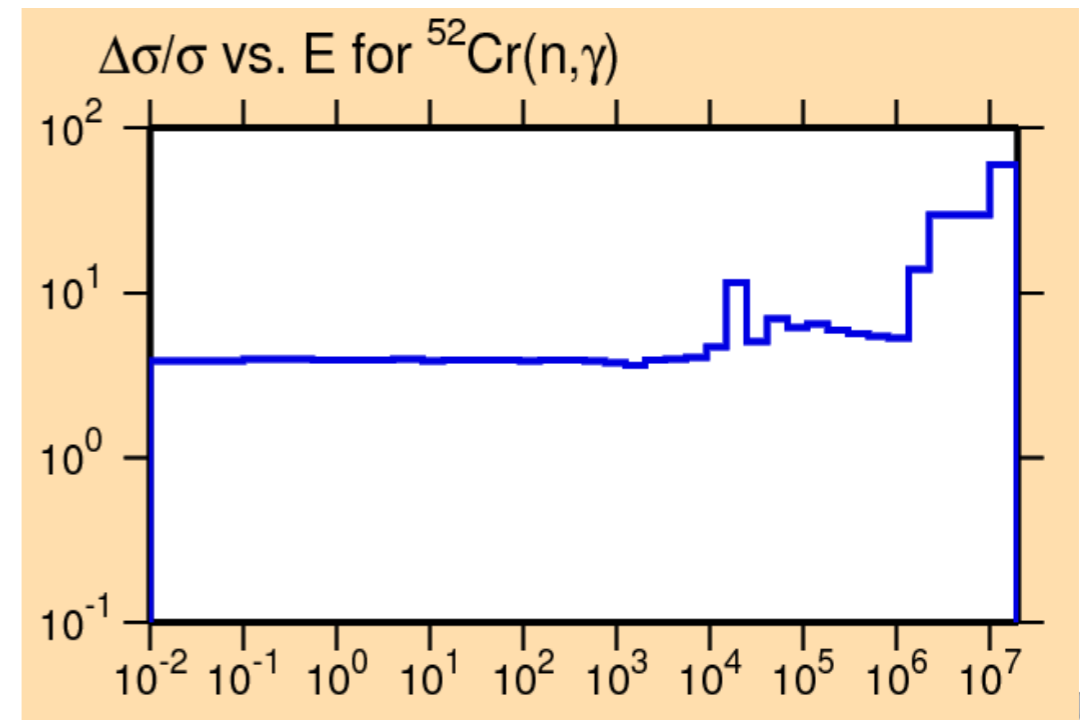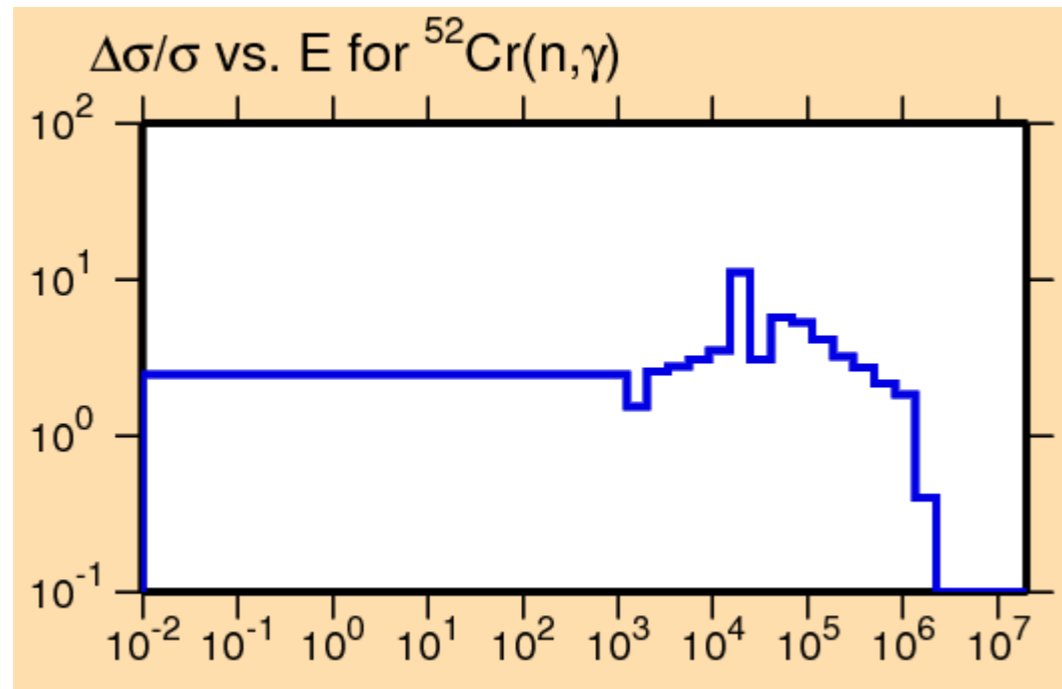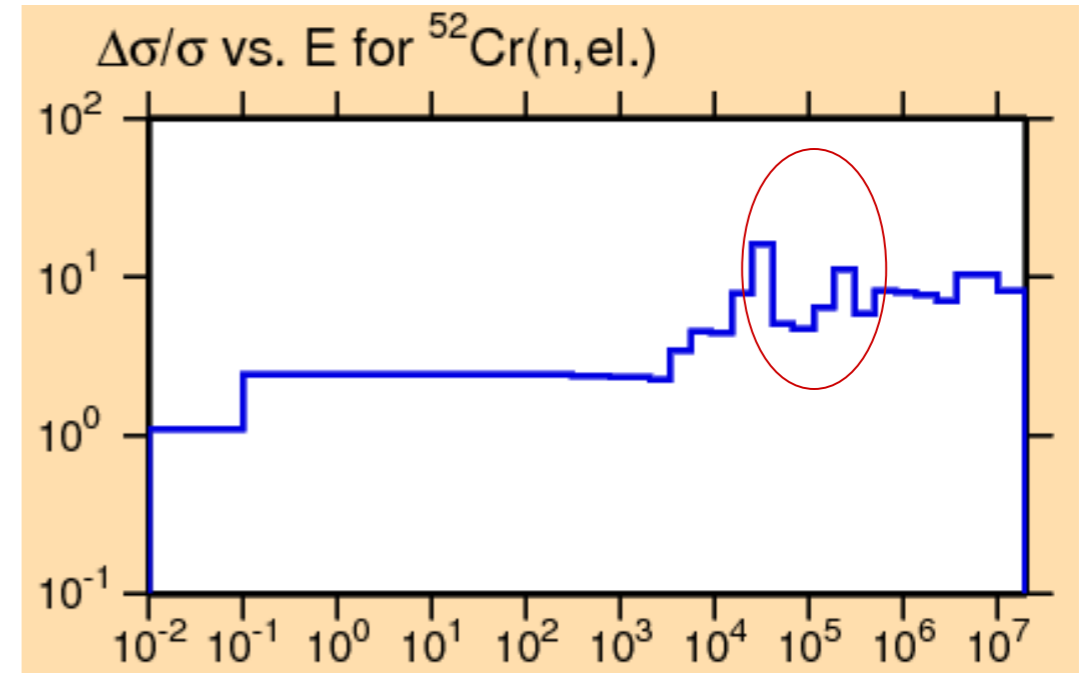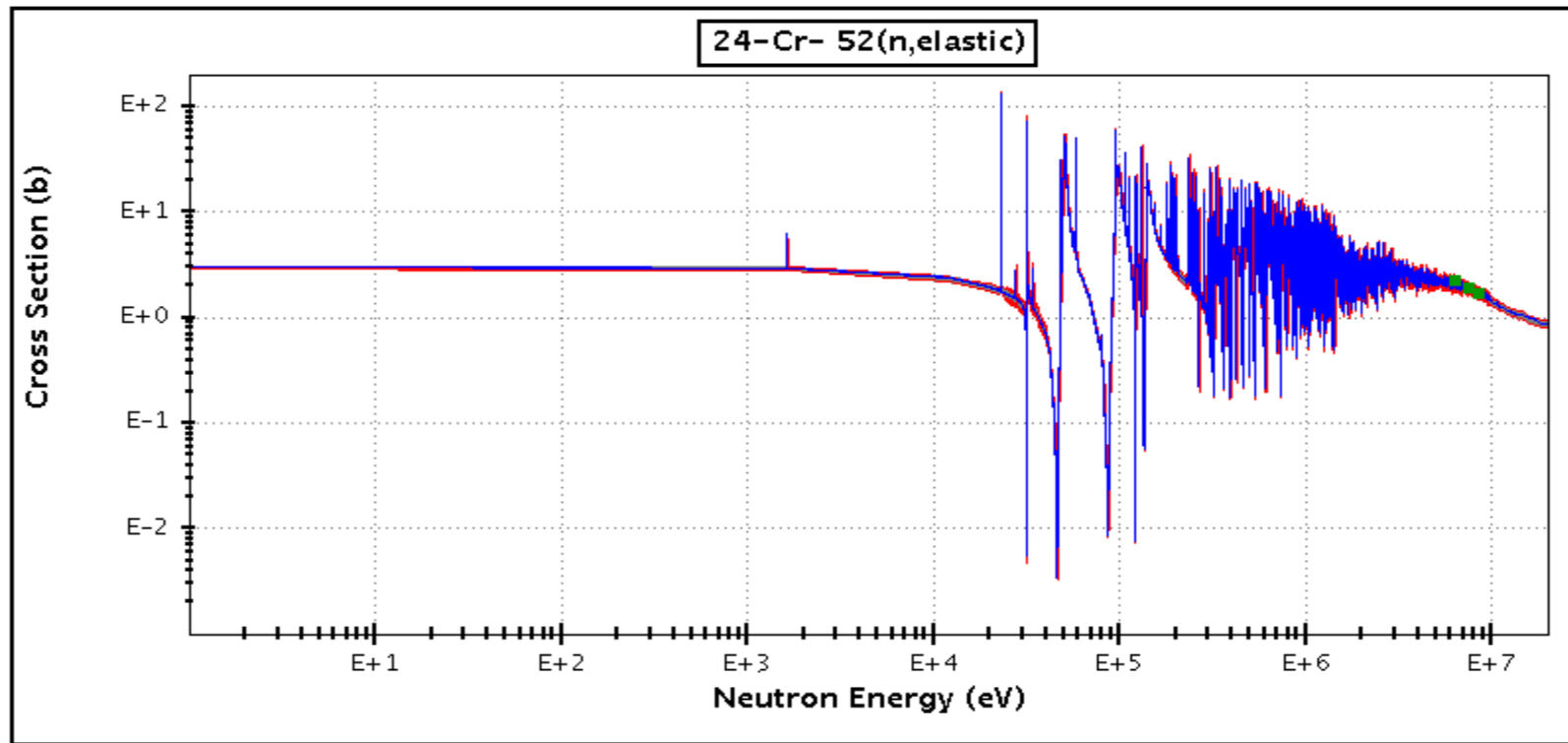
β4

Sigma ^{52}Cr

^{6}Li

- (n,t) taken from new LANL R-matrix analysis; other reaction channels from COMMARA-2.0
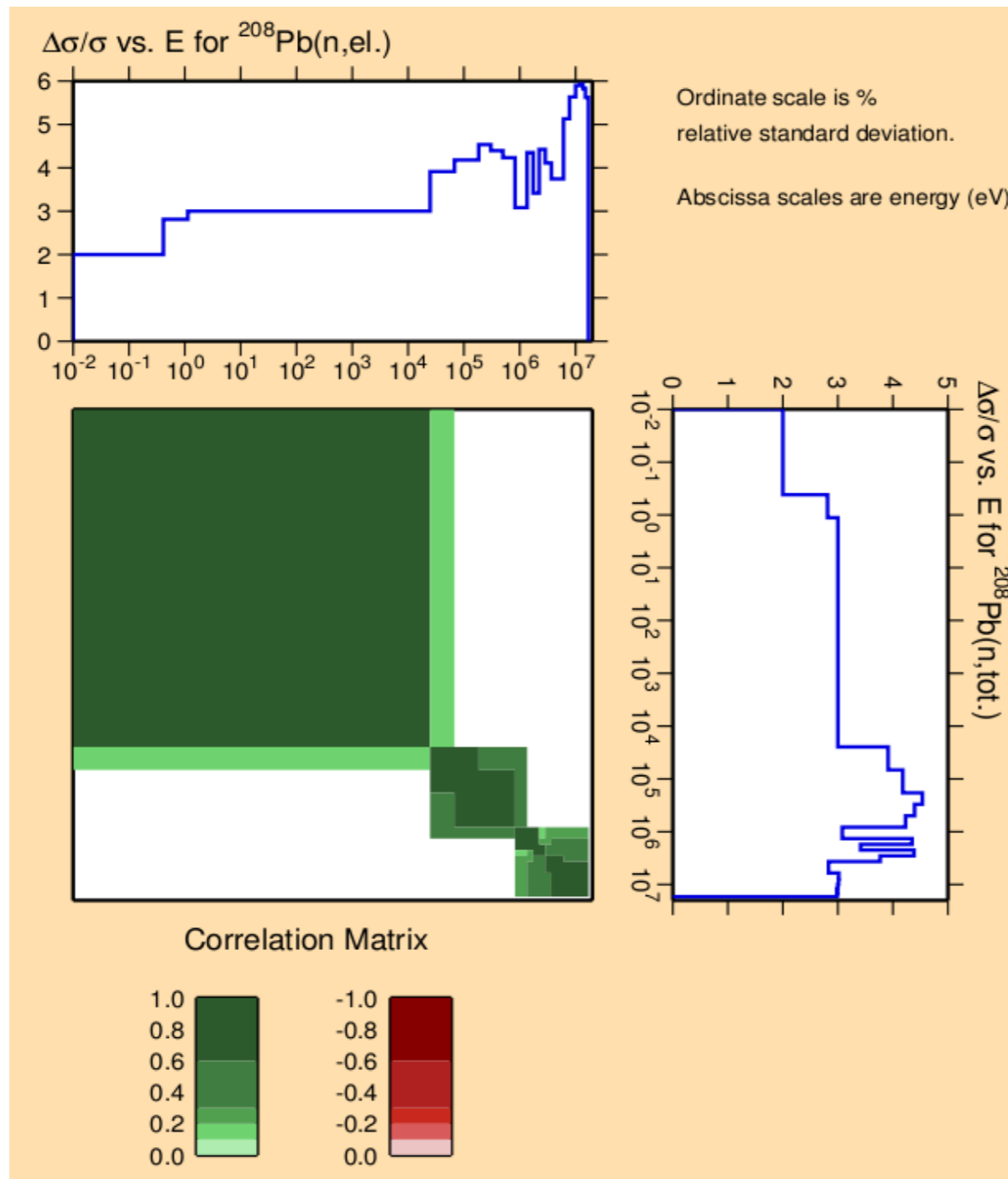
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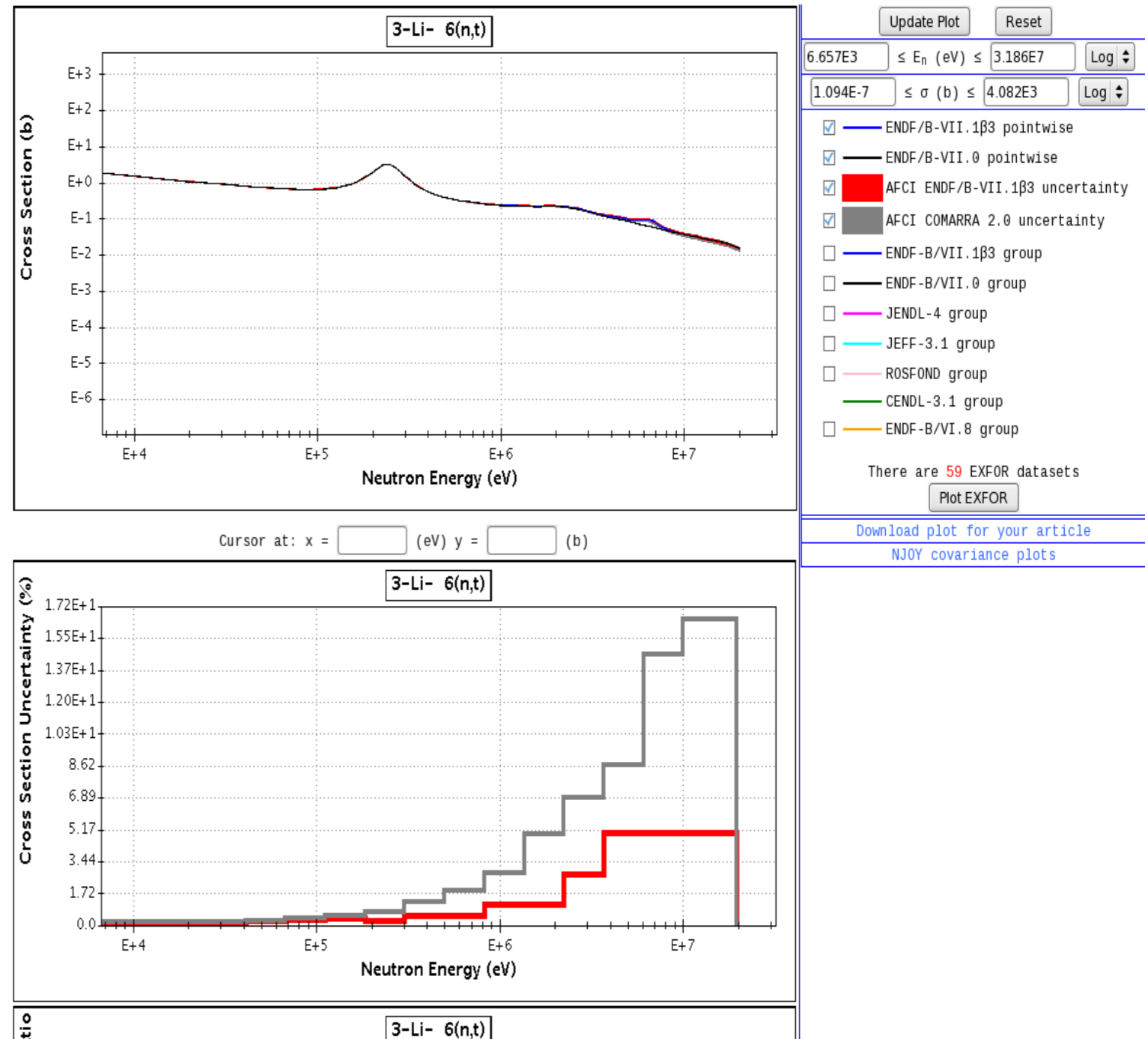
^{56}Fe
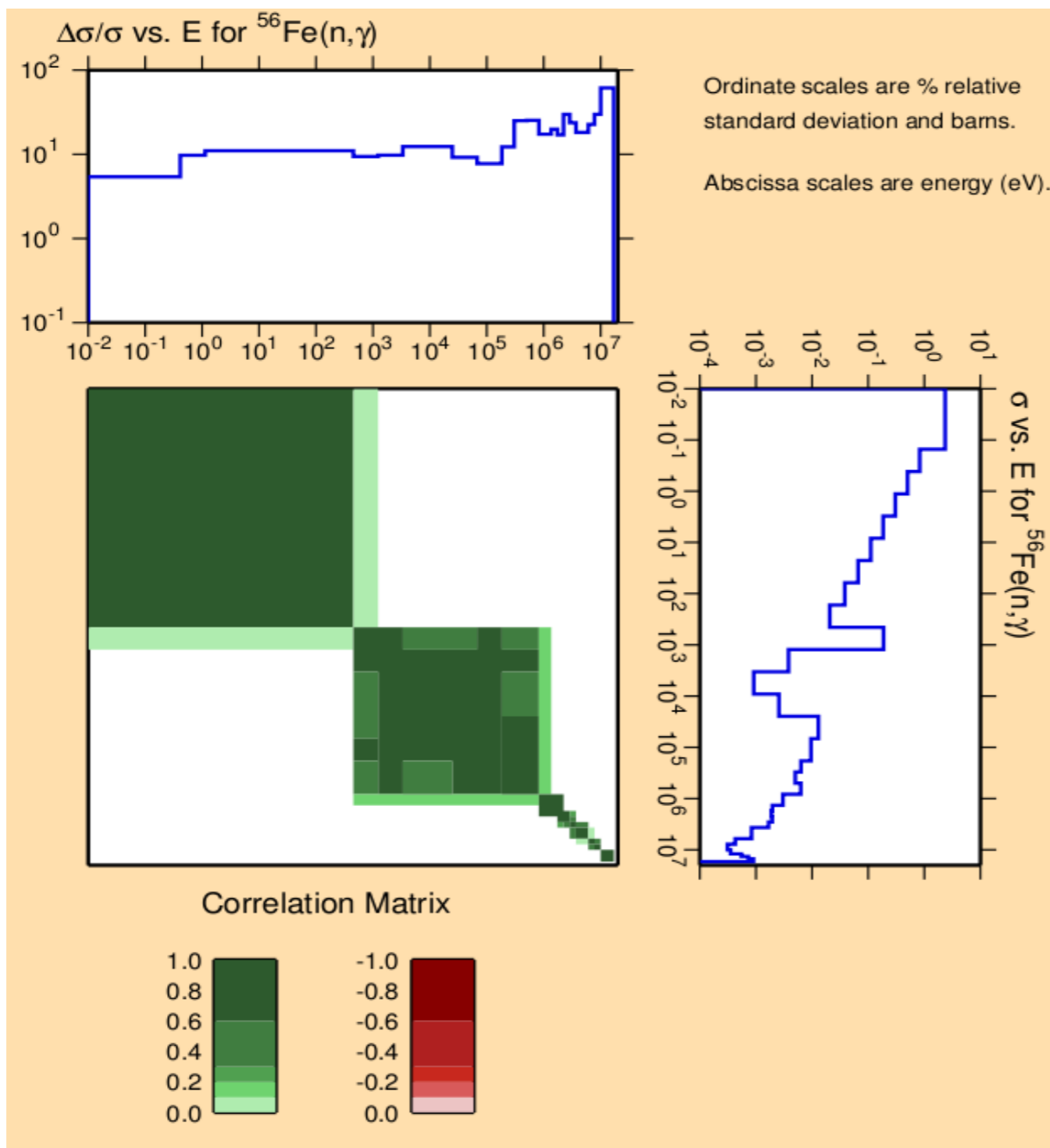
Kernel method in resonance region;

Modified VI.8 in fast region, based on dispersion analysis

^{208}Pb

Kernel method in resonance region;
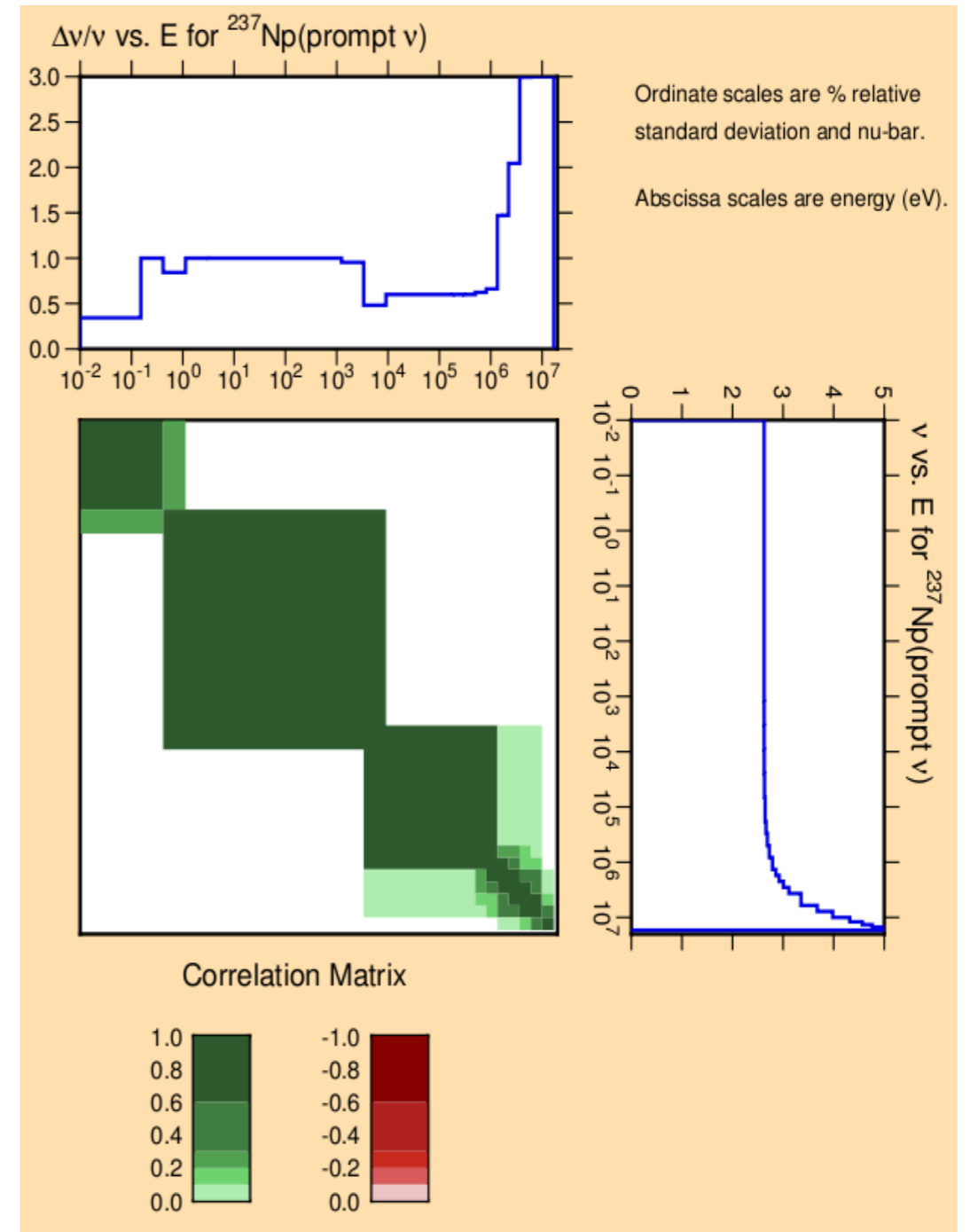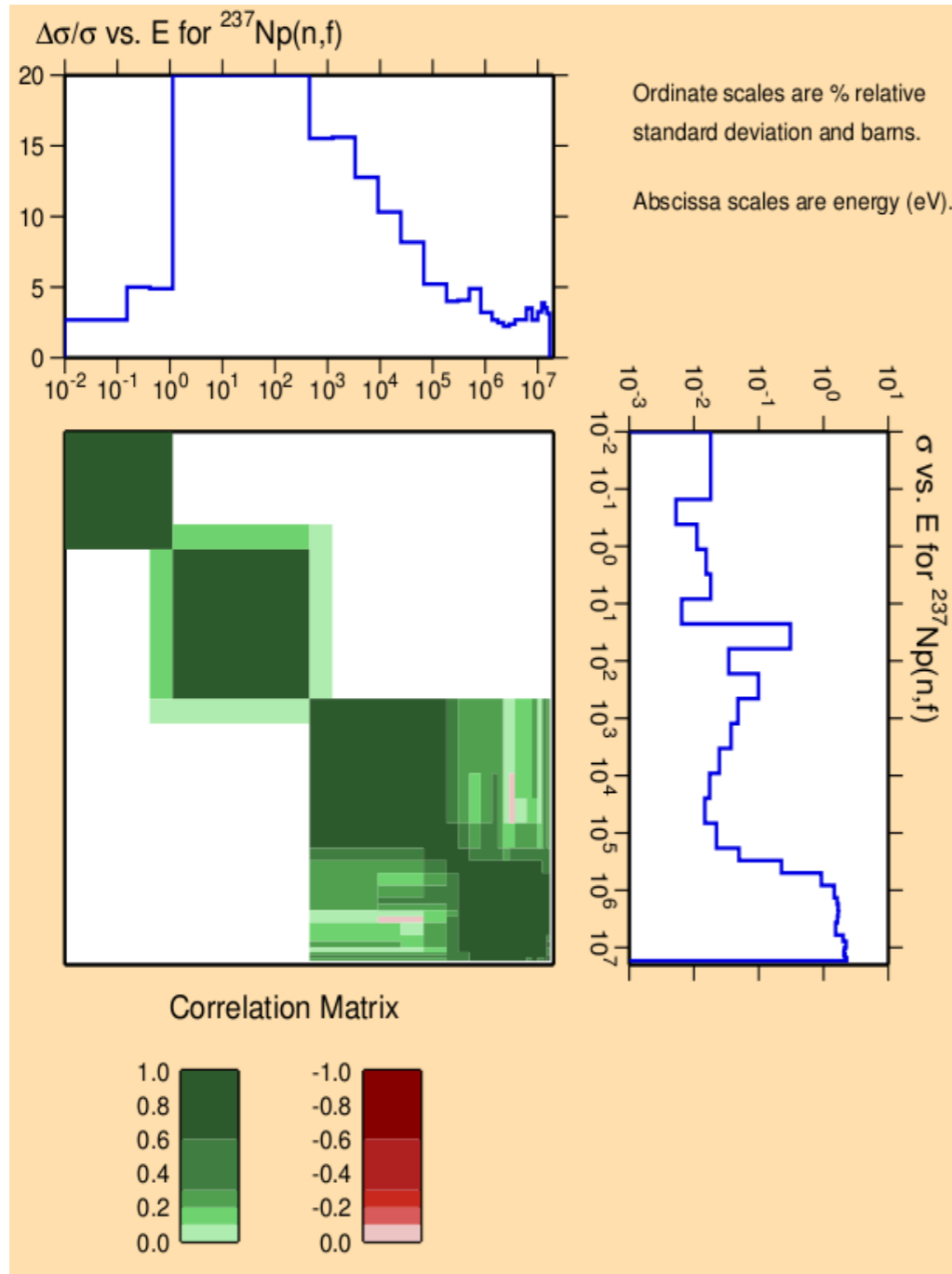
Empire/Kalman in fast

Am-242m,243 Np-237

No covariances present in ENDF/B-VII.1

MF33 covariances from AFCI moved directly into ENDF/B-VII.1

Differences between 7.0 (AFCI) and 7.1 less than quoted uncertainty from AFCI

^{237}Np

Δσ/σ vs. E for ^{237}Np(n,f)

Ordinate scales are % relative standard deviation and barns.

Abscissa scales are energy (eV).

σ vs. E for ^{237}Np(n,f)

Correlation Matrix

Δν/ν vs. E for ^{237}Np(prompt ν)

Ordinate scales are % relative standard deviation and nu-bar.

Abscissa scales are energy (eV).

ν vs. E for ^{237}Np(prompt ν)

Correlation Matrix

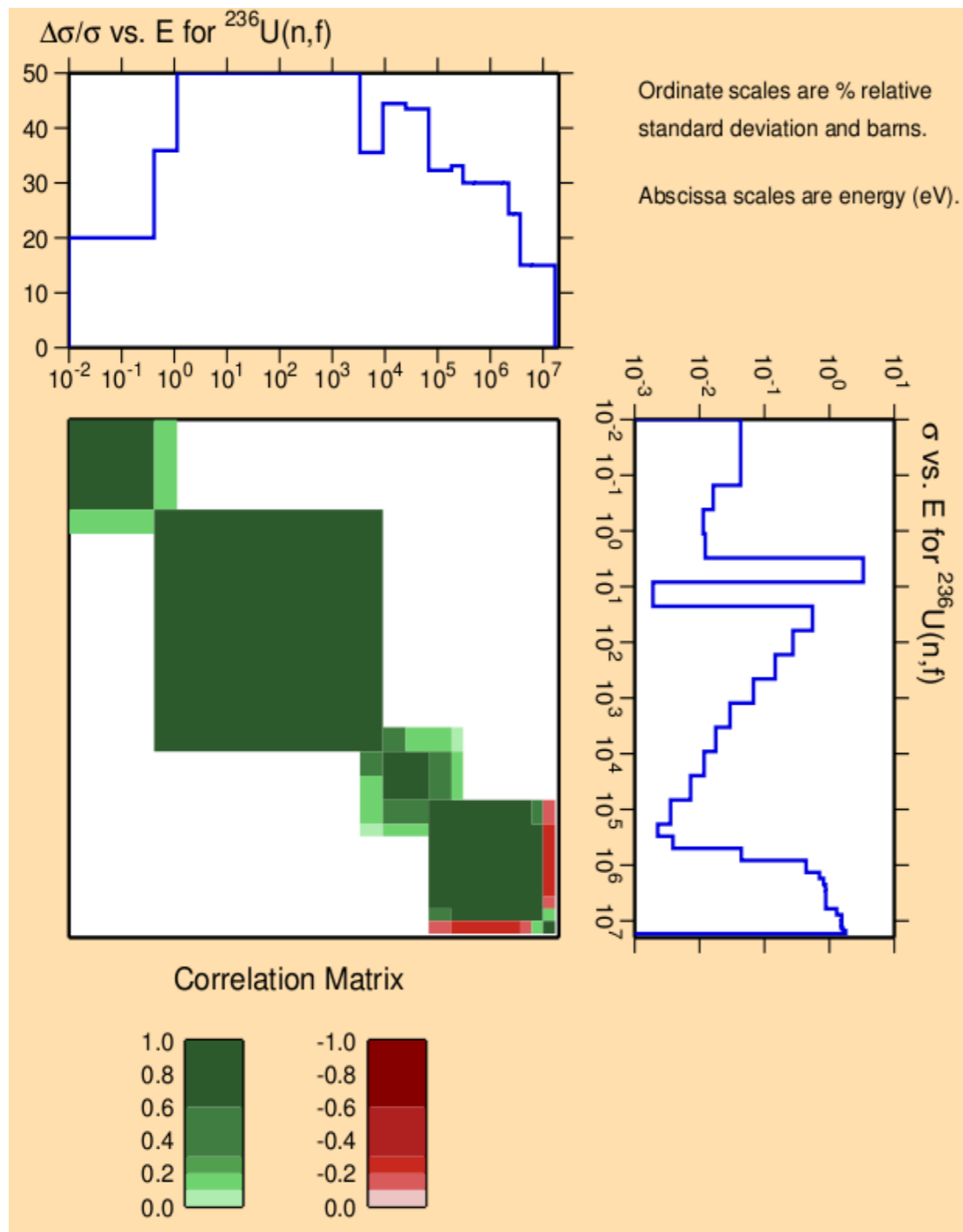NNDC

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^{234,236}U

No covariances present in ENDF/B-VII.1

MF33 covariances taken directly from AFCI 2.0

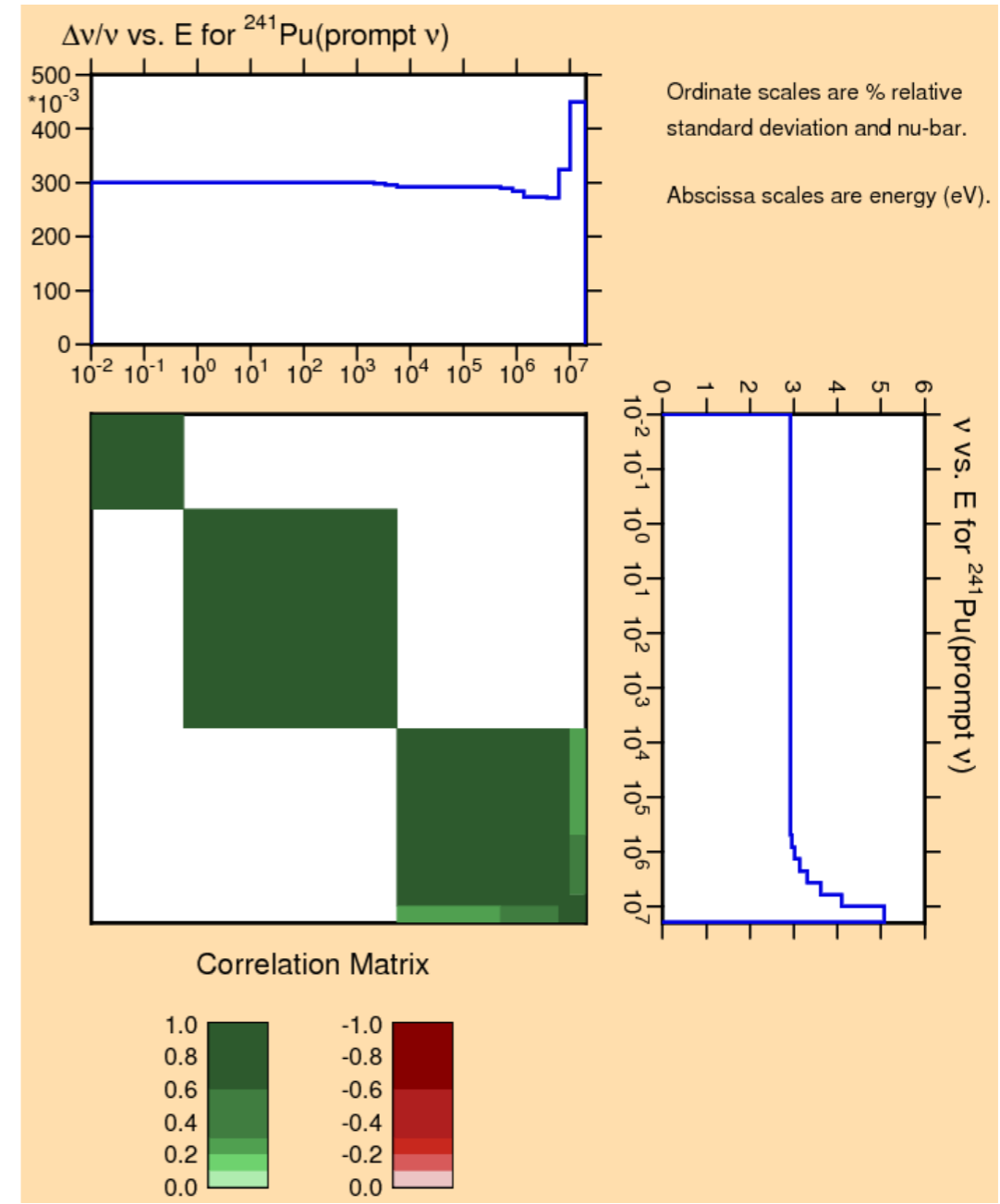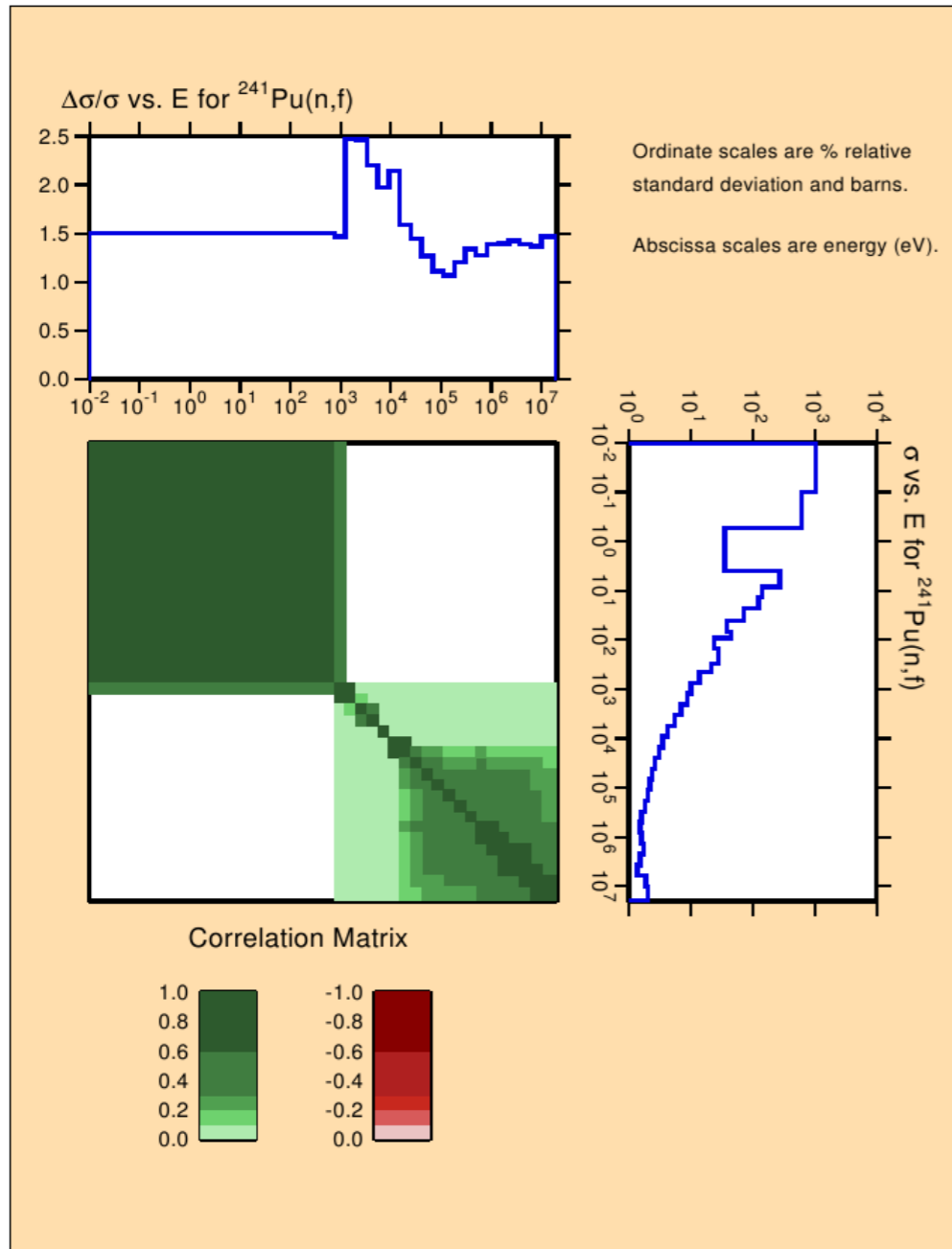^{236}U Difference in capture cross sections since VII.0 above 100 keV within uncertainty band.

^{234}U extended from 20 to 30 MeV.

^{236}U
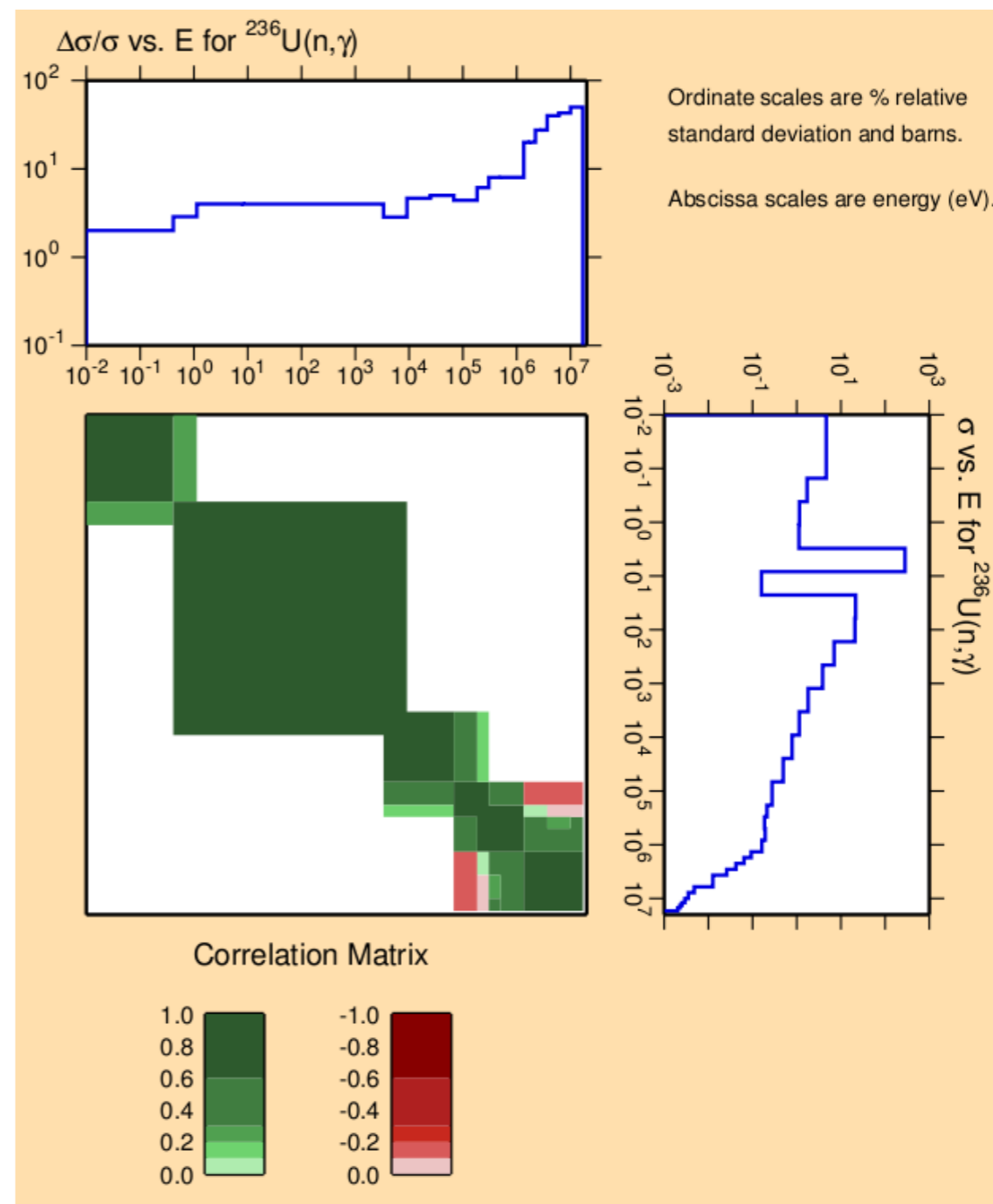
Pu-241

New LANL COMMARA eval adopted in ENDF/B-VII.1

Summary

- ENDF/B-VII.1 – β5 closed Oct 31, 2011, SVN version 458

- Total materials with covariance data: 190
  - Nubar: 73
  - Res param: 55
  - Cross sections: 183
  - Ang dist: 68
  - Energy spec: 64

Summary

- Review of entire covariance library:

  - Use of Sigma package for β5
  - Scan entire library with checking routines
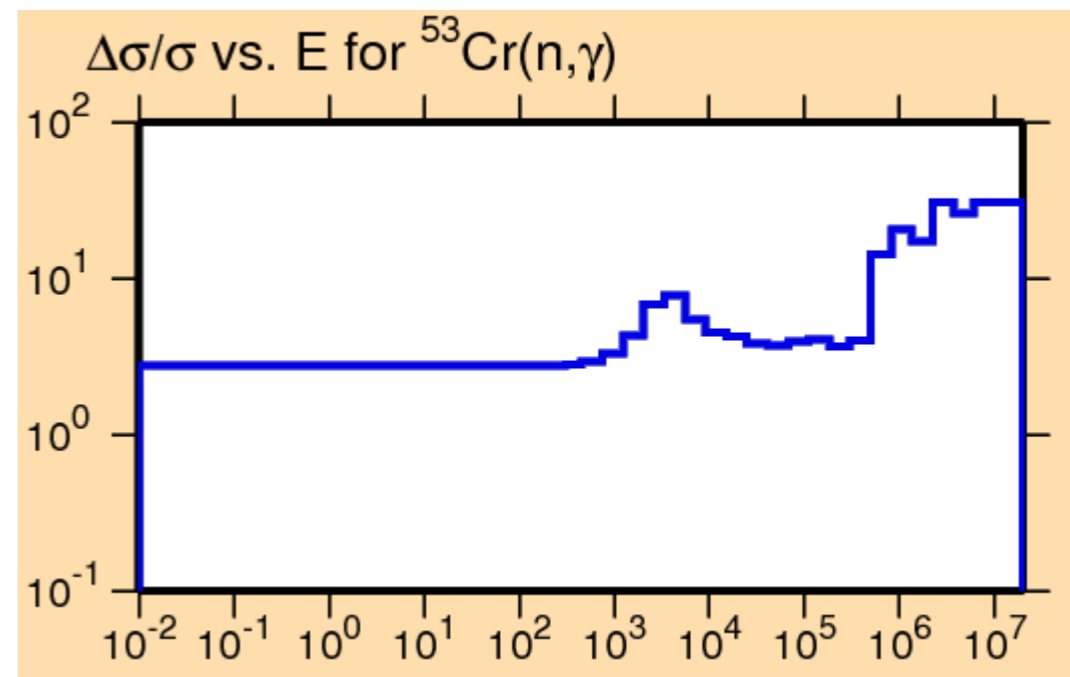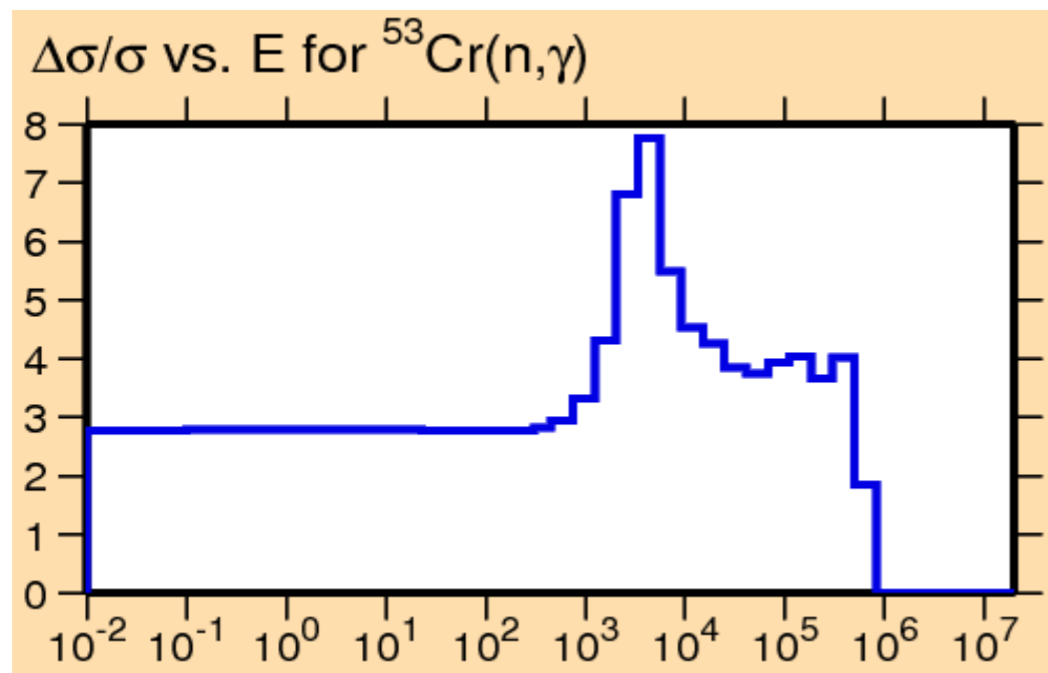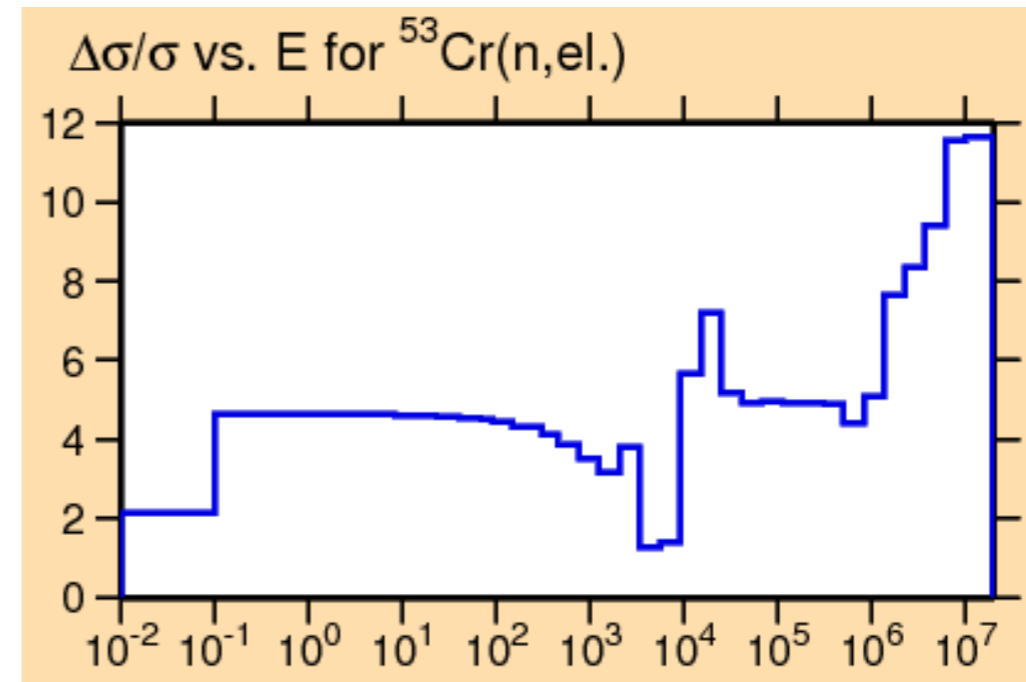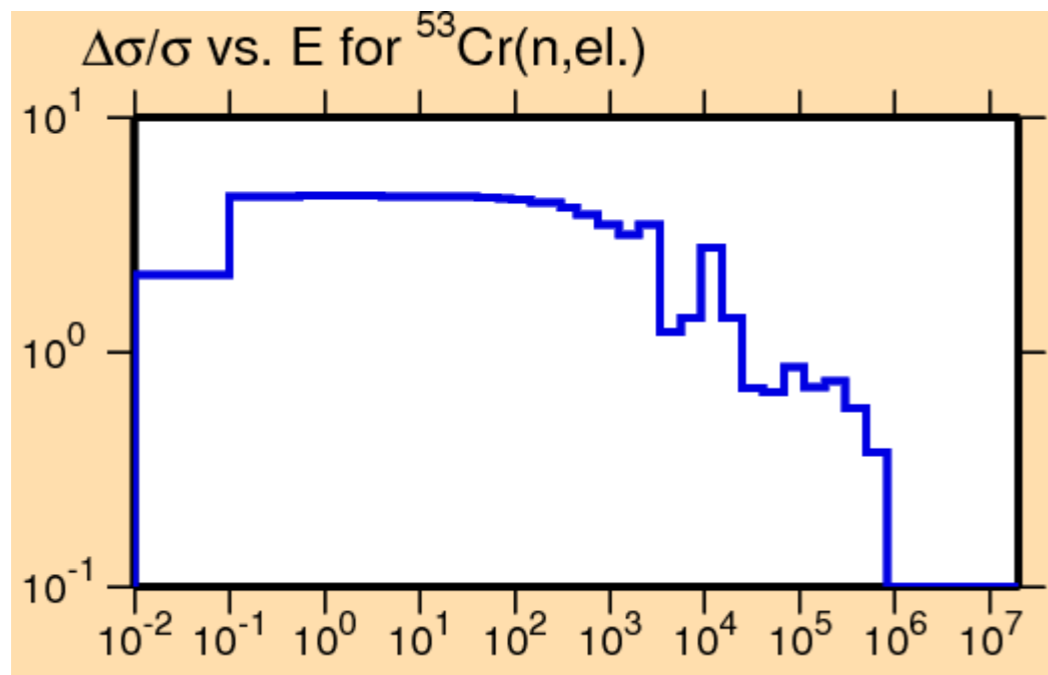 - Examination of fudge & unCor warnings
  - Users' feedback

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Extra slides

^{53}Cr

MF32 Resonance region only
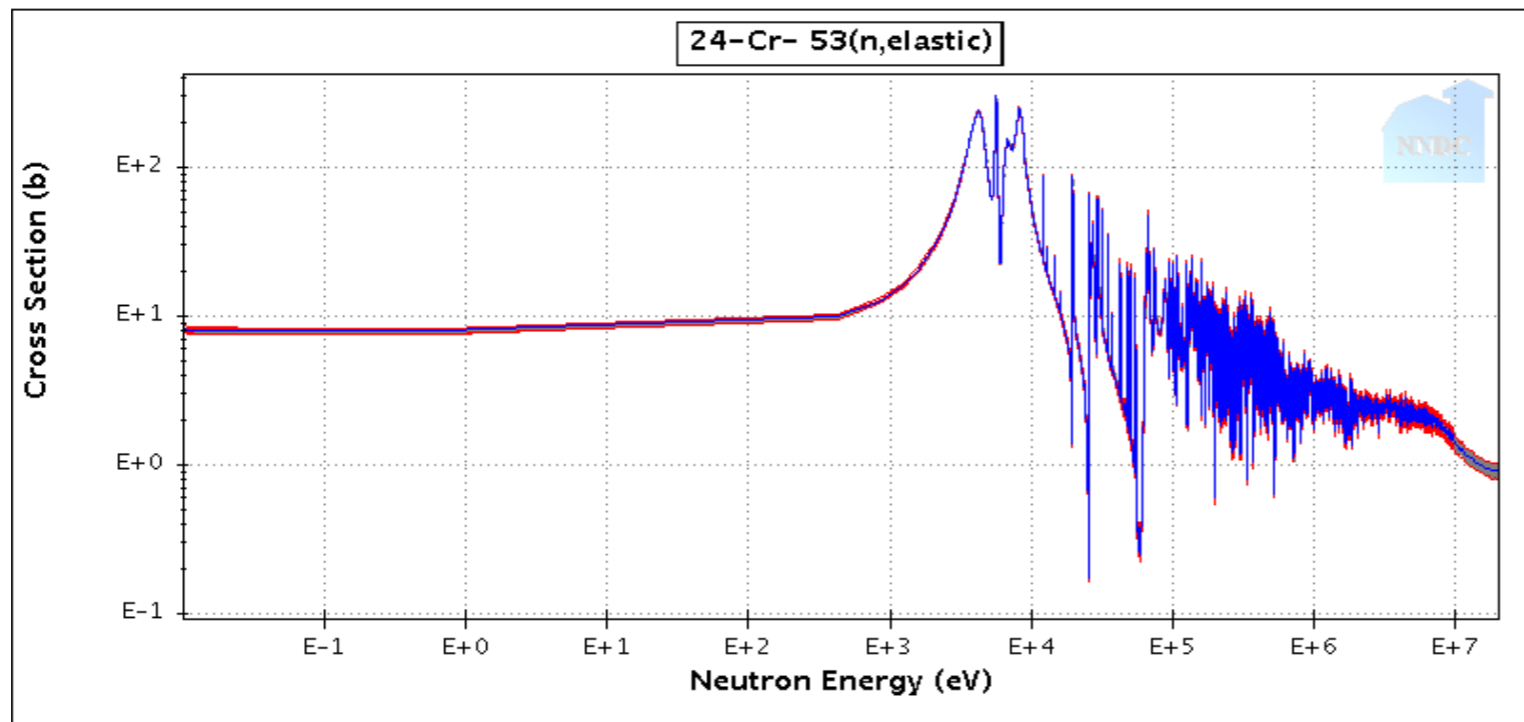
β4

Sigma ^{53}Cr
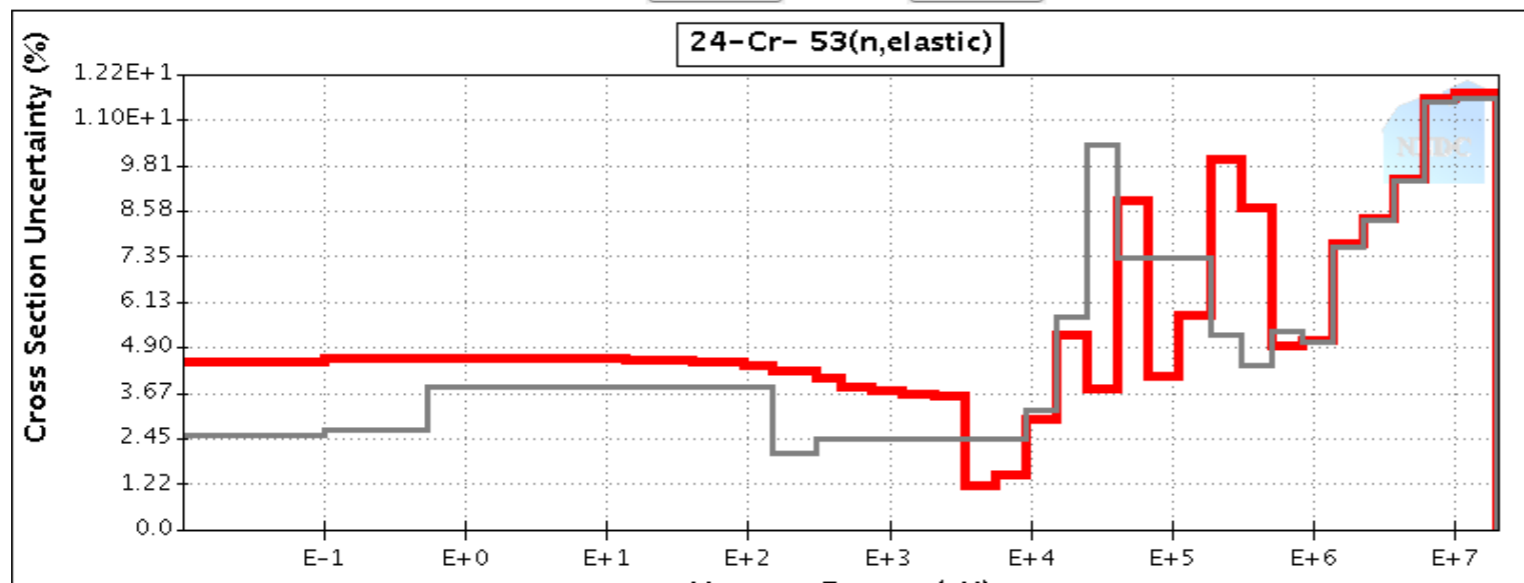
Final status

- O-16: capture cross section from JENDL-4.0 wrong parent state in MF14,Mt103 corrected

- Am-243: new (n,2n) isomeric ratio, new eval for RRR, URR and fast capture regions.

- Pu-242: New BNL eval for RRR, URR and fast capture. Remaining JENDL-4 eval not modified.

- Pu-238: Corrected MF3,MT19,20, MF4,MT18, MF6, MT37

- Am-241: Capture modified

^{58}Ni

MF32 Resonance region only

β4
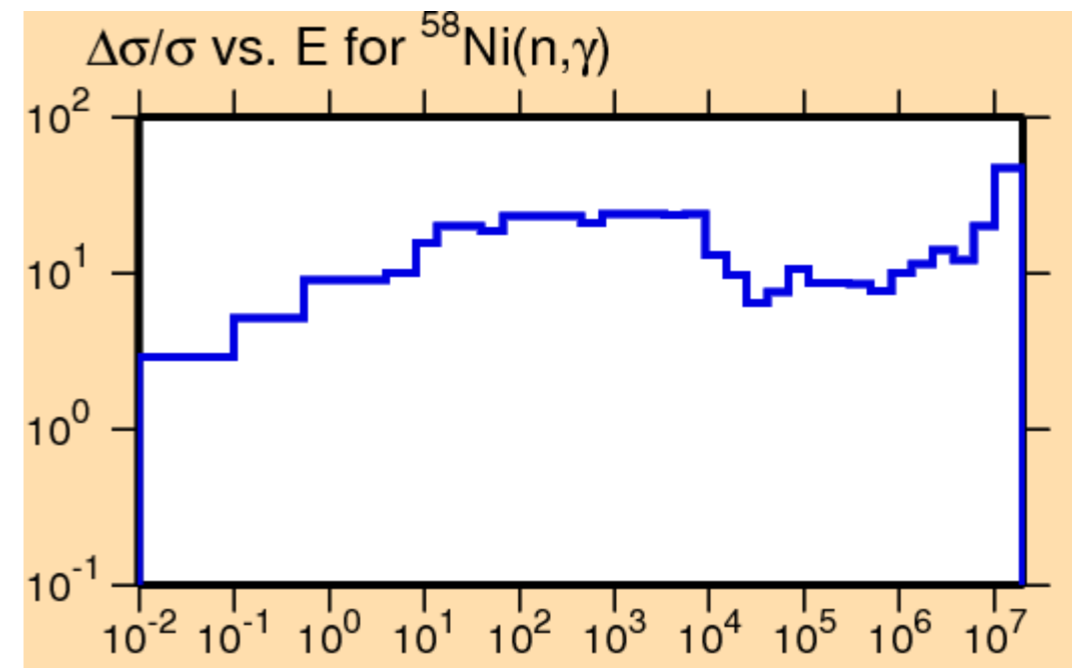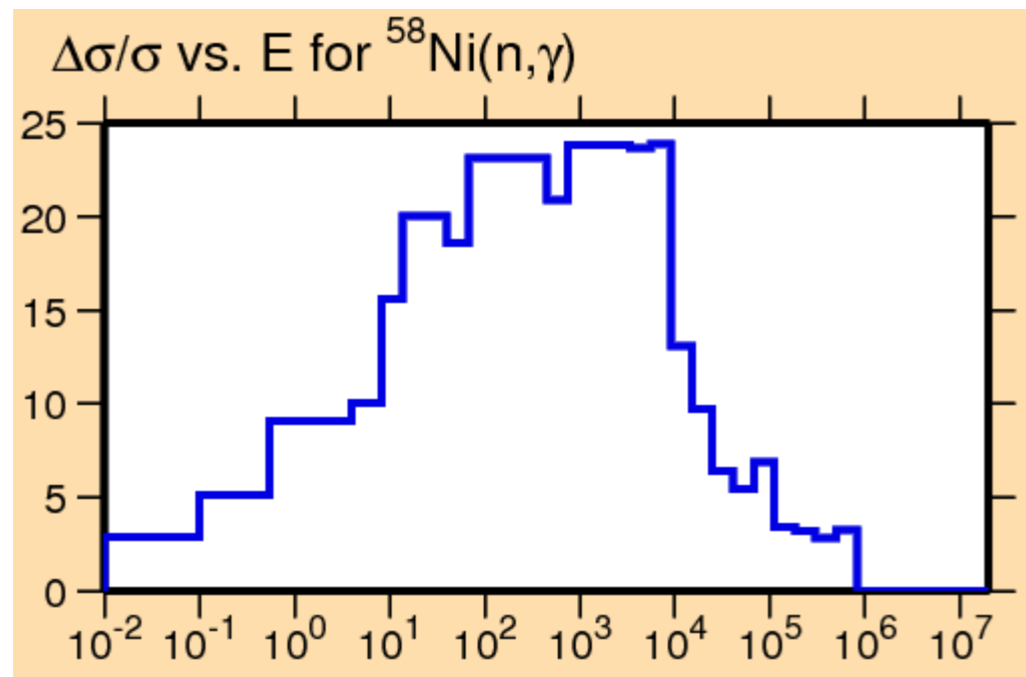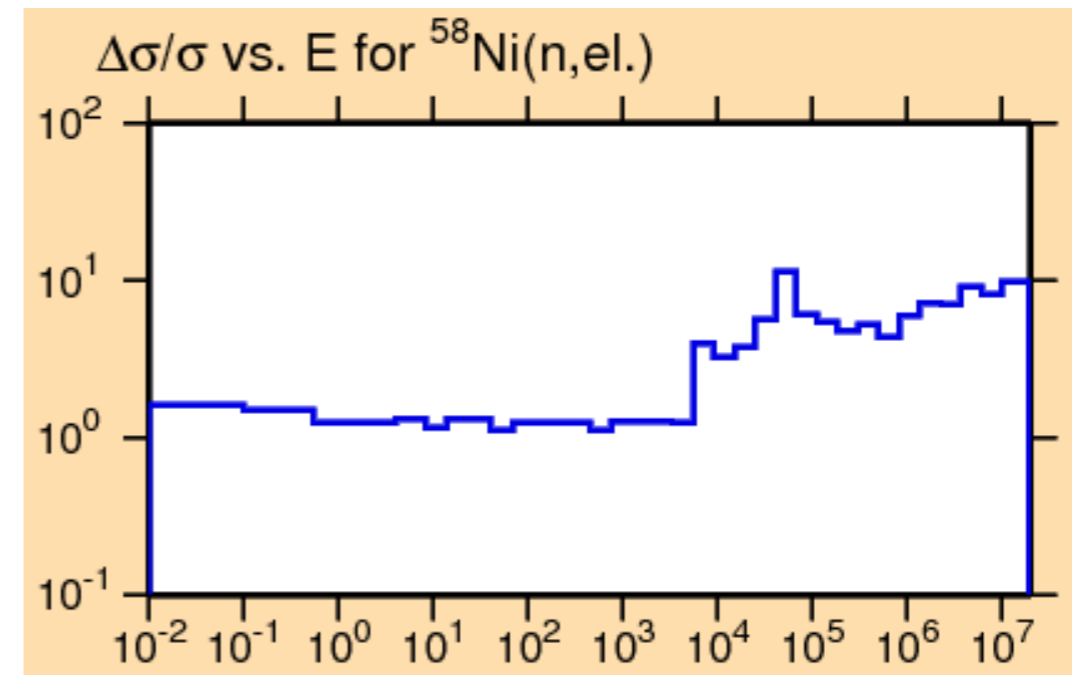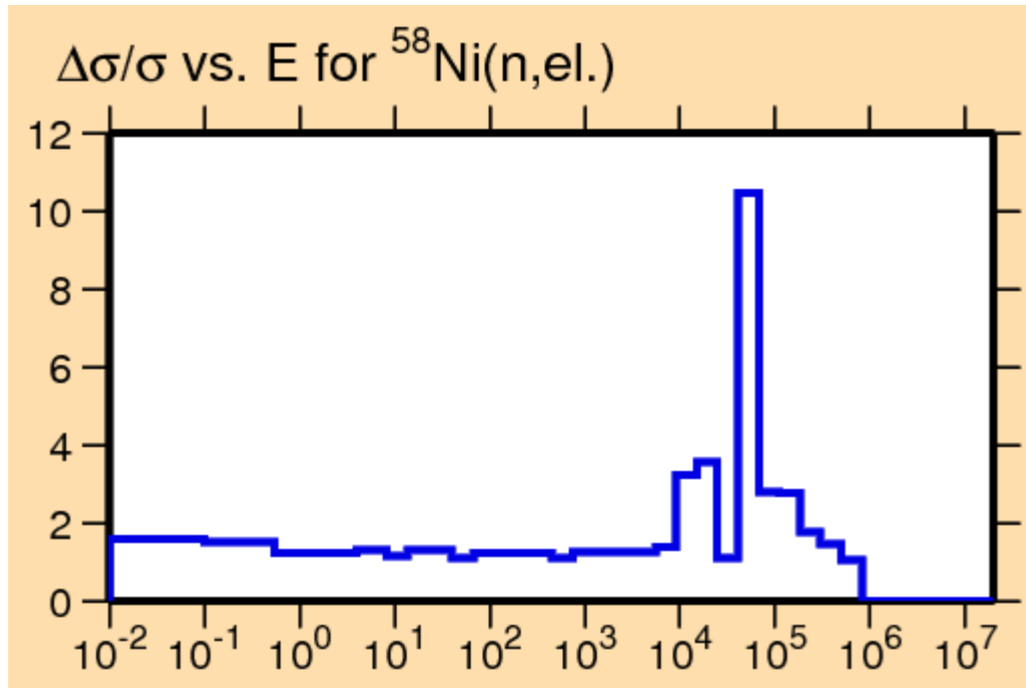
^{96}Mo
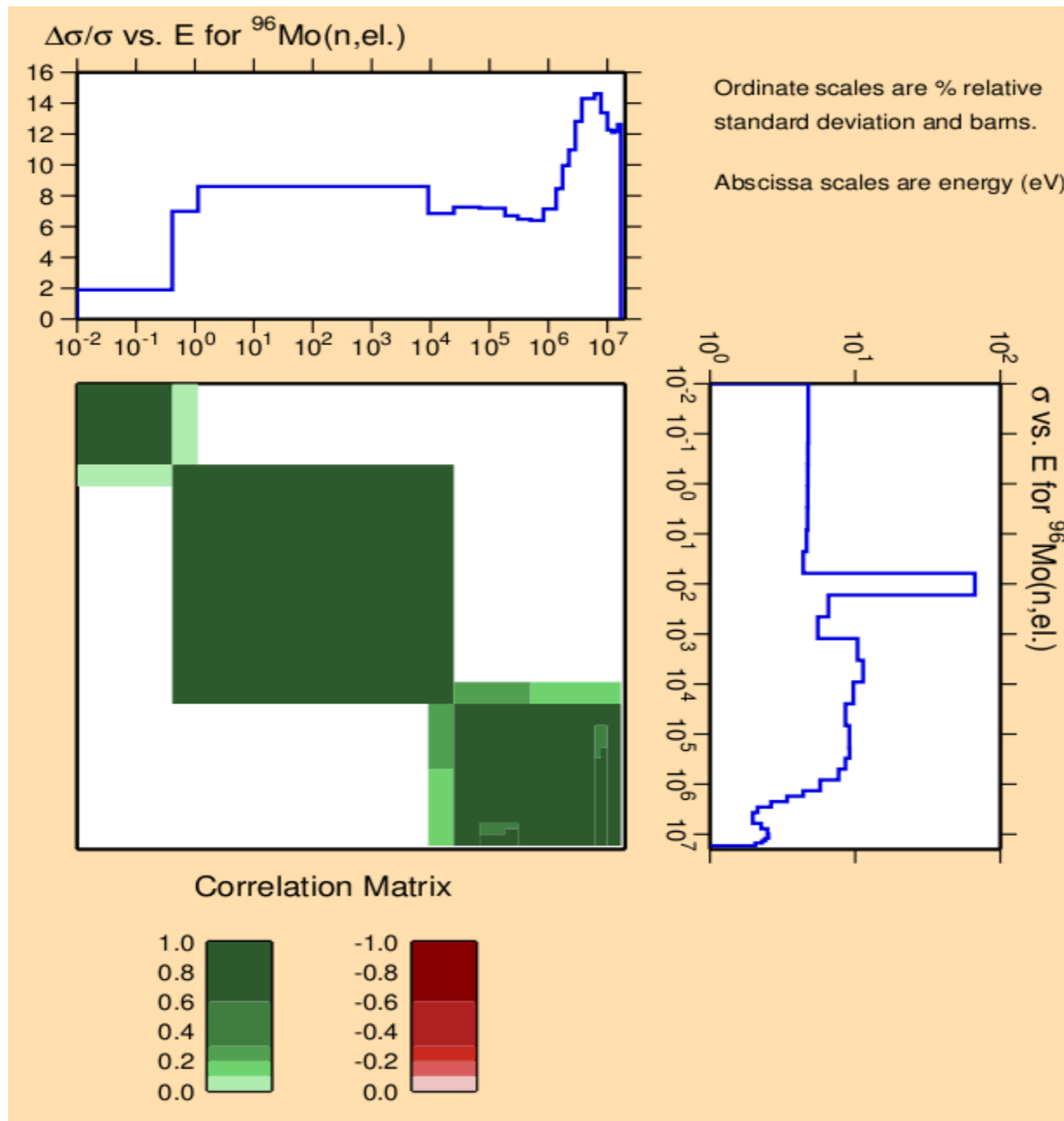
Kernel method in resonance region;

Empire/Kalman in fast

Methodology

- Move MF33 covariance data into ENDF file
- Process with checking codes
- Repair, if needed
- Process with NJOY (R. Arcilla)
- Use online Sigma package to compare to ENDF/B-VII.0 & COMMARA-2.0 (Sonzogni)
- ⇨make addition modifications, as required.

COMMARA Materials

- 110 materials most relevant to fast reactor R&D
  - 12 light nuclei (LANL)
  - 78 structural materials (BNL)
  - 20 major and minor actinides (LANL + BNL)

- 135 files
  - 110 cross section covariances,
  - 20 nubars,
  - 3 PFNS,
  - 2 mubars

|					
^{1}H	^{28}Si	^{92}Mo	^{106}Ag	^{149}Sm	^{232}Th
^{2}H	^{29}Si	^{94}Mo	^{127}I	^{151}Sm	^{233}U
^{4}He	^{30}Si	^{95}Mo	^{129}I	^{152}Sm	^{234}U
^{6}Li	^{50}Cr	^{96}Mo	^{131}Xe	^{153}Eu	^{235}U
^{7}Li	^{52}Cr	^{97}Mo	^{132}Xe	^{155}Eu	^{236}U
^{9}Be	^{53}Cr	^{98}Mo	^{134}Xe	^{155}Gd	^{238}U
^{10}B	^{55}Mn	^{100}Mo	^{133}Cs	^{156}Gd	^{237}Np
^{11}B	^{54}Fe	^{99}Tc	^{135}Cs	^{157}Gd	^{238}Pu
^{12}C	^{56}Fe	^{101}Ru	^{139}La	^{158}Gd	^{239}Pu
^{15}N	^{57}Fe	^{102}Ru	^{141}Ce	^{160}Gd	^{240}Pu
^{16}O	^{58}Ni	^{103}Ru	^{141}Pr	^{166}Er	^{241}Pu
^{19}F	^{60}Ni	^{104}Ru	^{143}Nd	^{167}Er	^{242}Pu
^{23}Na	^{90}Zr	^{106}Ru	^{145}Nd	^{168}Er	^{241}Am
^{24}Mg	^{91}Zr	^{103}Rh	^{146}Nd	^{170}Er	^{242m}Am
^{25}Mg	^{92}Zr	^{105}Pd	^{148}Nd	^{204}Pb	^{243}Am
^{26}Mg	^{93}Zr	^{106}Pd	^{147}Pm	^{206}Pb	^{242}Cm
^{27}Al	^{94}Zr	^{107}Pd		^{207}Pb	^{243}Cm
	^{95}Zr	^{108}Pd		^{208}Pb	^{244}Cm
	^{96}Zr			^{209}Bi	^{245}Cm
	^{98}Nb				^{246}Cm

AFCI Structural Materials

RRR		Fast	
Integral	40	Empire/Kalman	30
Kernel	20	Model-based	30
SAMMY	9	6.8	3
Empire	2	6.8 & mods	8