COMMARA-3

Processed ENDF/B-VII.1 covariance library

S. Hoblit
National Nuclear Data Center
Brookhaven National Laboratory

hoblit@bnl.gov

Brookhaven Science Associates

COMMARA-3.0 - ENDF/B-VII.1 Covariance Materials

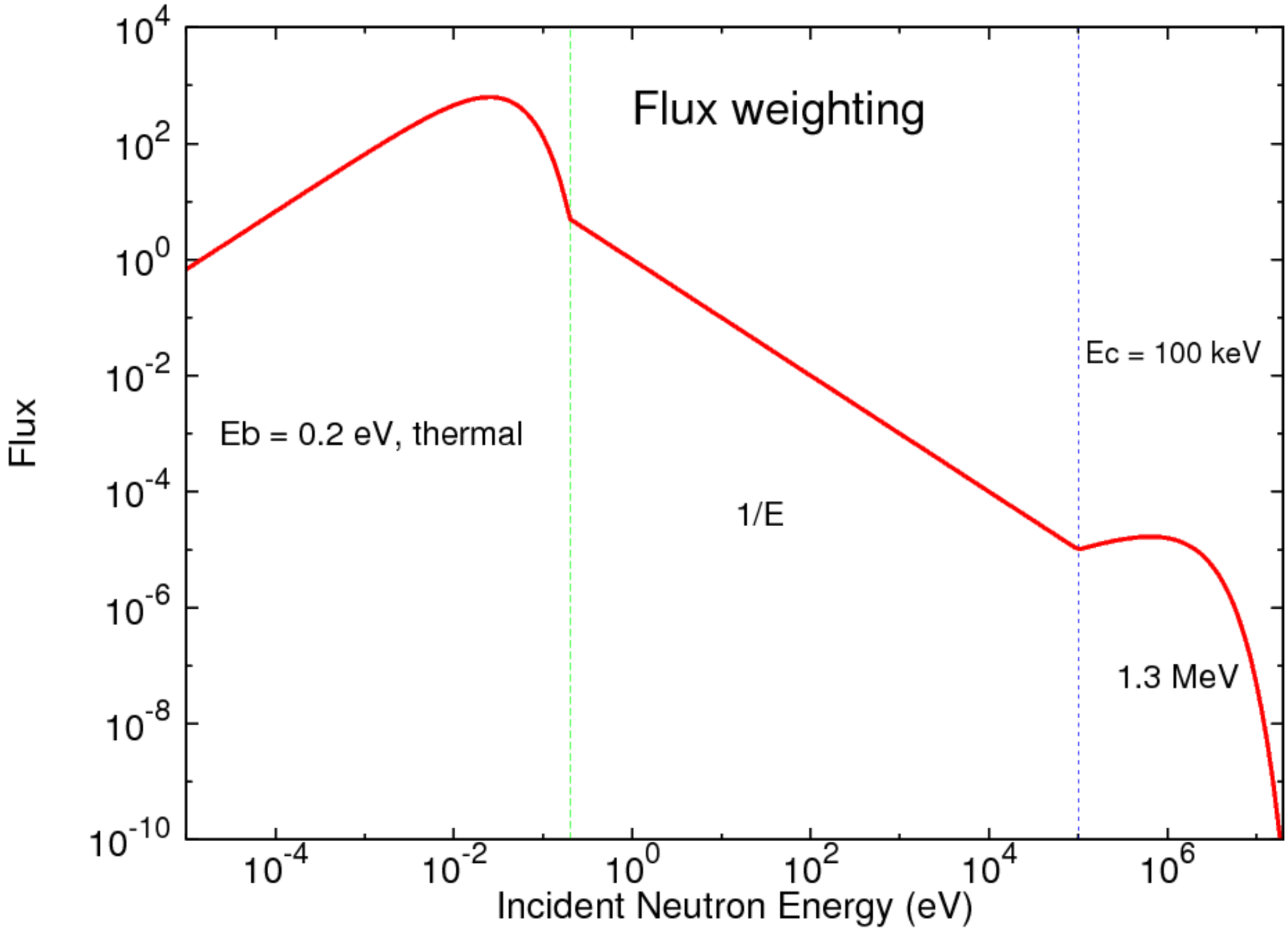
184 materials: 12 Light, 99 structural, 73 Actinides

- ^{1}H, ^{2}H, ^{4}He, ^{6}Li ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{0}C, ^{15}N, ^{16}O, ^{19}F, ^{24}Mg, ^{25}Mg, ^{26}Mg, ^{27}Al, ^{28}Si, ^{29}Si, ^{30}Si, ^{35}Cl, ^{37}Cl, ^{39}K, ^{41}K, ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, ^{50}Ti, ^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr, ^{55}Mn, ^{54}Fe, ^{56}Fe, ^{57}Fe, ^{59}Co, ^{58}Ni, ^{60}Ni, ^{89}Y, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{93}Zr, ^{94}Zr, ^{95}Zr, ^{96}Zr, ^{95}Nb, ^{92}Mo, ^{94}Mo, ^{95}Mo, ^{96}Mo, ^{97}Mo, ^{98}Mo, ^{100}Mo, ^{99}Tc, ^{101}Ru, ^{102}Ru, ^{103}Ru, ^{104}Ru, ^{106}Ru, ^{105}Pd, ^{107}Pd, ^{108}Pd, ^{109}Ag, ^{127}I, ^{129}I, ^{131}Xe, ^{132}Xe, ^{134}Xe, ^{133}Cs, ^{135}Cs, ^{139}La, ^{141}Ce, ^{141}Pr, ^{143}Nd, ^{145}Nd, ^{146}Nd, ^{148}Nd, ^{147}Pm, ^{149}Sm, ^{151}Sm, ^{142}Sm, ^{153}Eu, ^{155}Eu, ^{152}Gd, ^{153}Gd, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{160}Gd
- ^{166}Er, ^{167}Er, ^{168}Er, ^{170}Er, ^{180}W, ^{182}W, ^{183}W, ^{184}W, ^{186}W, ^{191}Ir, ^{193}Ir, ^{197}Au, ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{209}Bi, ^{225}Ac, ^{226}Ac, ^{227}Ac, ^{227}Th, ^{229}Th, ^{230}Th, ^{231}Th, ^{232}Th, ^{233}Th, ^{234}Th, ^{229}Pa, ^{230}Pa, ^{232}Pa, ^{230}U, ^{231}U, ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{234}Np, ^{235}Np, ^{236}Np, ^{237}Np, ^{238}Np, ^{239}Np, ^{236}Pu, ^{237}Pu, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{244}Pu, ^{246}Pu, ^{240}Am, ^{241}Am, ^{242m1}Am, ^{243}Am, ^{240}Cm, ^{241}Cm, ^{242}Cm, ^{243}Cm, ^{244}Cm, ^{245}Cm ^{246}Cm, ^{248}Cm, ^{249}Cm, ^{250}Cm, ^{245}Bk, ^{246}Bk, ^{247}Bk, ^{248}Bk, ^{250}Bk, ^{246}Cf, ^{249}Cf, ^{250}Cf, ^{251}Cf, ^{252}Cf, ^{253}Cf, ^{254}Cf, ^{251}Es, ^{252}Es, ^{253}Es, ^{254}Es, ^{254m1}Es, ^{255}Es, ^{255}Fm

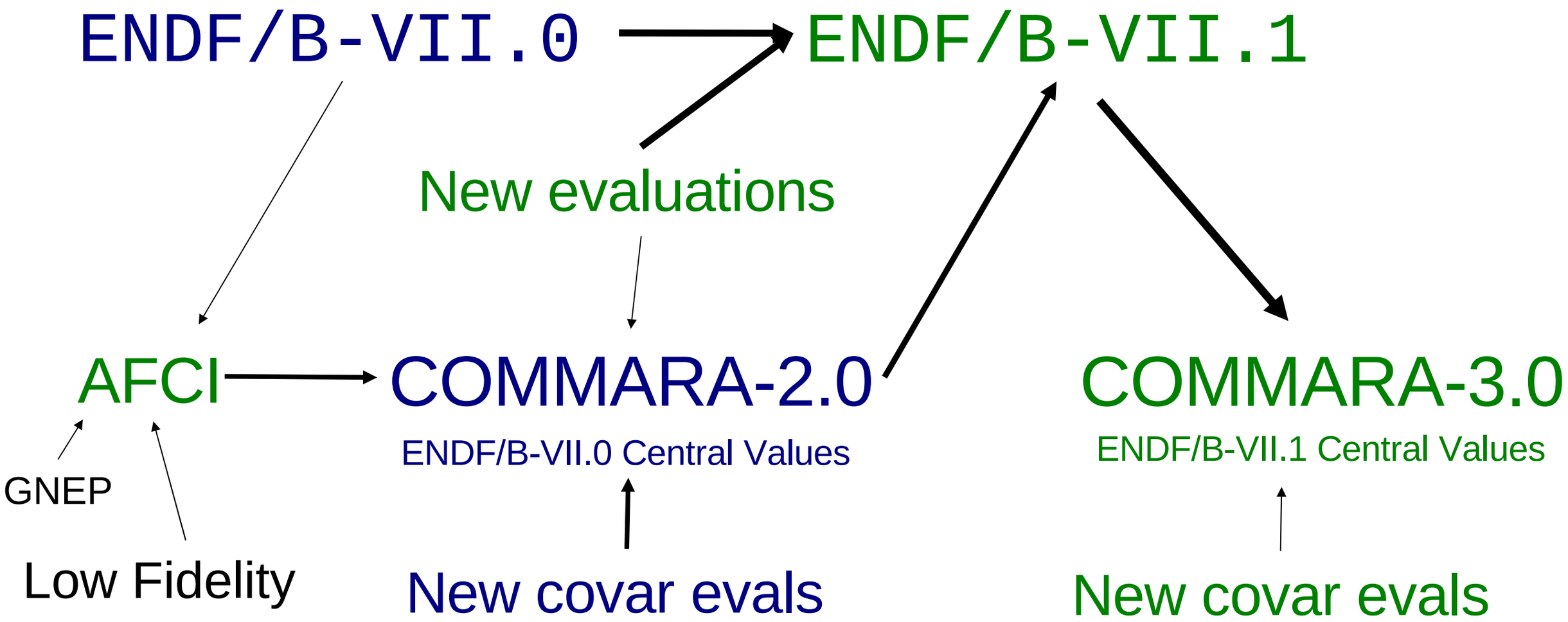
Scope

- Associated with neutron cross sections from ENDF/B-VII.1
- Multigroup (processed) covariances with uniform lethargy energy groups (33 groups, flux: thermal–1/E–fiss spec)
- Reaction channels:
  - (n,el), (n,inl), (n,2n), (n,γ)
  - (n,f) & nubar MF31 (73)
  - prompt fission neutron spectra (PFNS, ^{238,239,240}Pu LANL, JENDL-4 MF35 (85), plus cross-material covariances (LANL)
  - Mubars MF34 (116 & additional from JENDL)

NJOY flux weighting



Recent Covariance Evolution



Quality Assurance

- Web-based Sigma-QA (A. Sonzogni) allows visual and also quantitative inspection of:
  - Differential uncertainties (dynamic)
  - Integral uncertanties (static)
- UnCor applied to full library, performs 8 tests, warnings for possible problems including:
  - small uncertainties: (n,tot)<1%, (n,el) and (n,γ)<2%, etc.
  - non-positive-definite matrices (fixable for all but PFNS)
  - PFNS covariance not summing to zero (not usually a problem)
- non-positive-definite matrices are usually fixable by slightly reducing the off-diagonal elements. If not, slightly more drastic measures may be required.

COMMARA Checklist

- Test for small uncertainties:

Total with small uncertainties : 174

Total with too large uncertainties : 91

Uncertainty test 1

Reation	Max % Unc
(n,total)	1.0
(n,elas)	2.0
(n,inel)	3.0
(n,2n)	3.0
(n,f)	0.7
(n,g)	2.0
Total nubar	0.7
Prompt nubar	0.7
other	2.0

COMMARA Checklist

- 2nd test for too small uncertainties:

  If cross section < 3mb ⇨ uncert ≥ 25%

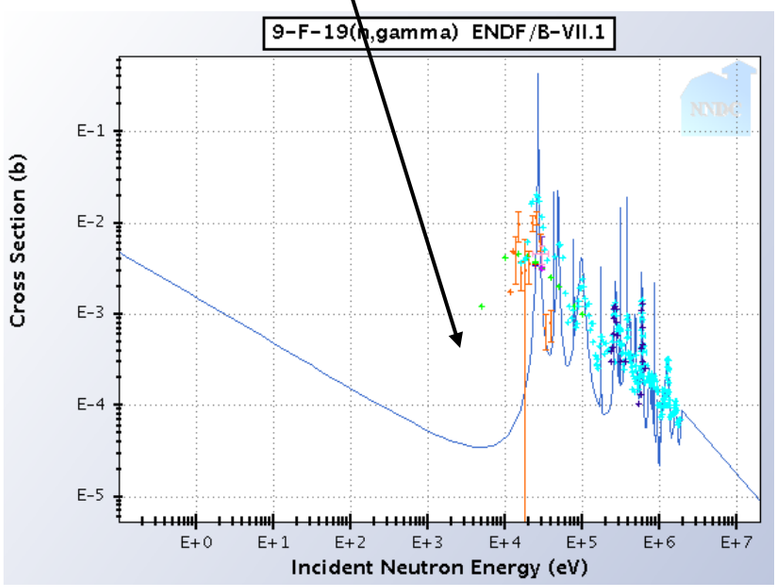
  Total materials : 128

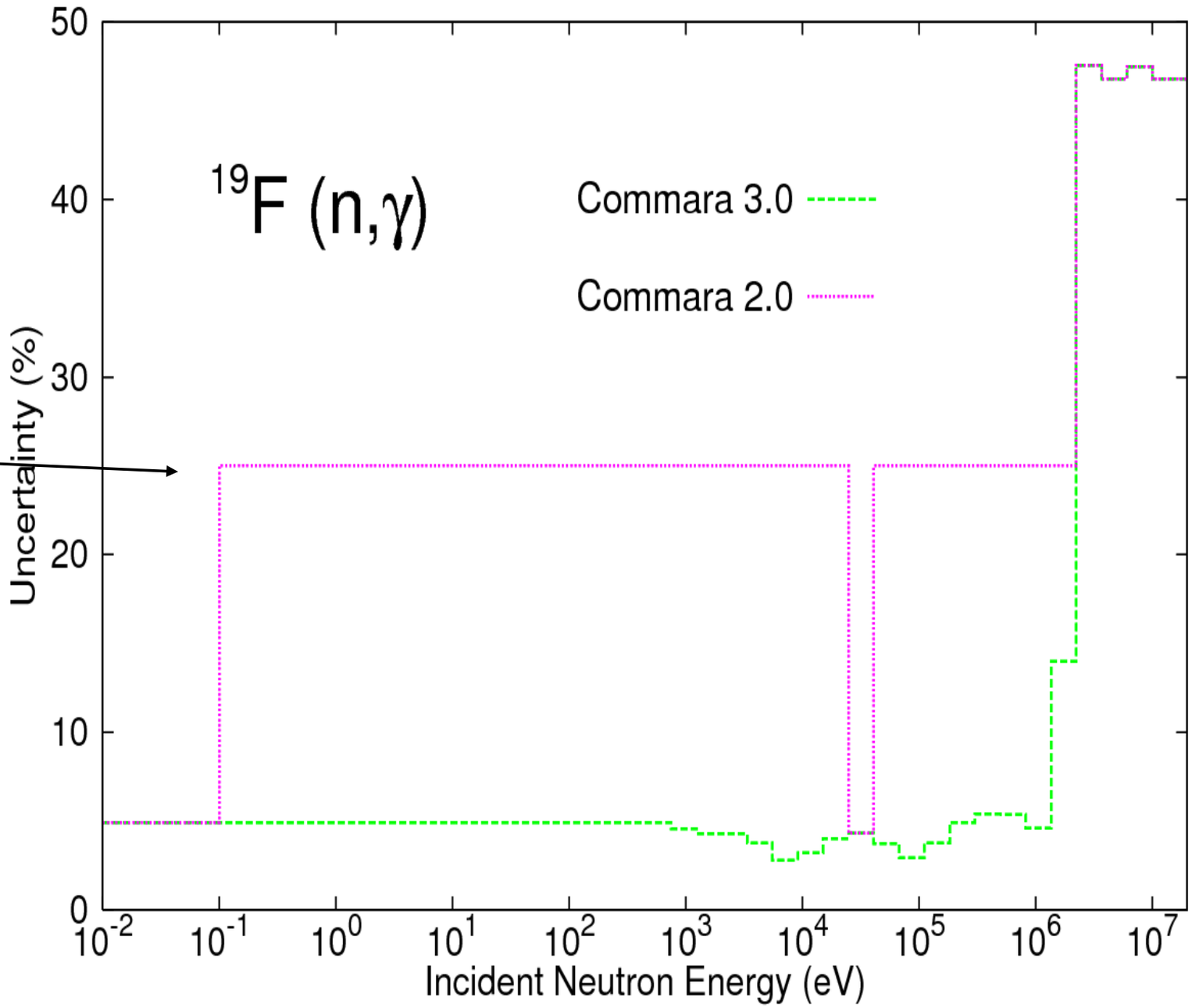
- Optical model peaks in elastic: 44
- Zero unc with non-zero cross section: 90
- Peaks/jumps in uncertainties: 33 (more than factor of 8)
- Negative eigenvalues : only PFNS (all ~2-3E-3, roundoff err)

^{19}F

3.0: LANL
MF33 estimates

2.0: LANL estimates
with 25% unc limit when
σ < 3mb

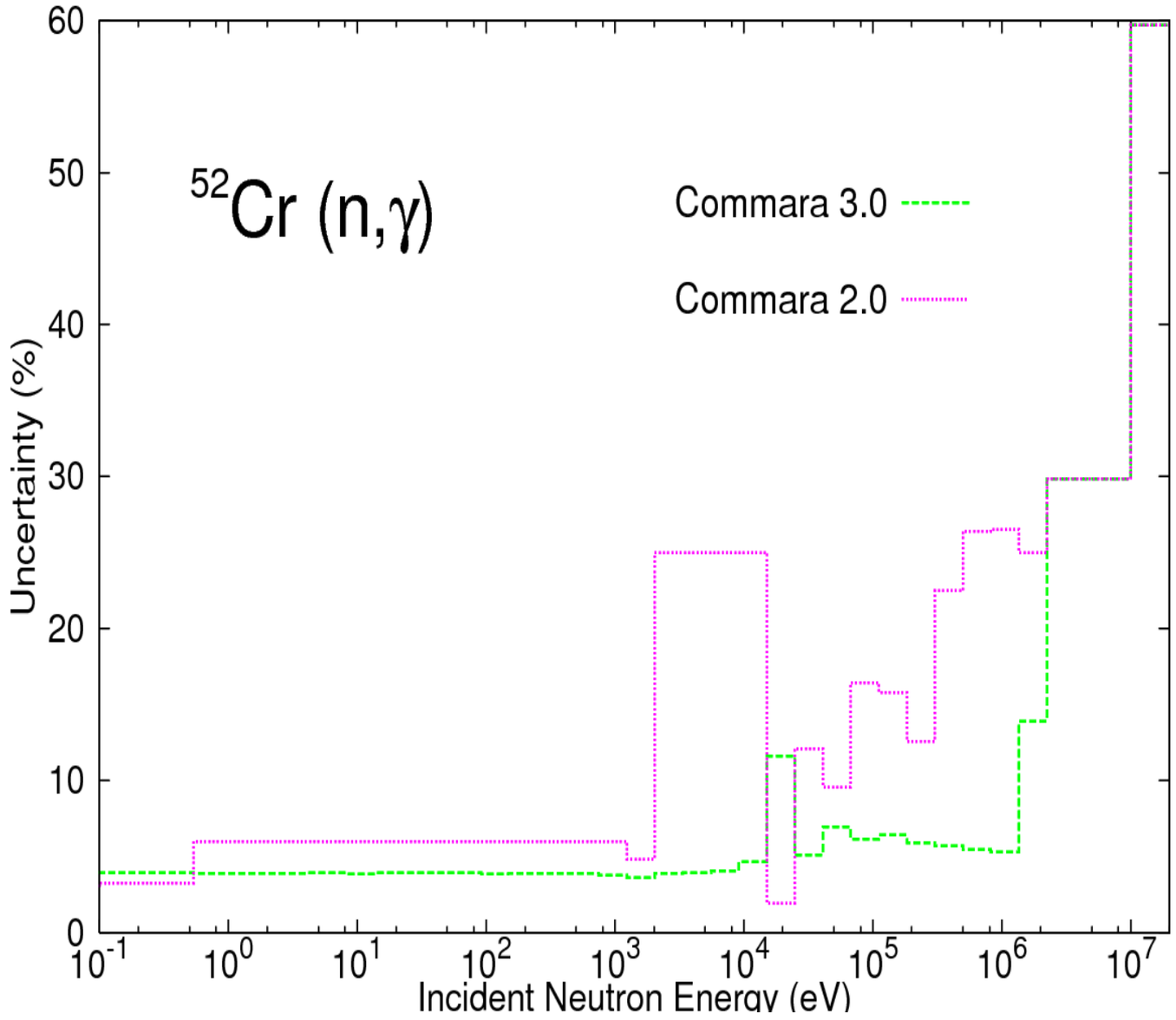




^{52}Cr

3.0: New ORNL RRR evaluation

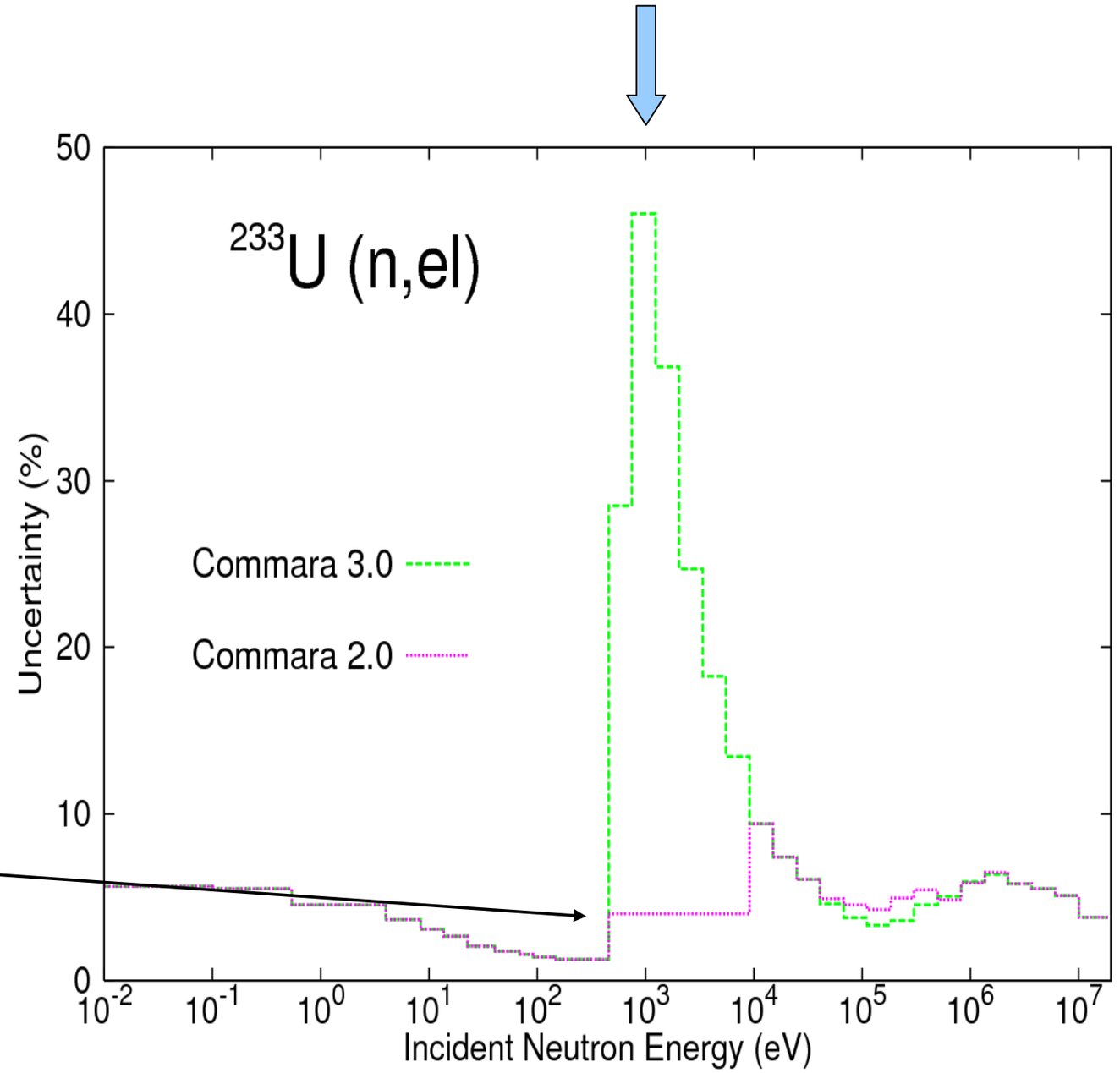
2.0: Estimate using kernel approximation



^{233}U

3.0: Updated LANL evaluation

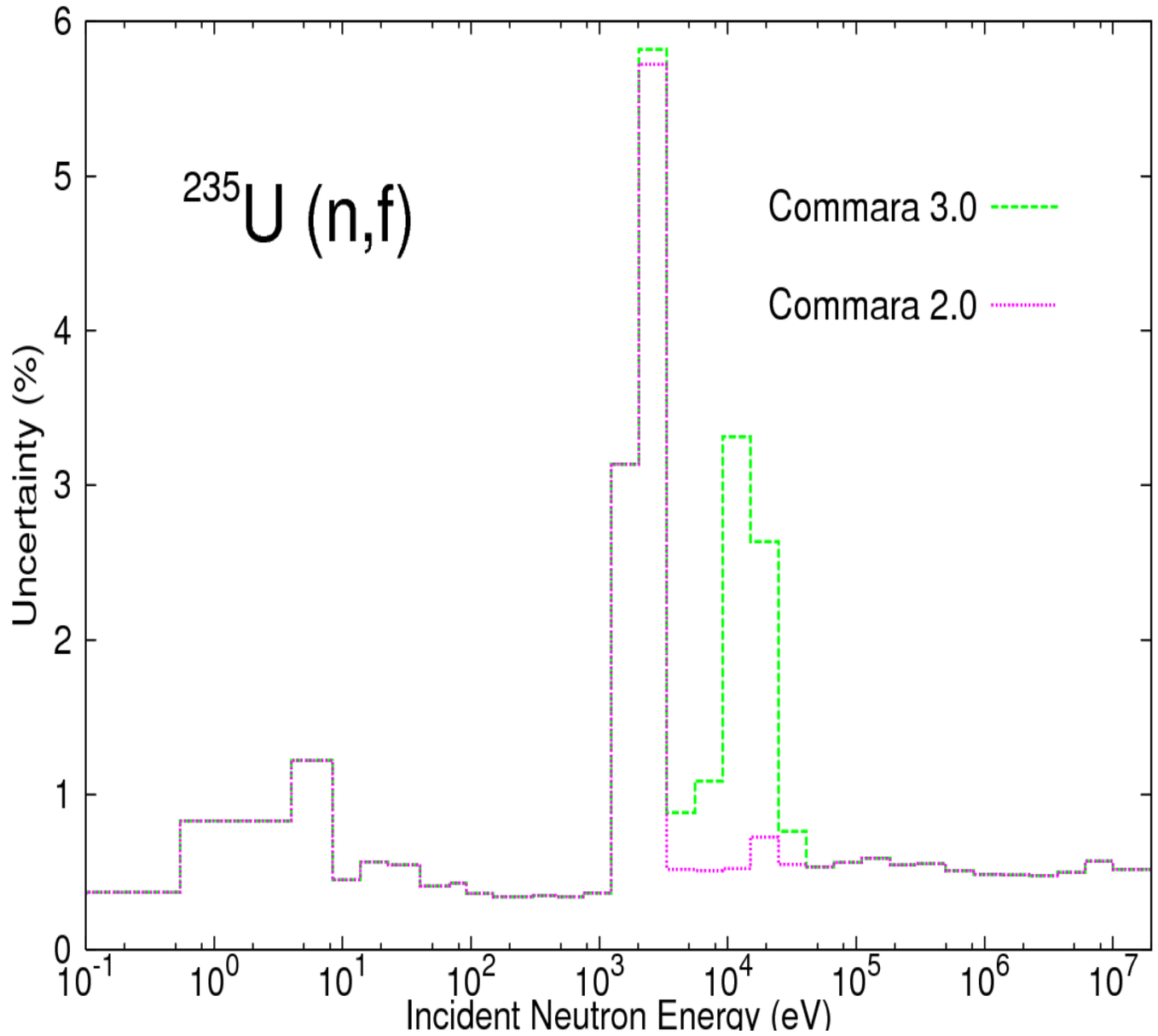
2.0: LANL evaluation, optical peak truncated to 4%



^{235}U

3.0: Updated MF33
V.G. Pronyaev,
IPPE/LANL

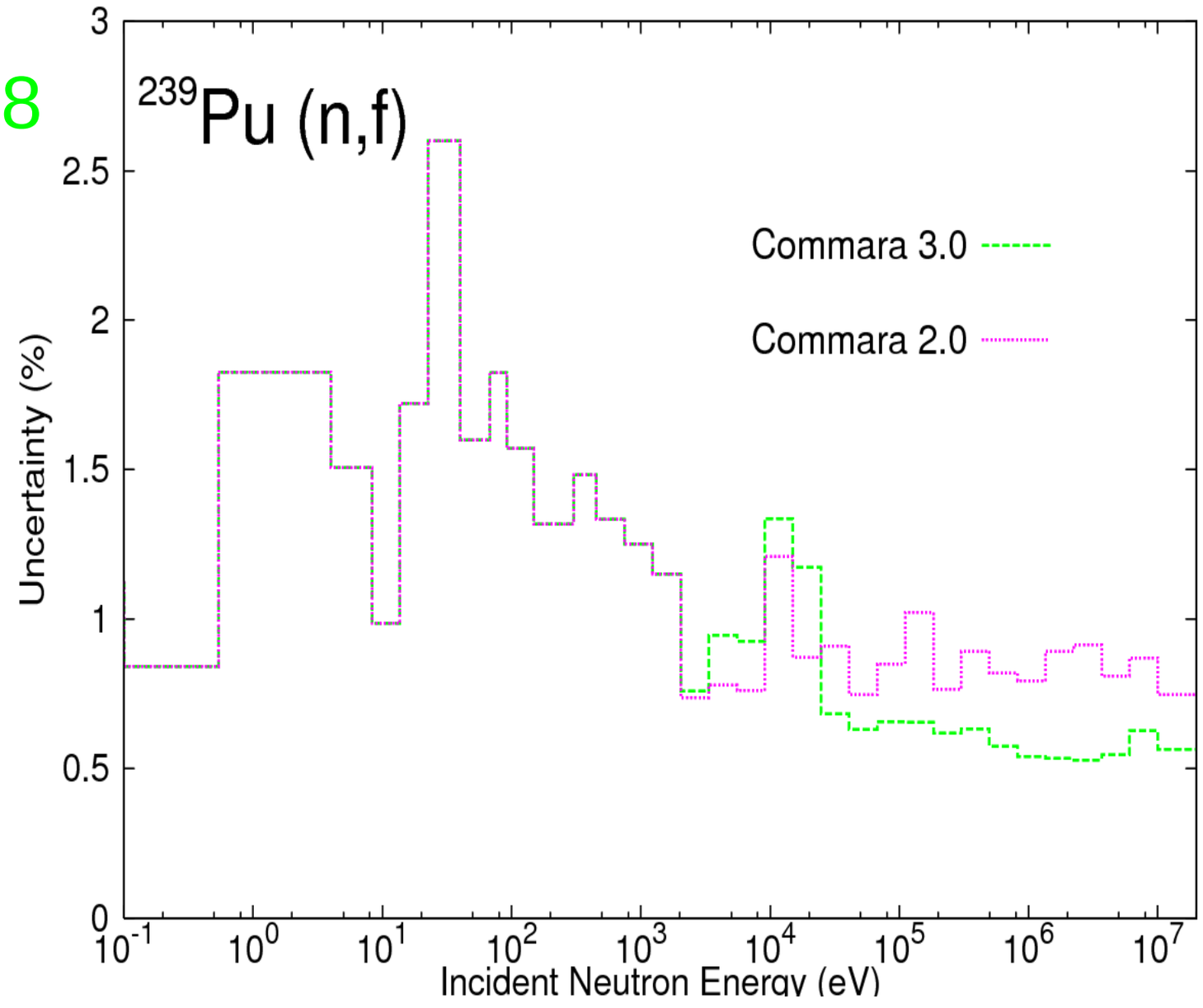
2.0: MF33 covariances
LANL/ORNL



^{239}Pu

3.0: Updated MF33/MT18 standards covariances, V.G. Pronyaev IPPE

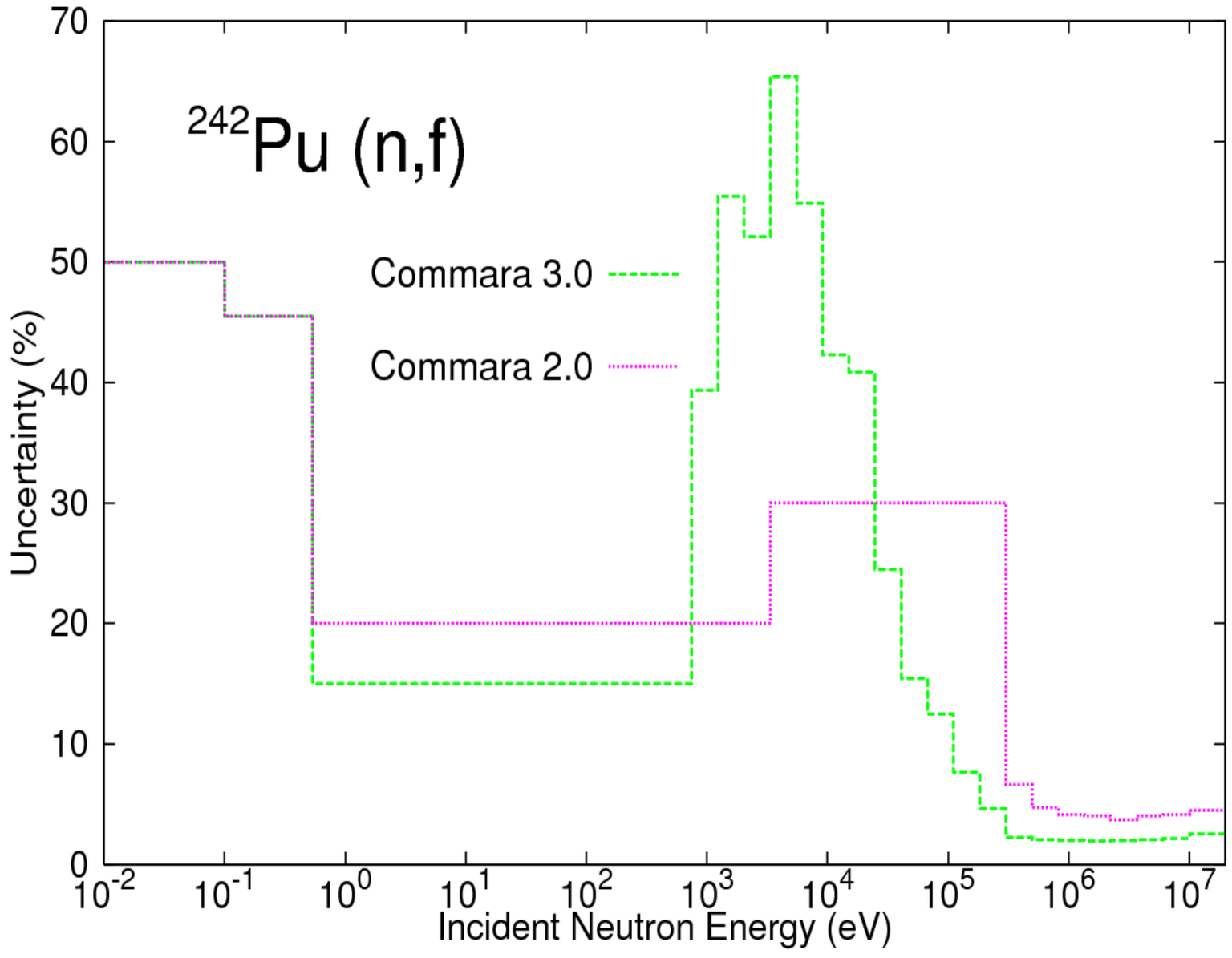
2.0: MF33 evaluation by LANL/ORNL



^{242}Pu

3.0: adopted JENDL-4

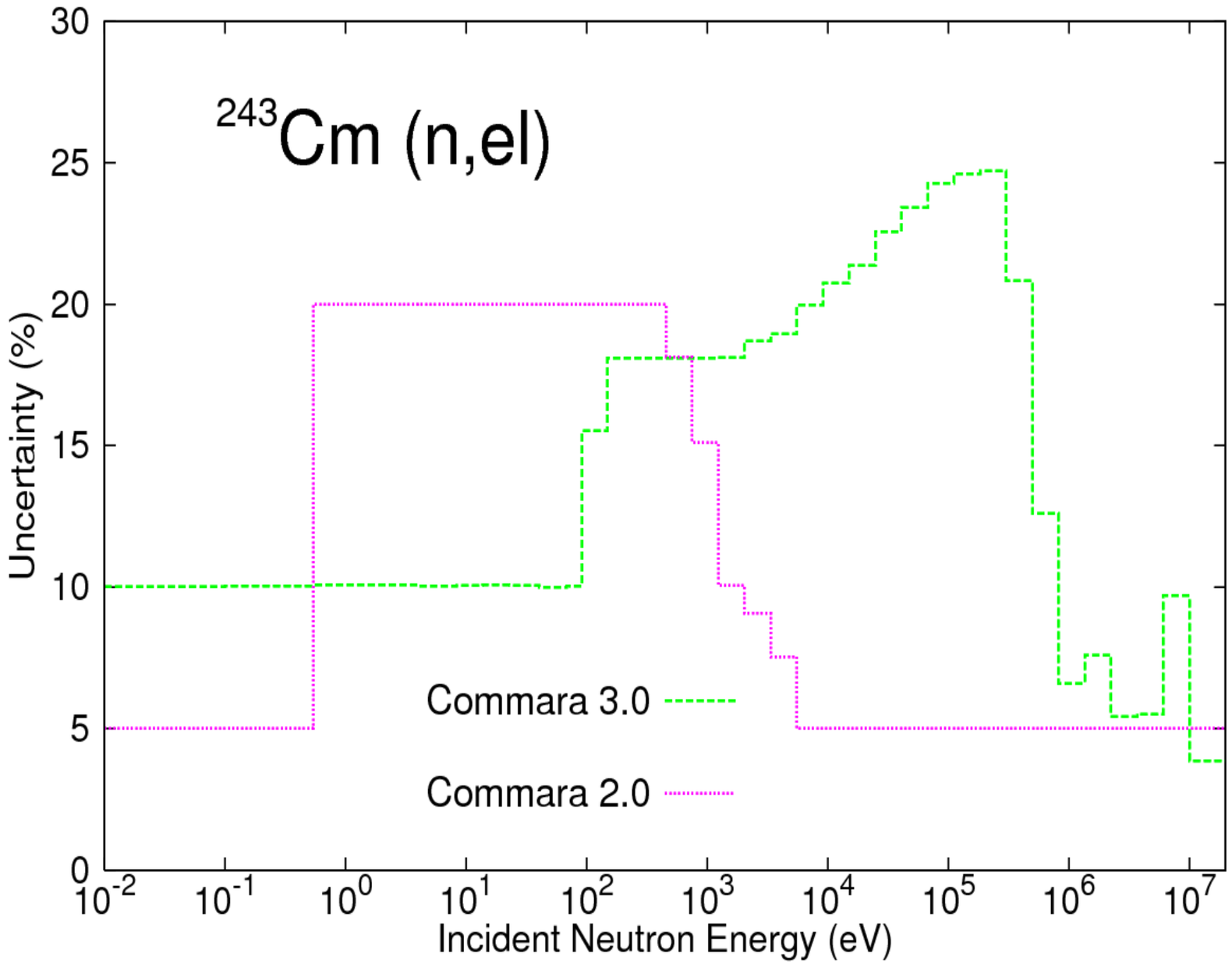
2.0: Empire/Kalman in fast region.
Low-fidelity estimates in thermal/RRR.



^{243}Cm

3.0: adopted JENDL-4

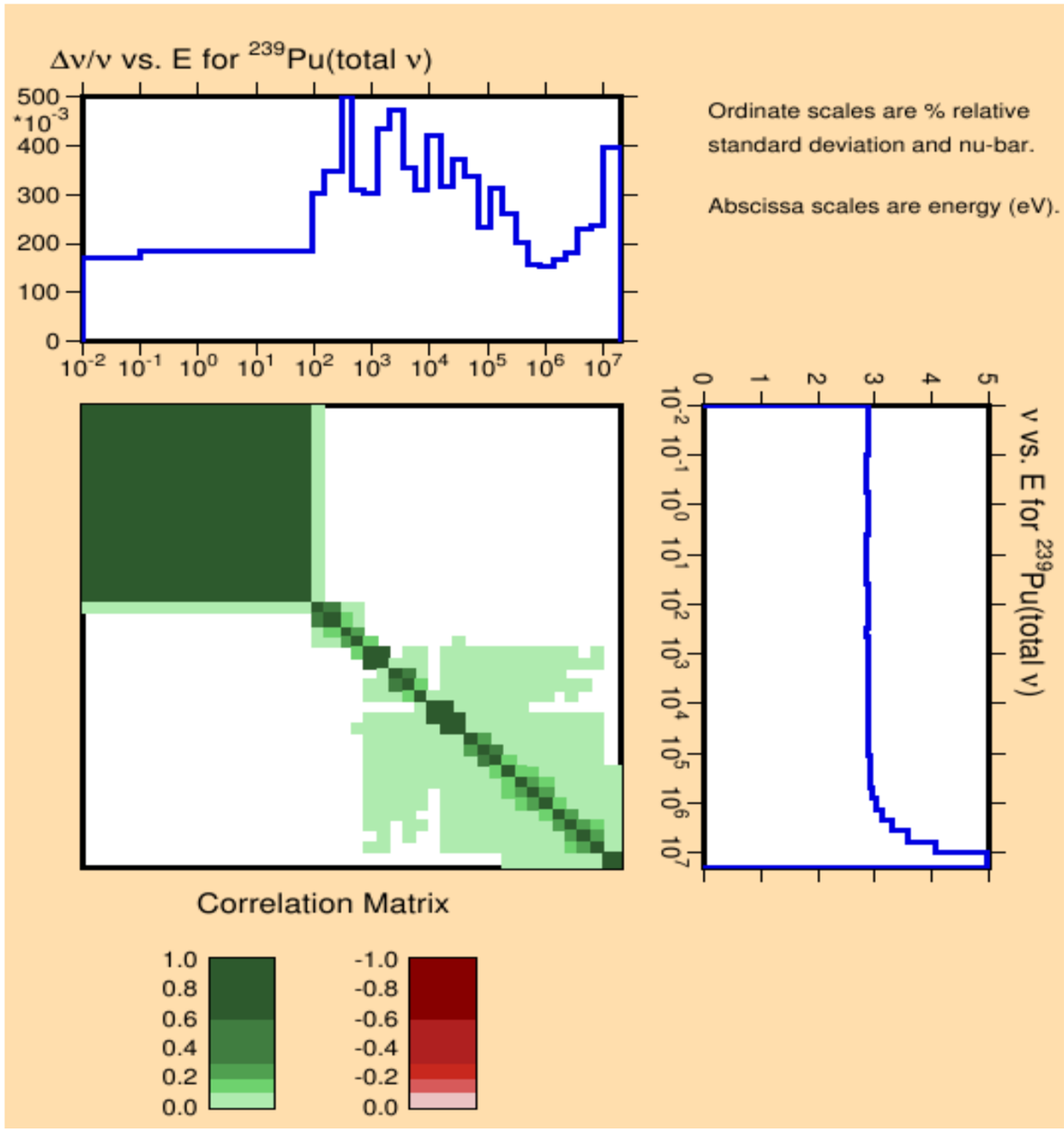
2.0: default Empire/Kalman with Low-fidelity estimates in thermal/RRR



Nubar covariances

^{239}Pu - LANL

Total materials with MF31: 73

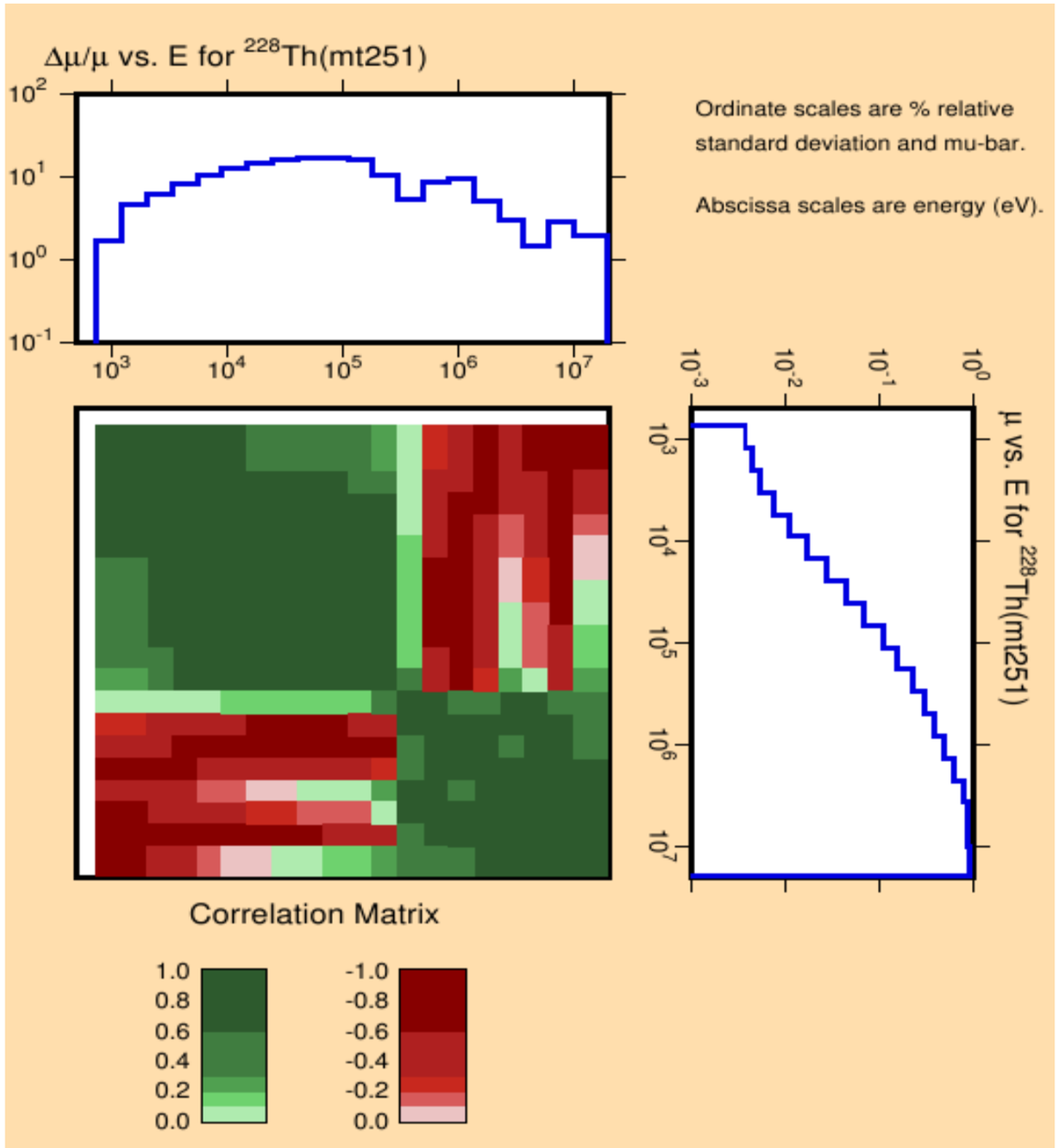


Mubar covariances

^{228}Th

JENDL-4

Most mubar covariances in ENDF/B-VII.1 from JENDL



Missing Mubars (MF34)

- ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U
- ^{237}Np
- ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu
- ^{241}Am, $^{242m1}Am$, ^{243}Am
- $^{242\text{-}246}Cm$

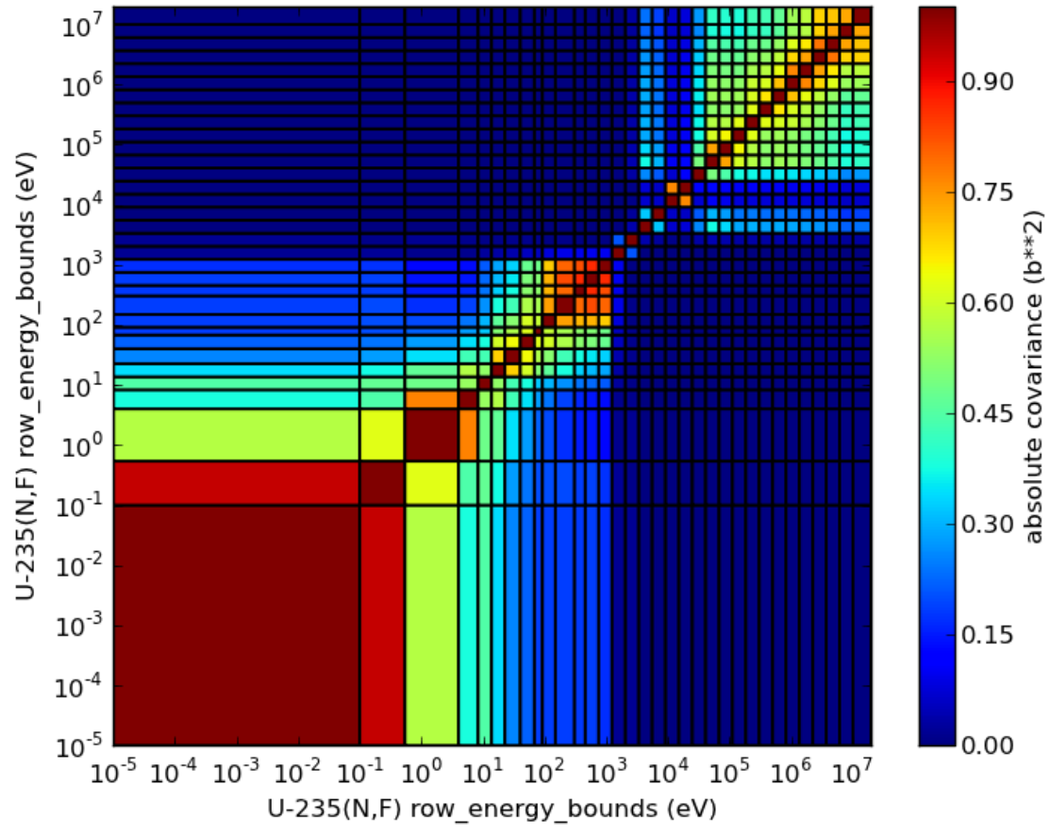
Possible Sources:
LANL
Empire estimates
JENDL

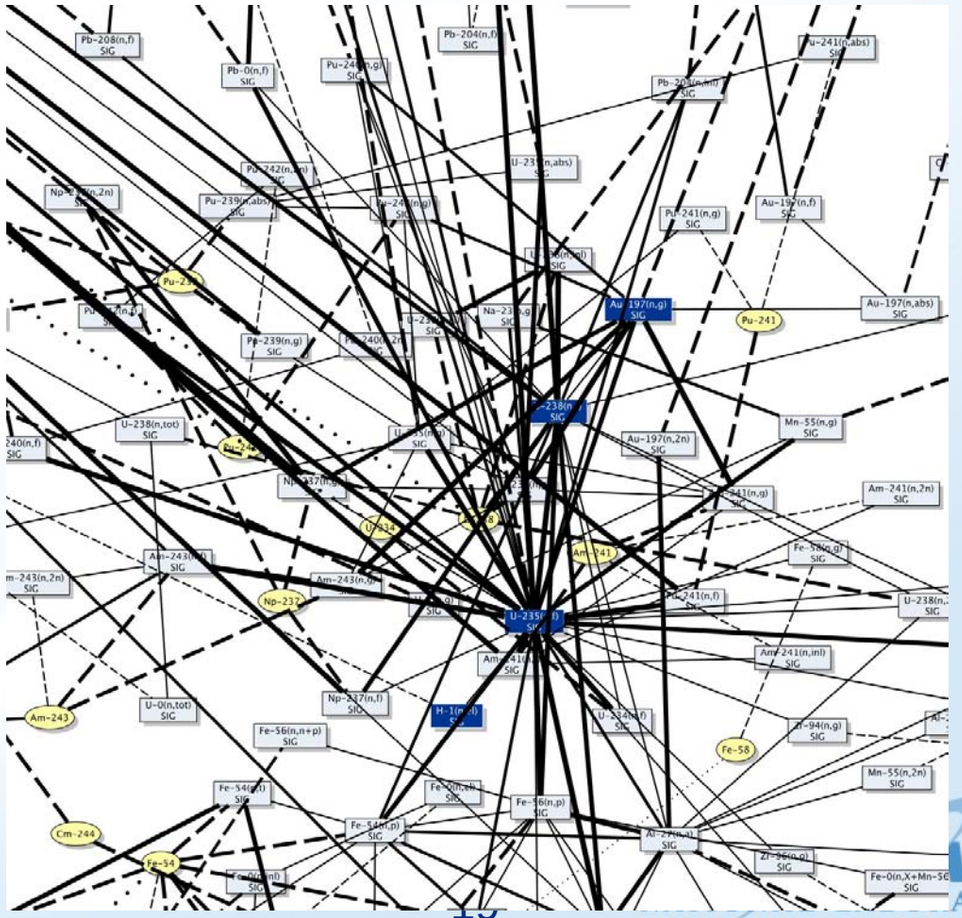
Only structural materials with MF34
^{23}Na, ^{55}Mn, ^{56}Fe, $^{180\text{-}186}W$

Developing cross-isotope cross-reaction covariances

- EXFOR contains many forms of coupled cross section data:
  - reaction combinations
  - reactions on elemental targets
  - non-elastic data
  - ratios to monitors (unused)
  - “isomers math” (unused)
- Goal: Refit all COMMARA-2.0 priority cross sections simultaneously
  - 33-group structure
  - ENDF/B-VII.1 covariances for prior
    - includes “on-diagonal” covariance
    - includes standards “off-diagonals”
  - use EXFOR entry’s REACTION string to construct linearized kernel

End product is covariance, not mean values





Integral experiment uncertainty simulations using COMMARA 2 & 3.0β

SFR

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
^{240}Pu	206	241	439	39	113	169	0	580
^{56}Fe	195	0	0	320	321	0	88	501
^{245}Cm	8	444	50	0	3	0	0	447
^{238}U	50	9	33	51	230	0	0	244
^{244}Cm	147	141	111	2	5	0	0	232
^{238}Pu	117	119	154	8	32	28	0	231
^{242}Pu	176	93	81	7	15	0	0	216
^{239}Pu	131	136	41	27	78	100	0	233
^{241}Pu	95	45	34	2	38	0	0	117
^{243}Am	55	58	13	2	18	0	0	83
^{23}Na	8	0	0	21	182	0	145	234
Total	423	567	492	329	459	198	170	1063

2.0

ADMAB

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
^{241}Am	231	122	172	11	116	0	0	333
^{241}Pu	73	42	33	0	57	0	0	107
^{245}Cm	13	1063	115	0	10	0	0	1070
^{244}Cm	505	651	516	1	37	0	0	973
^{243}Am	300	449	95	3	229	0	0	594
^{237}Np	183	171	65	1	97	0	0	277
^{209}Bi	64	0	0	66	166	0	0	190
^{240}Pu	56	88	151	8	64	82	0	211
^{15}N	1	0	0	216	13	0	0	216
^{239}Pu	91	126	35	15	118	129	0	237
^{242m}Am	11	142	10	0	4	0	0	143
^{238}Pu	32	56	59	2	19	3	0	89
Total	674	1360	593	227	355	153	0	1690

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
^{240}Pu	153	94	119	36	106	95	0	261
^{56}Fe	194	0	0	320	320	0	80	499
^{245}Cm	39	46	67	0	2	21	0	93
^{238}U	48	9	33	52	231	45	0	248
^{244}Cm	94	31	90	1	3	3	0	133
^{238}Pu	63	26	56	5	8	30	0	93
^{242}Pu	40	41	26	6	14	55	1	85
^{239}Pu	132	141	41	27	78	100	0	236
^{241}Pu	95	70	34	2	38	0	0	128
^{243}Am	55	58	13	2	18	0	0	83
^{23}Na	102	0	0	17	182	0	35	212
Total	345	206	186	327	456	160	87	738

3.0β

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
^{241}Am	230	122	172	11	116	0	0	333
^{241}Pu	73	74	33	0	57	0	0	123
^{245}Cm	57	112	149	0	6	69	0	207
^{244}Cm	311	148	416	1	25	45	1	543
^{243}Am	300	449	95	3	229	0	0	594
^{237}Np	314	171	65	1	64	0	0	369
^{209}Bi	63	0	0	66	166	0	0	190
^{240}Pu	44	34	37	8	60	60	0	109
^{15}N	1	0	0	216	13	0	0	216
^{239}Pu	91	131	35	15	118	129	0	240
^{242m}Am	0	0	0	0	0	0	0	0
^{238}Pu	17	10	21	1	5	14	0	33
Total	602	551	492	227	346	165	1	1052

Summary

- ENDF/B-VII.1 released Dec 2011
- ENDF files processed with NJOY using AFCI 33-group structure, flux = thermal, 1/E, fiss spec (E>100 keV)
- Preliminary files tested using Sigma-QA and UnCor procedures for Quality Assurance
- Subset provided as COMMARA-3.0β
- Final release dependent on funding

EXTRAS

Commara 2.0 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	^{109}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
	^{93}Nb				^{246}Cm

COMMARA-2 Methodology

- Covariance evaluation methodology determined by priorities:
  - Most important materials treated individually
  - Medium importance materials treated with simplified methods
  - Low priority materials (mostly fission products) treated with low-fidelity type approach

COMMARA-2 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

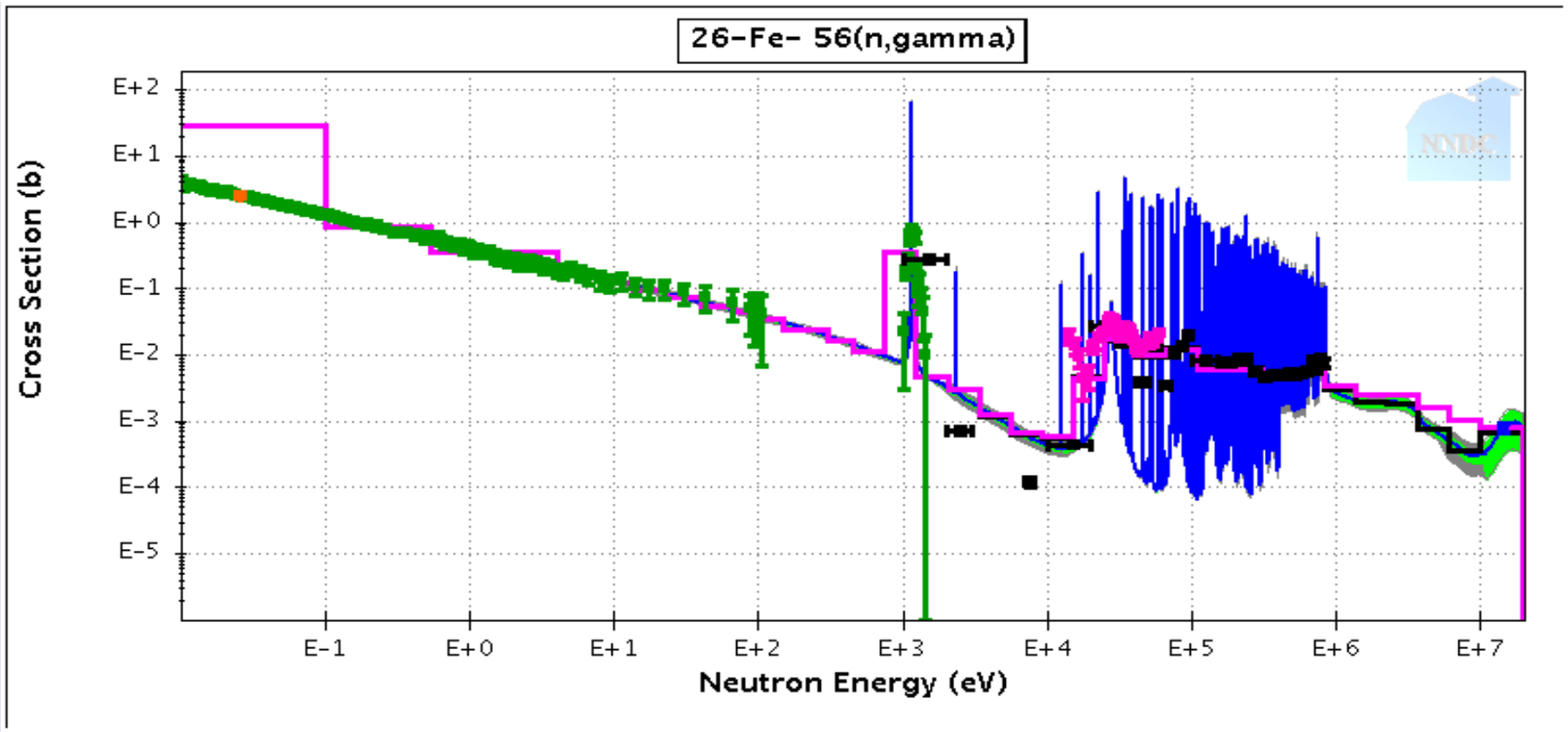
Fast neutron range (MF33)

- 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

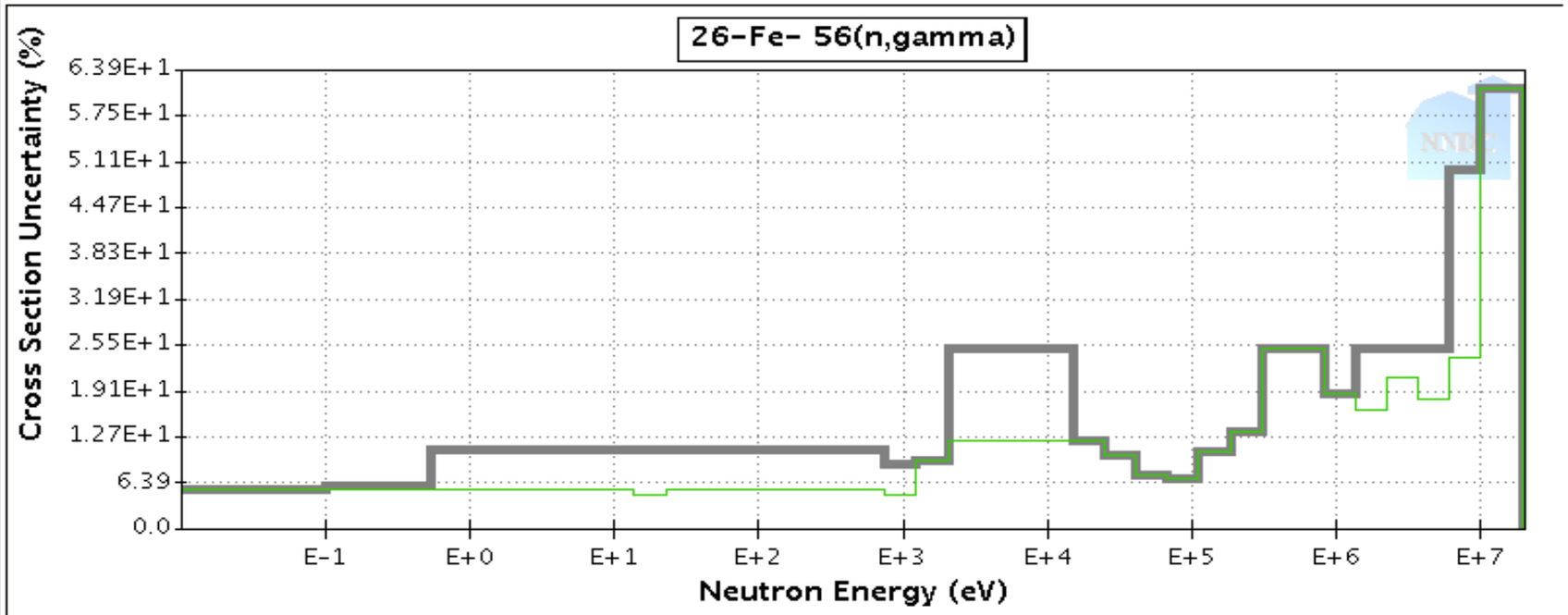
^{60}Ni capture integral quantities from Sigma-QA

Capture					
Library	THERMAL	RI 0.5-2E+7 eV	MACS 30 keV	^{252}Cf	14 MeV
ENDF/B-VII.0	2.772	1.412	2.826E-2	4.022E-3	2.859E-4
JEFF3.1	2.772	1.412	2.826E-2	6.033E-3	7.558E-4
JENDL4.0	2.913	1.472	2.792E-2	6.172E-3	6.992E-5
ROSFOND	2.772	1.412	2.826E-2	6.033E-3	7.558E-4
ENDF/B-VI.8	2.772	1.406	2.826E-2	4.022E-3	2.859E-4
CENDL3.1	2.772	1.413	2.826E-2	5.825E-3	1.131E-3
KADoNiS			2.990E-2		
Atlas	2.500	1.400			
Kadonis Δ			7.000E-4 2.34%		
Atlas Δ	6.000E-2 2.40%	2.000E-1 1.42E+1%			
AFCI2.0 Δ	1.386E-1 5.00%	1.183E-1 8.37%	1.811E-3 6.40%	2.902E-4 7.21%	6.591E-5 2.30E+1%
Recommended Δ	1.430E-1 5.15%	2.017E-1 1.42E+1%	7.968E-4 2.81%		

Example of Sigma-QA plot



Cursor at: x = 3.6826E-2 (eV) y = 2.0212E-2 (b)



Update Plot | Reset

1E-2 ≤ E_n (eV) ≤ 2E7 Log

1E-6 ≤ σ (b) ≤ 1.924E2 Log

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

Group cross sections with 1/E flux

- [x] ENDF/B-VII.0 group
- [x] 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
- [x] Huang Zheng-De 1980
- [x] Shcherbakov 1977
- [x] Shcherbakov 1977
- [x] Allen 1982
- [ ] Allen 1976
- [x] Macklin 1964
- [x] Pomerance 1952

Remove EXFOR

Download plot for your article