COMMARA-3

Processed ENDF/B-VII.1 covariance library

M. Herman & S. Hoblit
National Nuclear Data Center
Brookhaven National Laboratory

mwherman@bnl.gov

Brookhaven Science Associates

Office of Science
U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY

COMMARA-2.0 materials

^{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**
	^{95}Nb				^{246}**Cm**

- 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

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, χ + 1/E flux)
- Reaction channels:
  - (n,el), (n,inl), (n,2n), (n,γ)
  - (n,f) & nubar MF31 (73)
  - prompt fission neutron spectra (PFNS, 238,239,240Pu by LANL & JENDL-4 MF35 (85)
  - Mubars MF34 (116 & additional from JENDL)

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

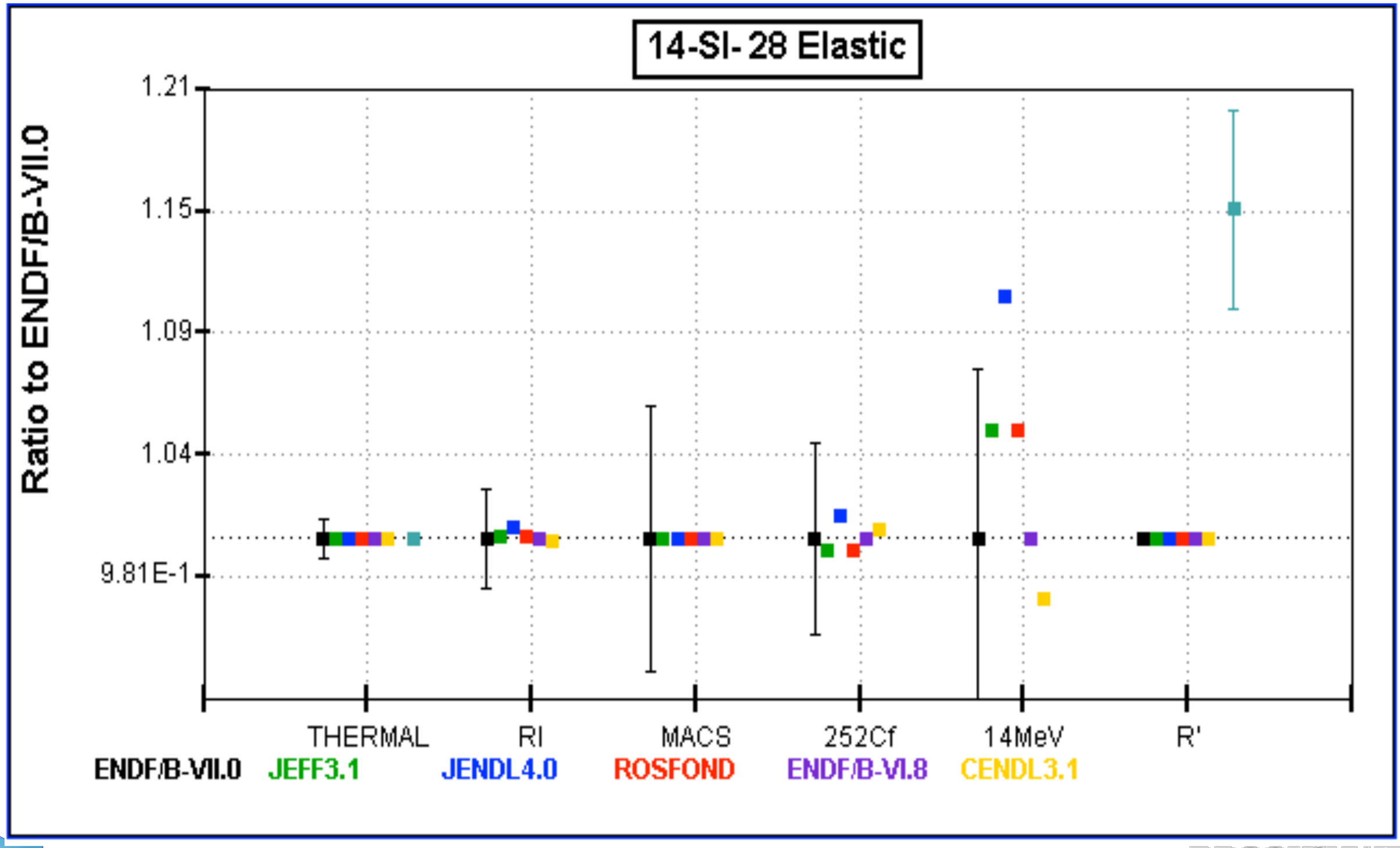
Fast neutron range (MF33)

- 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

Quality Assurance

- New 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
  - PFNS covariance not summing to zero
- non-positive-definite matrices are usually fixable by slightly reducing the off-diagonal elements. If not, more drastic measures may be required.

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



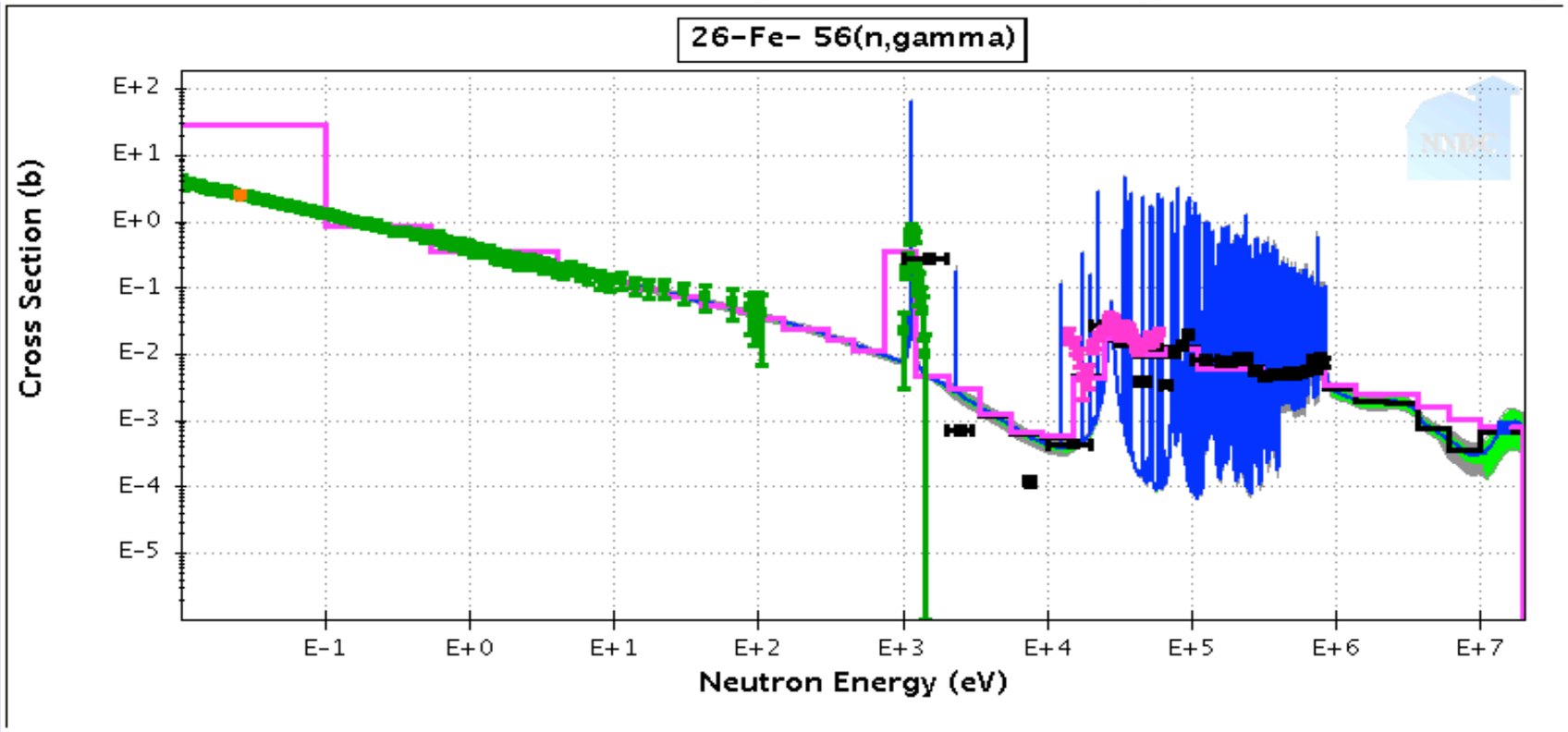
^{28}Si elastic integral quantities from Sigma-QA

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%

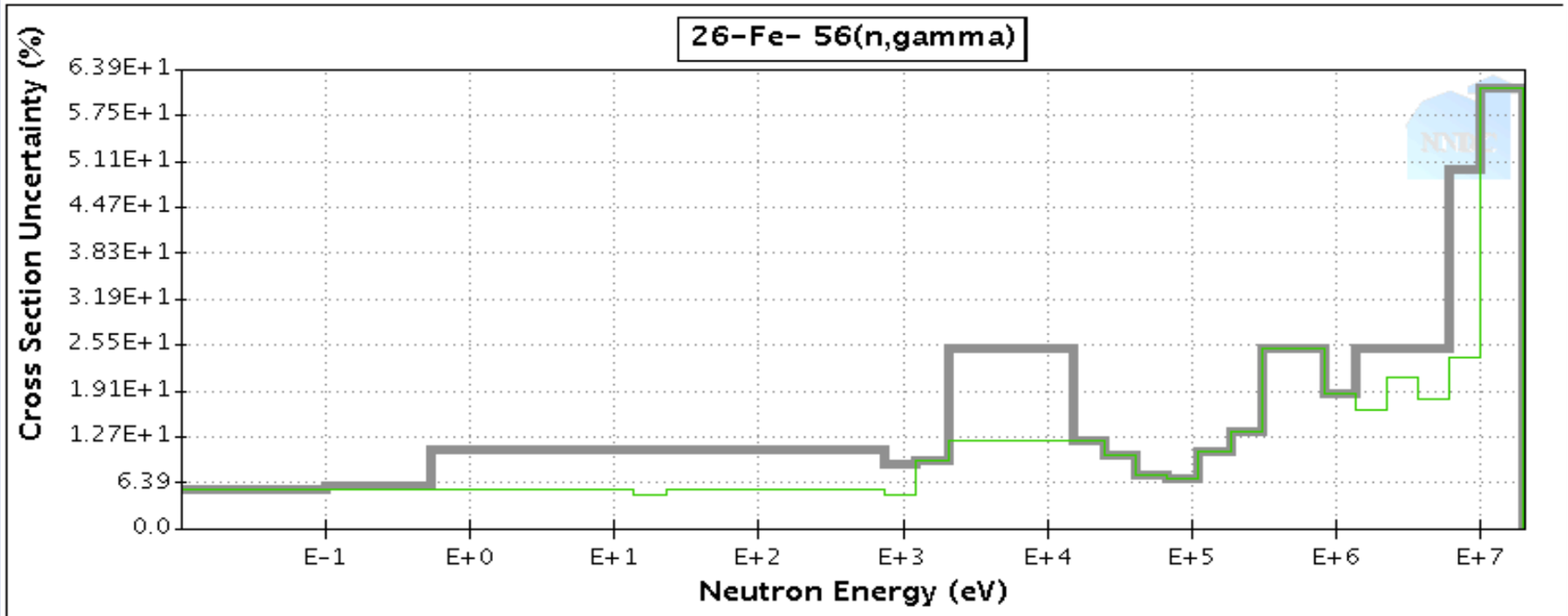
^{60}Ni capture integral quantities from Sigma-QA

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

- ☑ 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

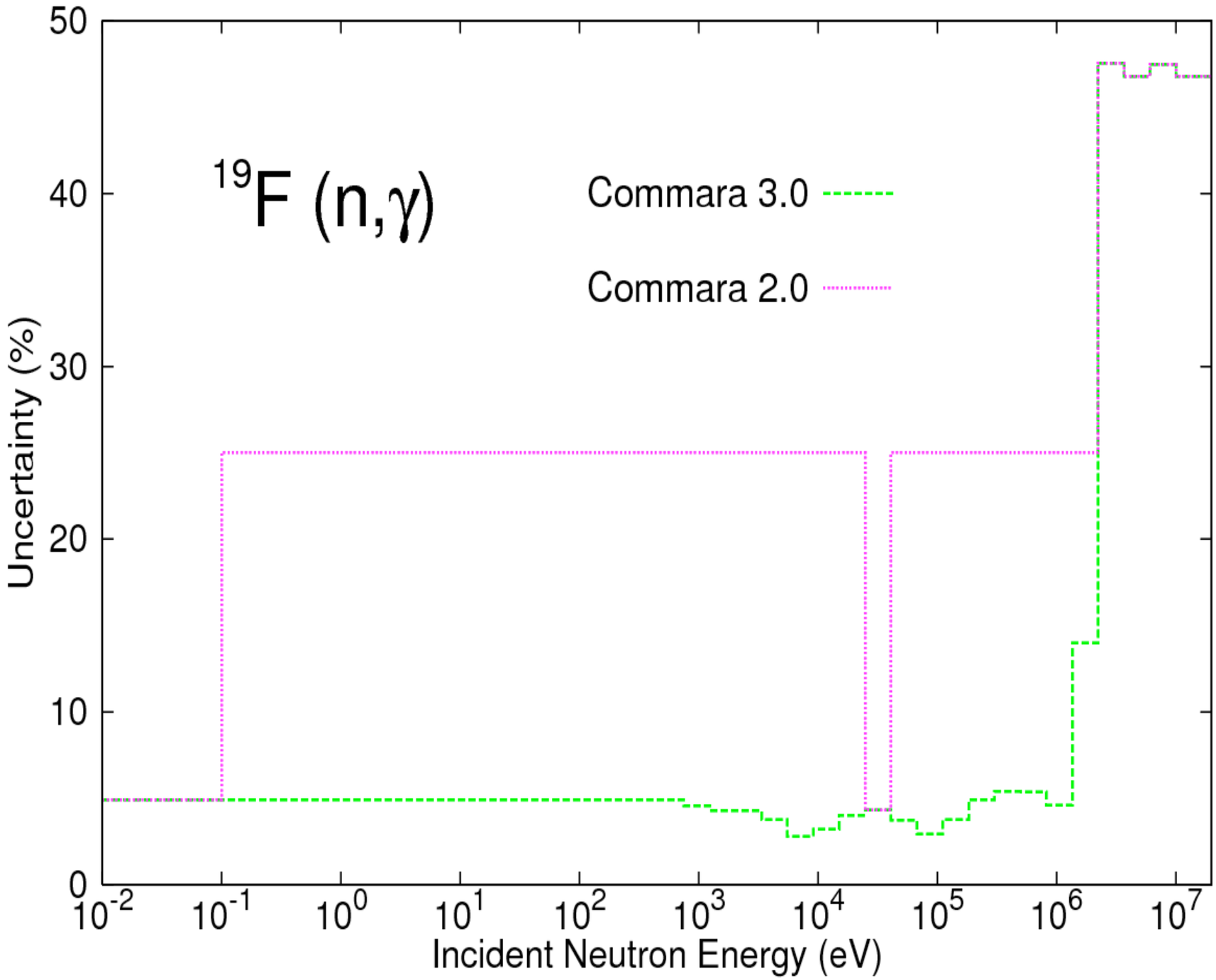
There are 7 EXFOR datasets

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

Remove EXFOR

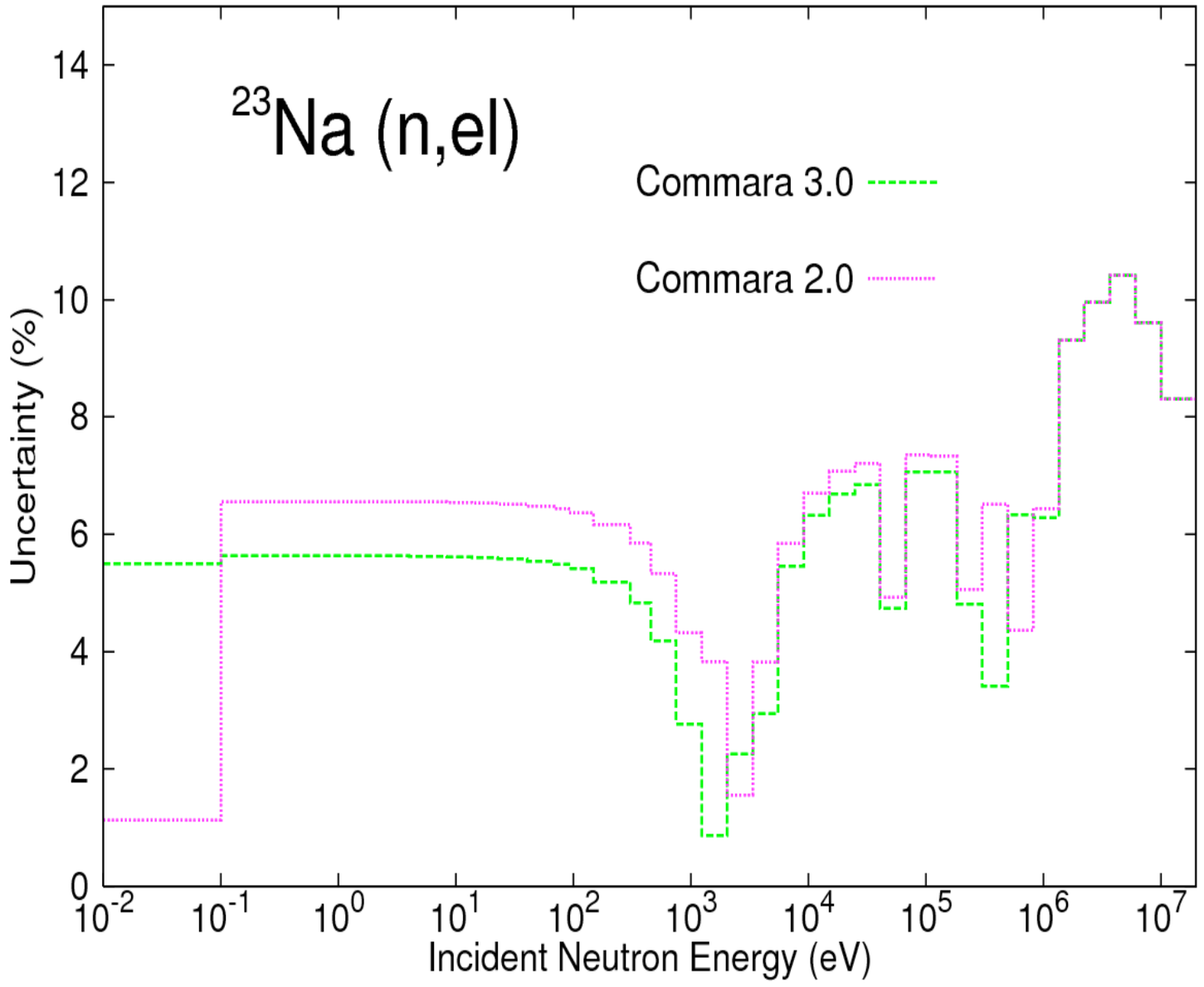
Download plot for your article

^{19}F (new ORNL evaluation)

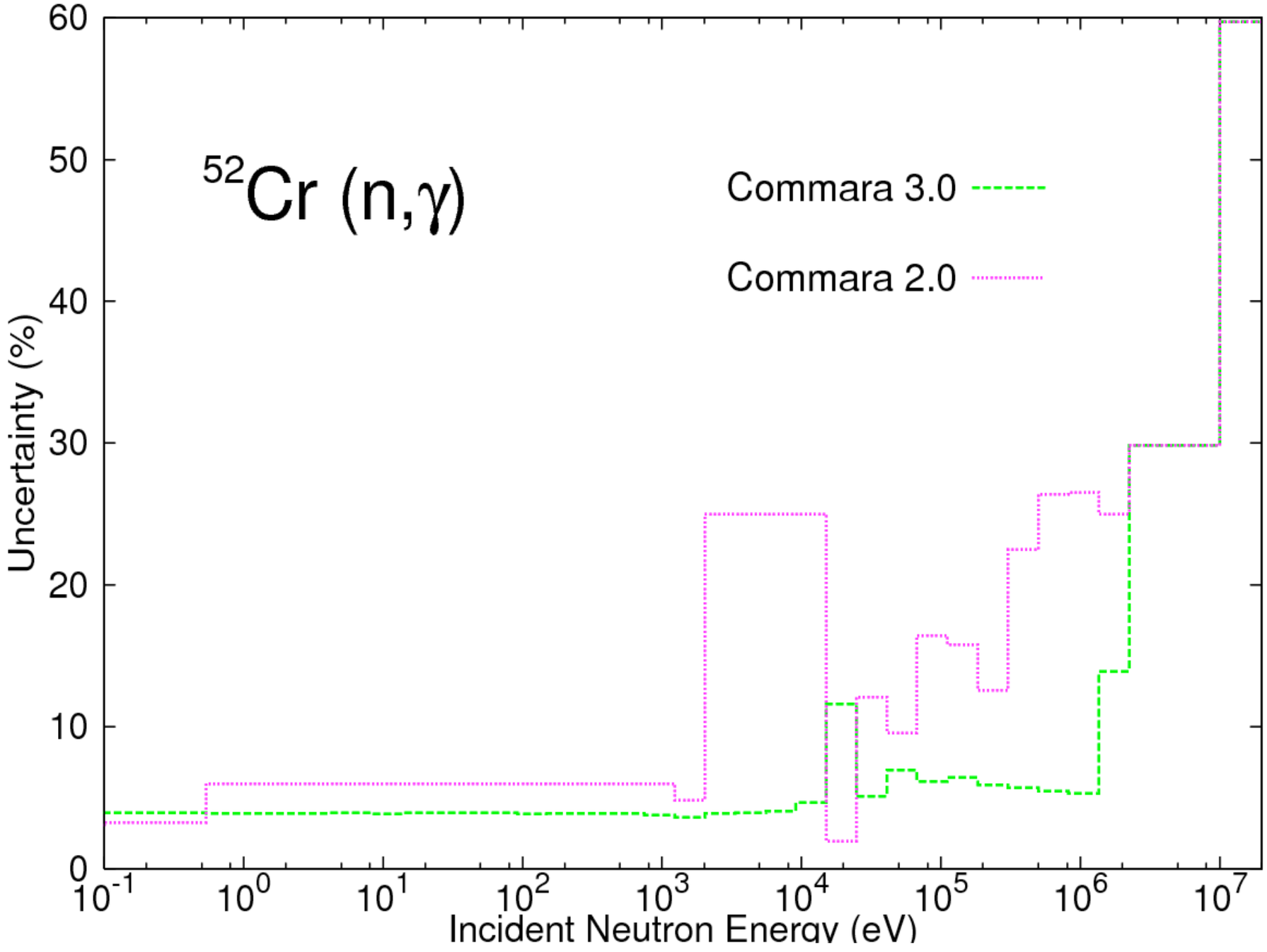


^{23}Na (reverted to ENDF/B-VII.0)

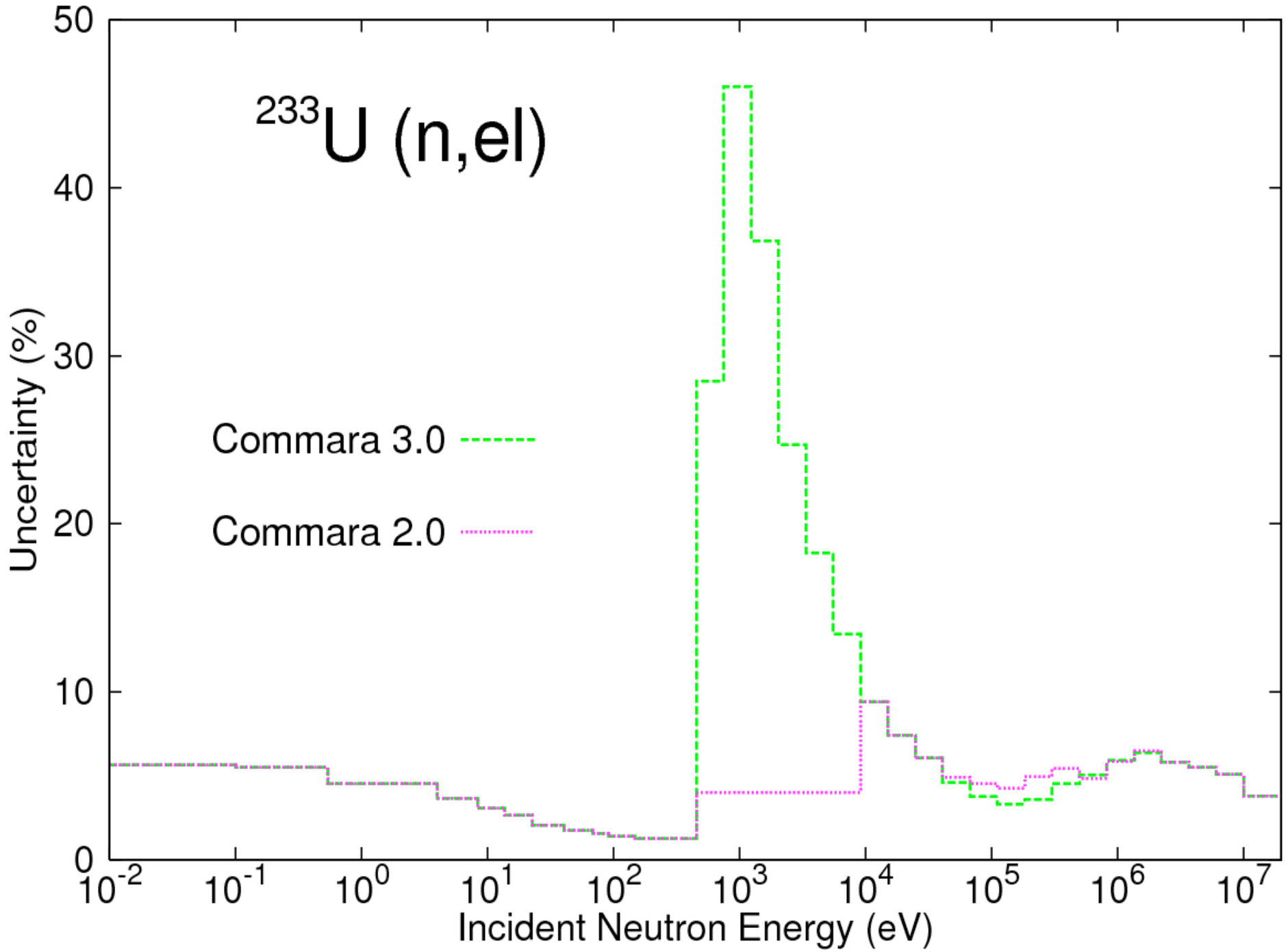
COMMARA 2.0 Covariances backported, w/ modifications



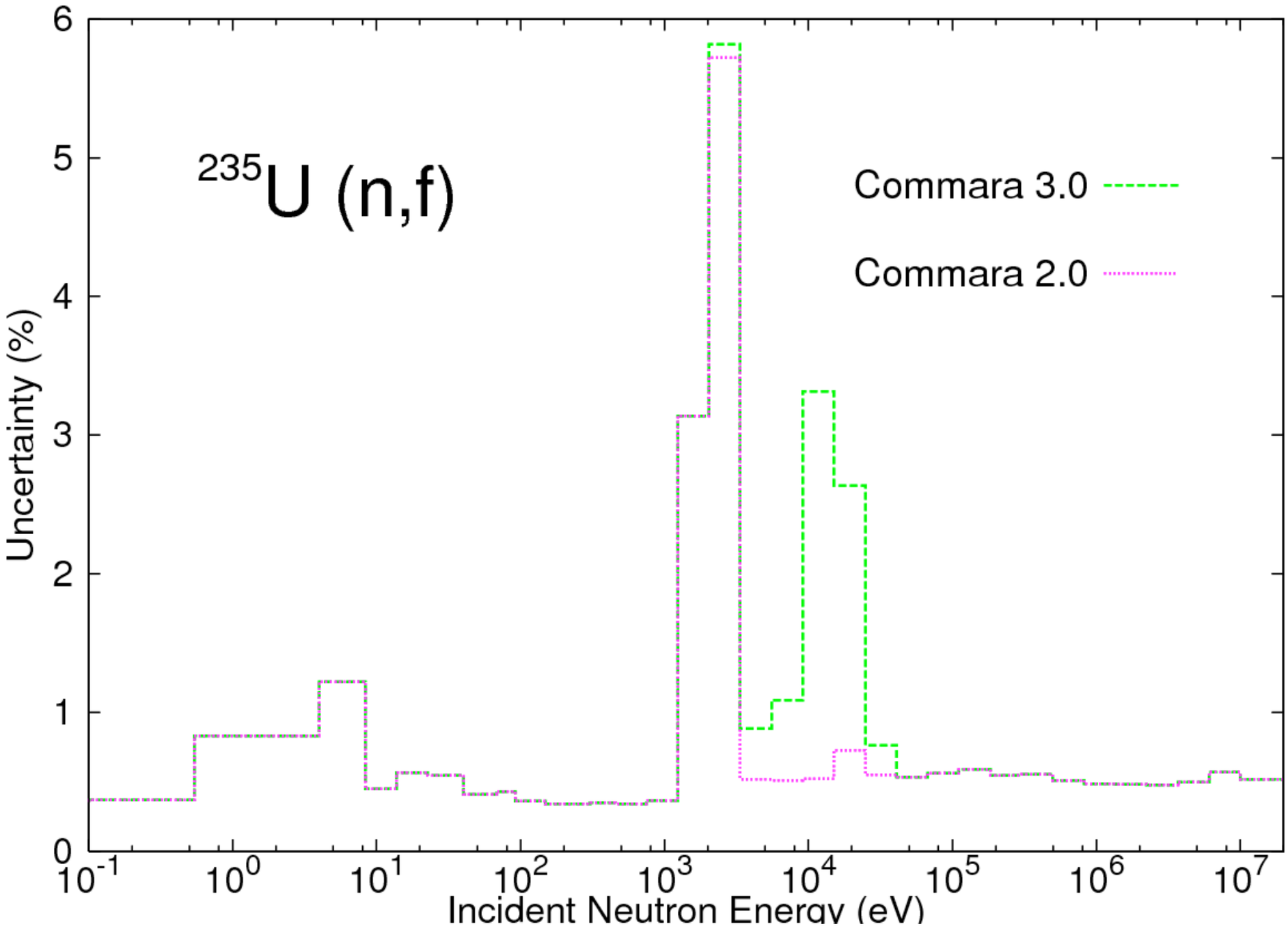
^{52}Cr (New ORNL RRR evaluation)



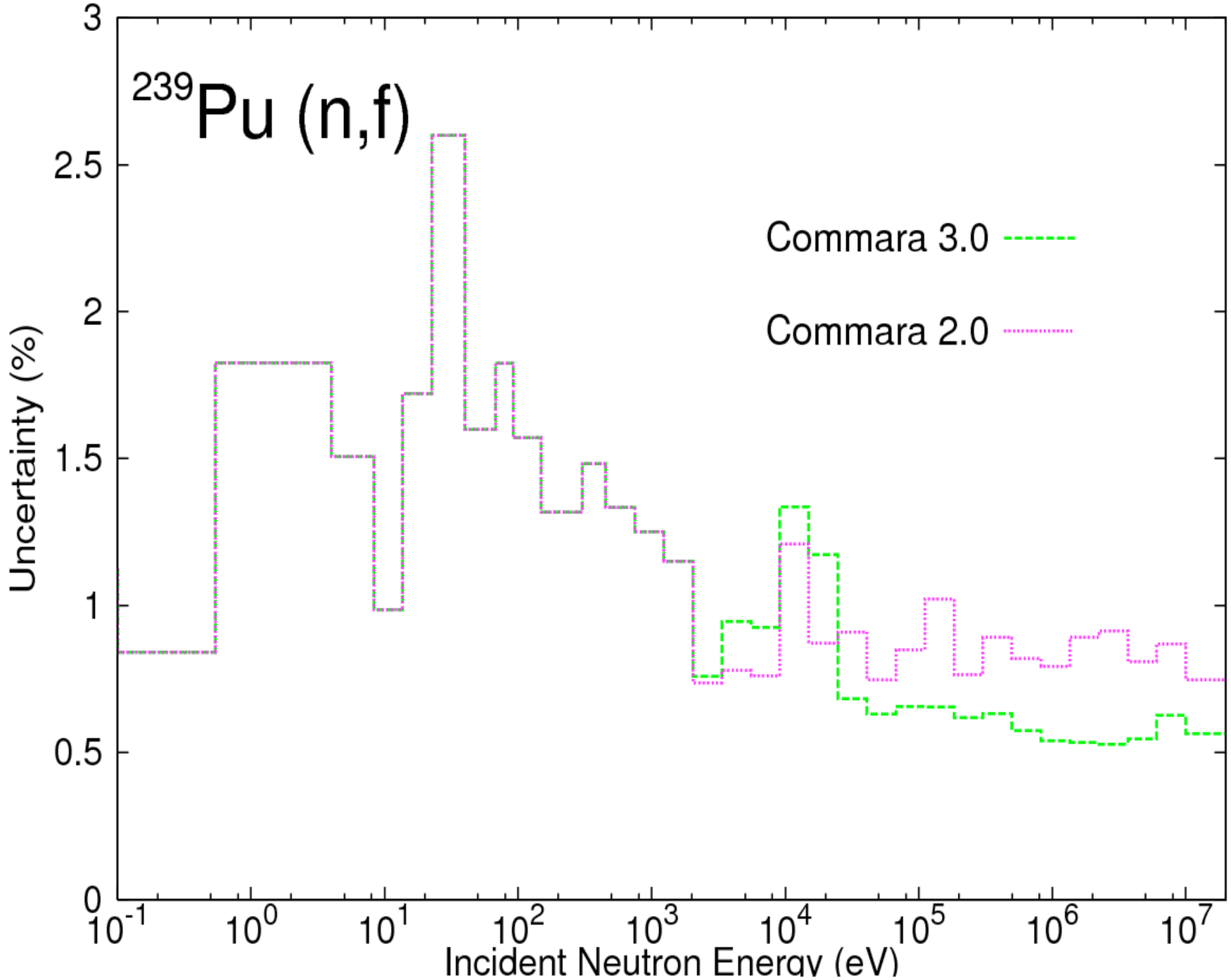
^{233}U(ORNL RRR MF32 replaced with LANL MF33)



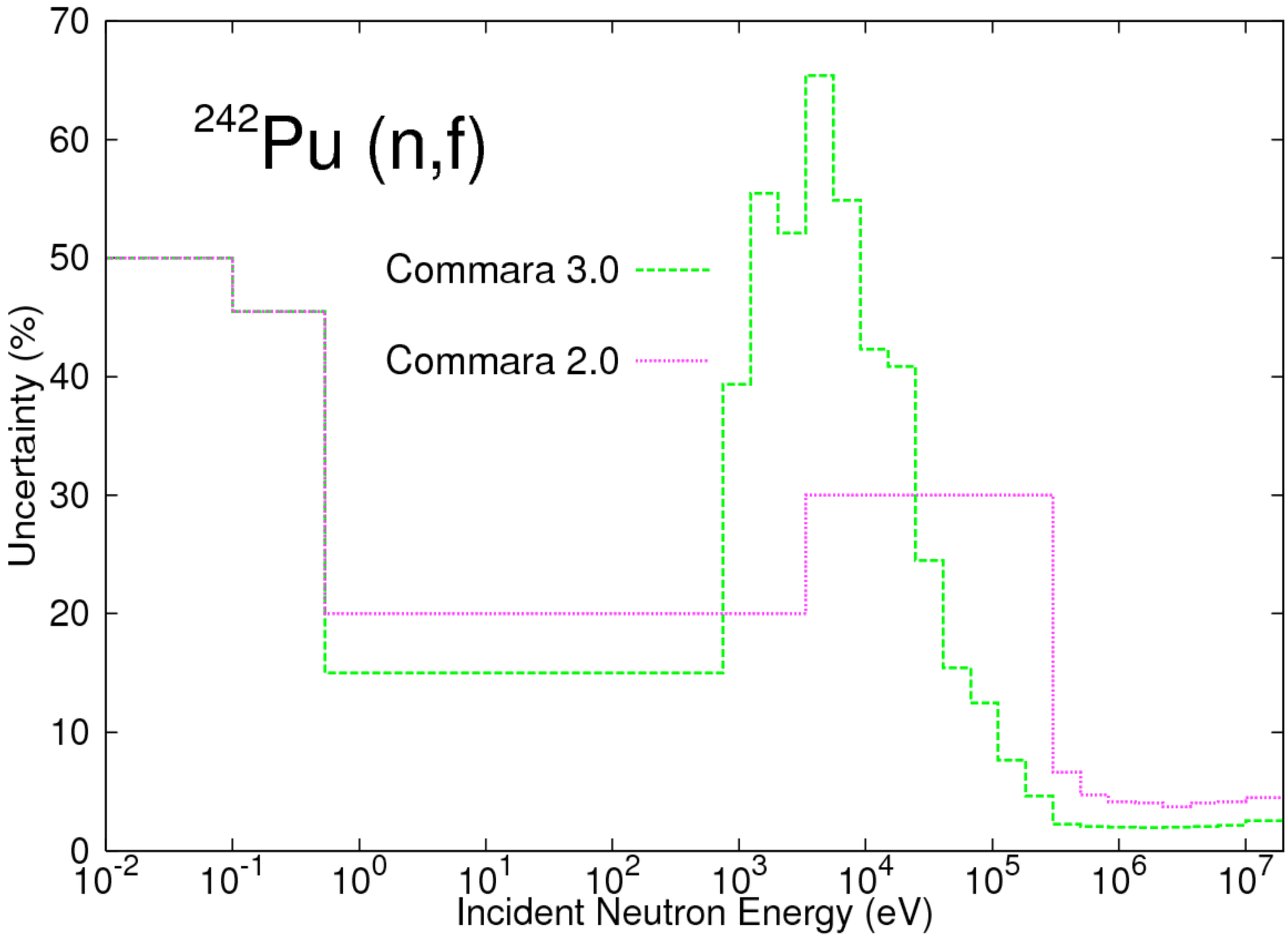
^{235}U (New MF33 eval by LANL/ORNL)



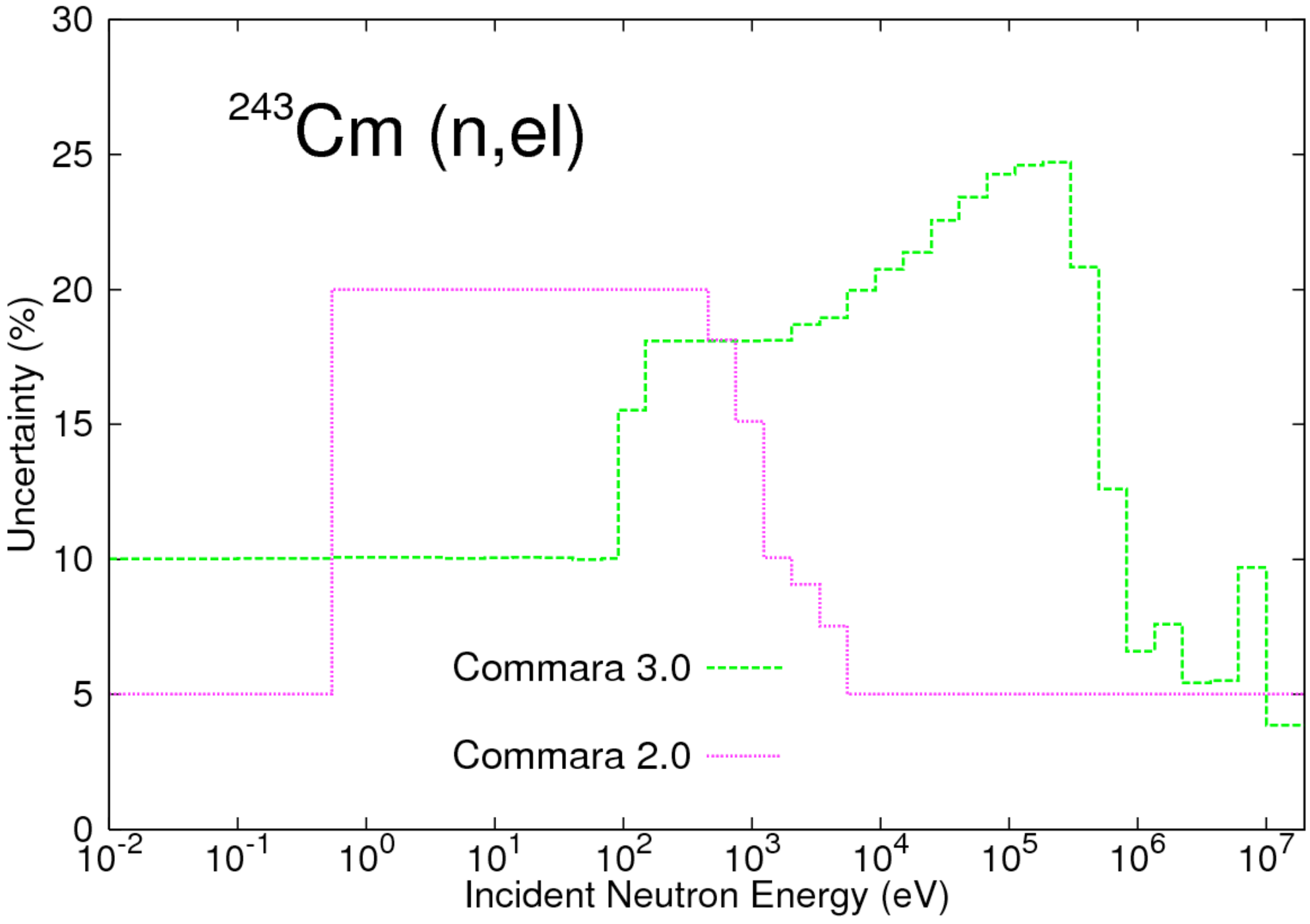
^{239}Pu (New MF33 eval. by LANL/ORNL)



^{242}Pu (from JENDL-4)



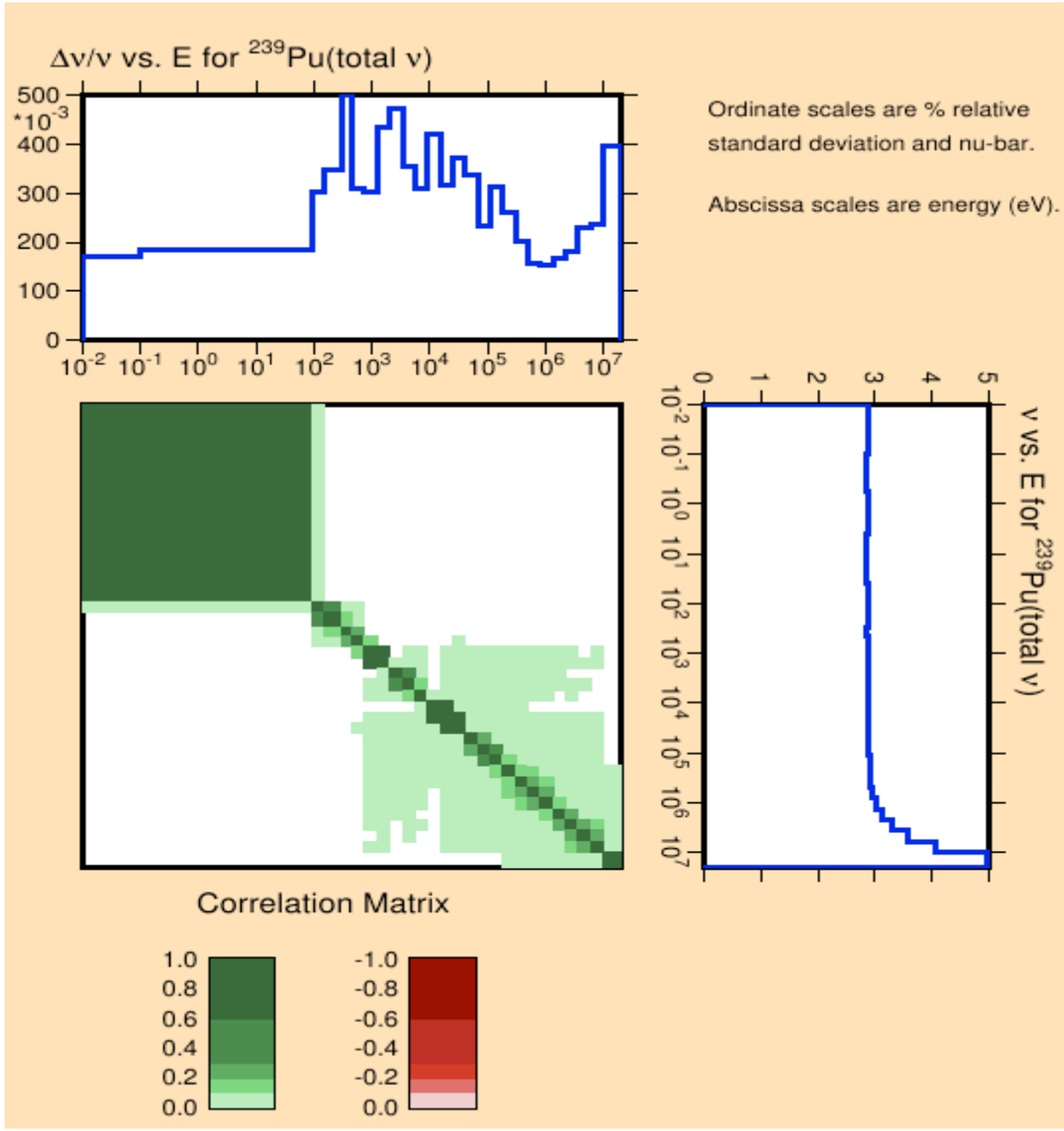
^{243}Cm (from JENDL-4)



Nubar covariances

- ^{239}Pu

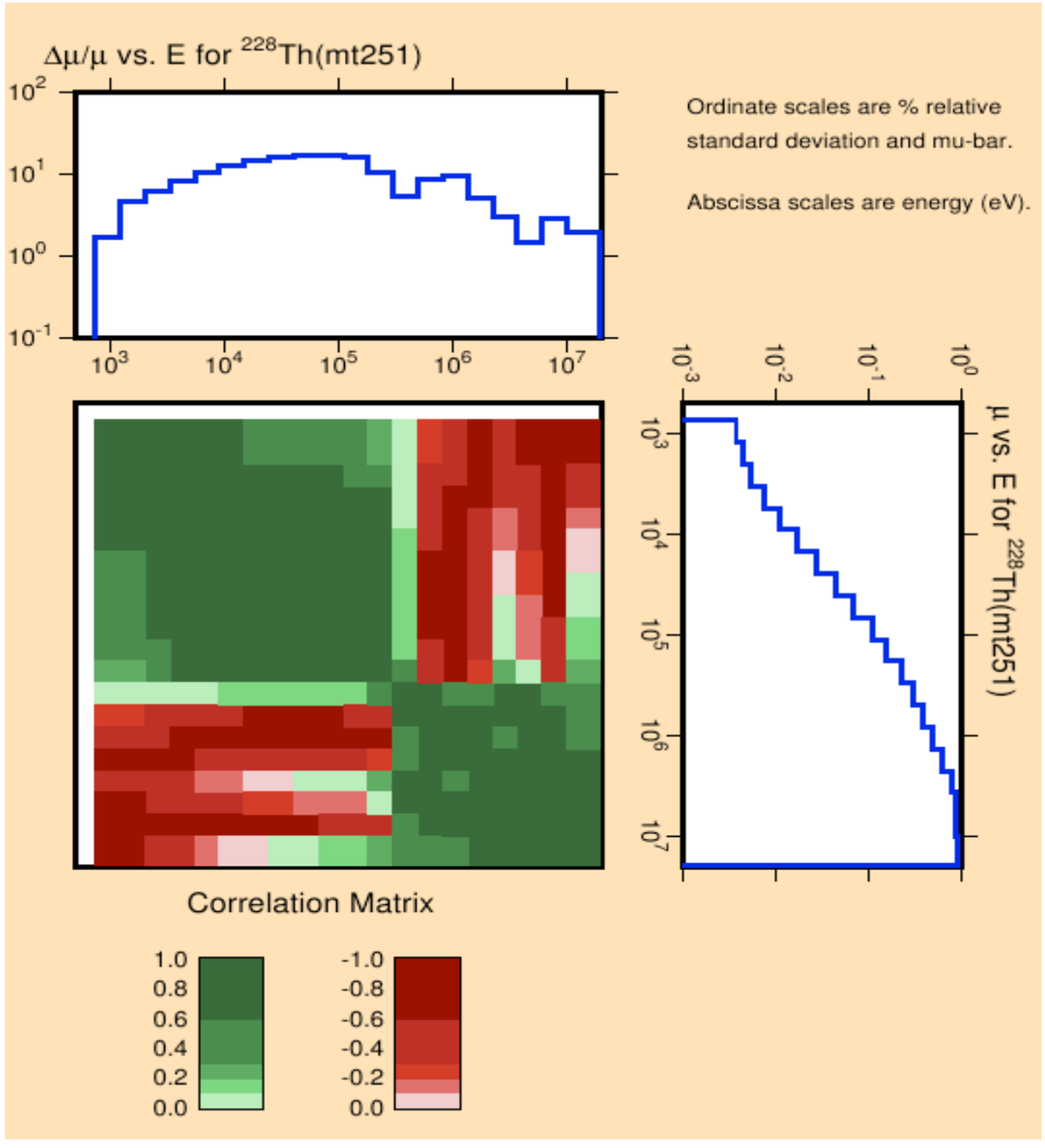
From LANL



Mubar covariance

^{228}Th

JENDL-4



COMMARA-3 (release FY2013)

Using new features of EMPIRE will address cross-correlations, PFNS, and mu-bars

- Extended to include 184 materials with covariances from ENDF/B-VII.1
- Will be applicable to practically any reactor system and associated fuel cycle.
- Will also include new key features:
  - Major cross-correlations among reactions of the same isotope and among selected isotopes
  - Correlations for elastic angular distributions for most important isotopes (Pu-239, U-235, U-238, Fe, Na, O-16)
  - A complete set of prompt fission neutron spectra, including some cross-isotope correlations