Covariances in ENDF/B-VII.1

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BROOKHAVEN NATIONAL LABORATORY
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ENDF/B-VII.1 was released on Dec. 22, 2011

- Many more full evaluations in neutron sublibrary than in any other release
  - ENDF/B-VII.0 contains 393 evaluations
  - ENDF/B-VII.1 contains 423 evaluations
- Extensive collection of covariance data (190 evaluations)
- **Library summarized in Dec. 2011 issue of Nuclear Data Sheets**
- **See also http://www.nndc.bnl.gov/exfor/endfb7.1.jsp**

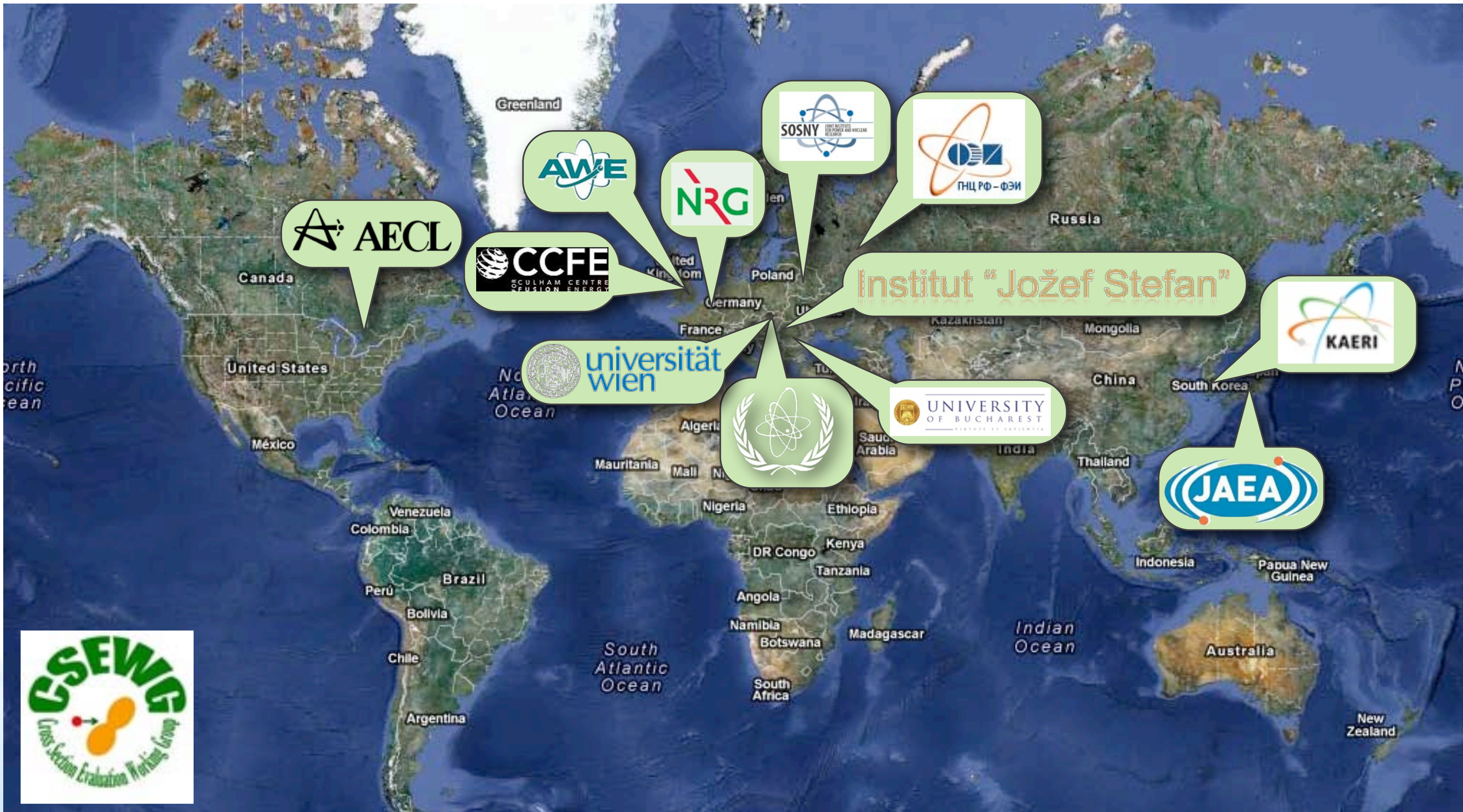
ENDF/B-VII.1 was the combined effort of collaborators from across the US...

ENDF B-VII.1

CSEWG Cross Section Evaluation Working Group

... and the world.

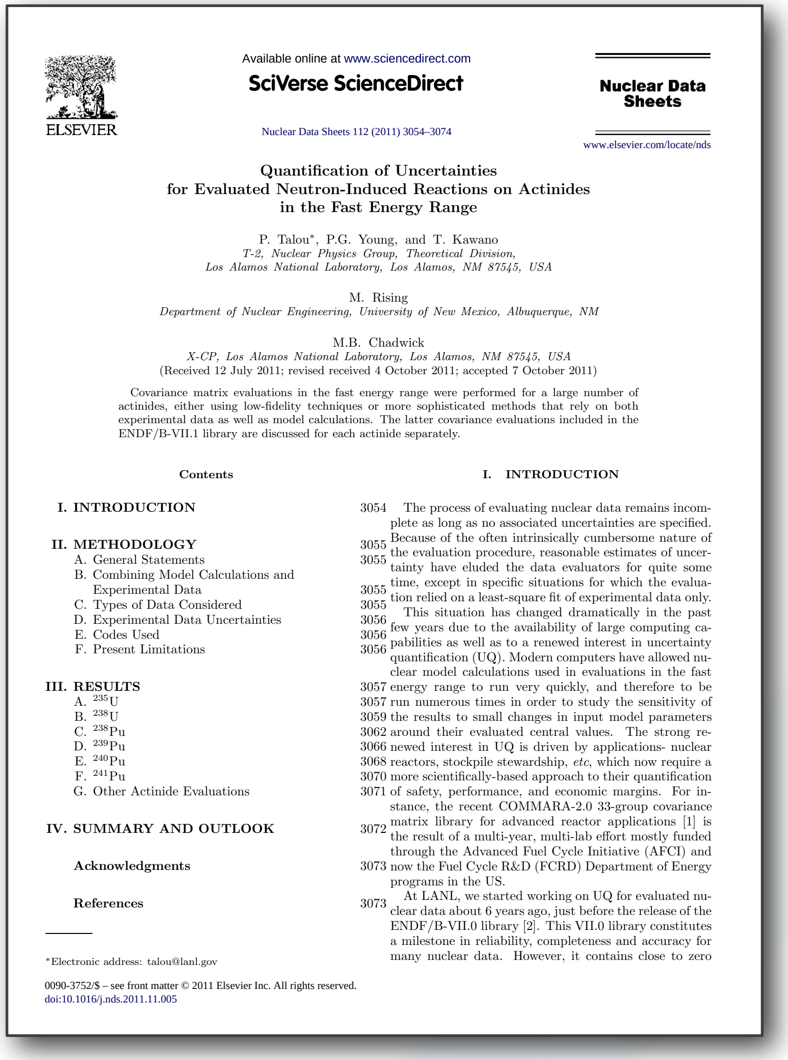
ENDF B-VII.1



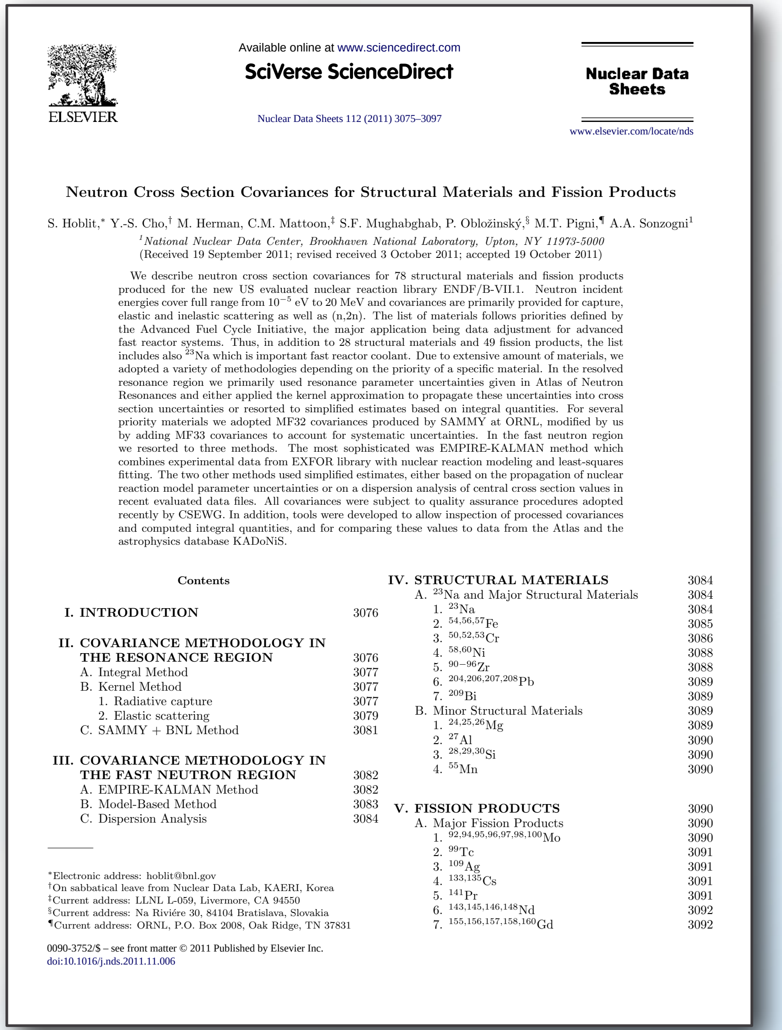
One of the main thrusts was the addition of covariance data; They are detailed in 3 papers

ENDF/B-VII.1

D. Smith, "Evaluated Nuclear Data Covariances: The Journey From ENDF/B-VII.0 to ENDF/B-VII.1", Nuclear Data Sheets, 112(12):3037-3053(2011).

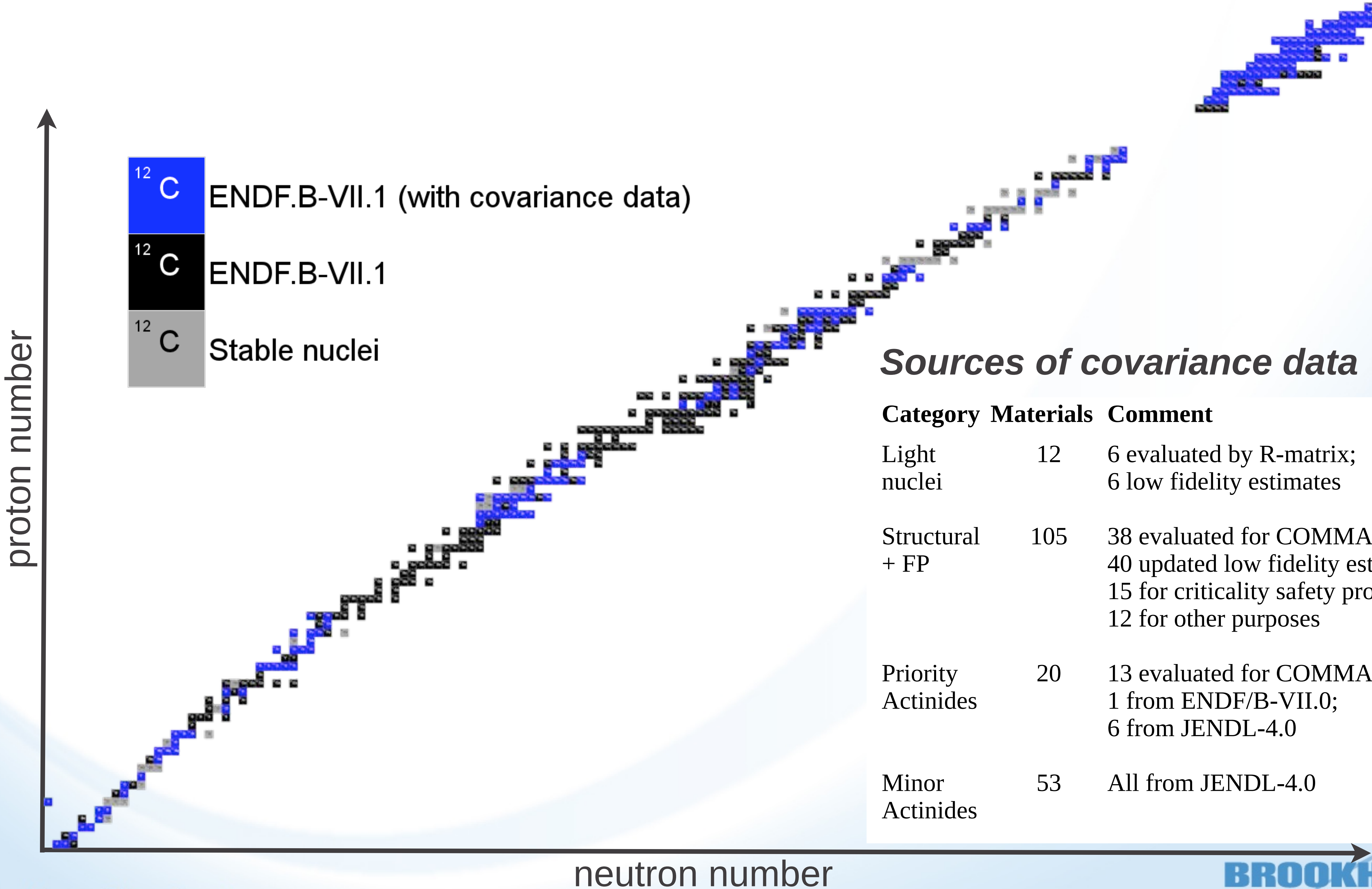


P. Talou, P. Young, T. Kawano, et al., "Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Region", Nuclear Data Sheets, 112(12): 3054-3074(2011).



S. Hoblit, Y.-S. Cho, M. Herman, et al., "Neutron Cross Section Covariances for Structural Materials and Fission Products", Nuclear Data Sheets, 112(12): 3075-3097(2011).

An overview of the library



Sources of covariance data

Category	Materials	Comment
Light nuclei	12	6 evaluated by R-matrix; 6 low fidelity estimates
Structural + FP	105	38 evaluated for COMMARA-2.0; 40 updated low fidelity estimates; 15 for criticality safety programs; 12 for other purposes
Priority Actinides	20	13 evaluated for COMMARA-2.0; 1 from ENDF/B-VII.0; 6 from JENDL-4.0
Minor Actinides	53	All from JENDL-4.0

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

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

Methodology

ENDF/B-VII.1

Thermal and Resonance Region

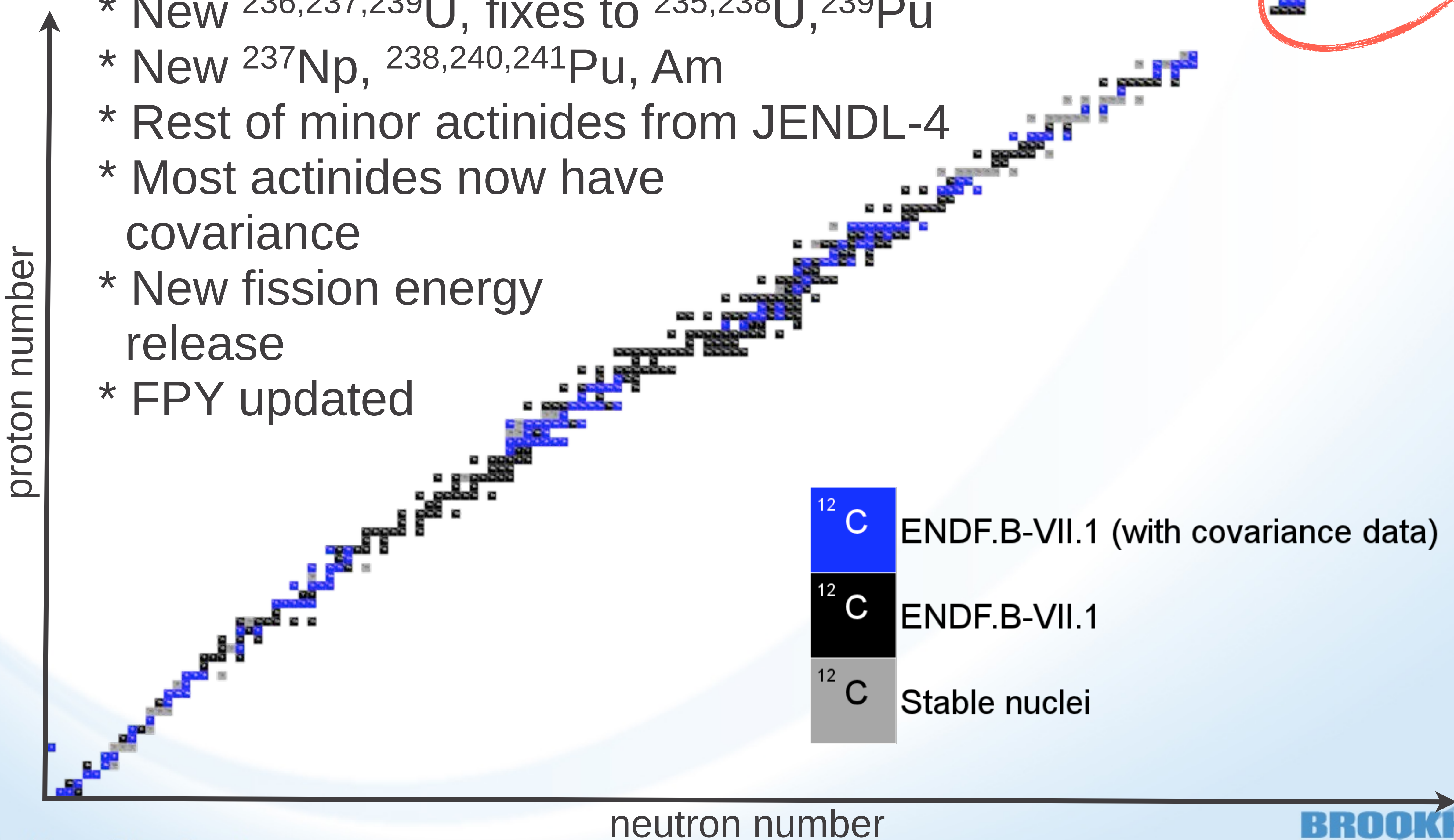
- Source of data
- Experiments
- ENDF file (retroactive method)
- Atlas of Neutron Resonances (ANR)
- SAMMY analysis
- full analysis (MF32, Exp. data)
- retroactive (MF32, ENDF file)
- EMPIRE Resonance Module (MF32, ANR, scattering radius and thermal point uncertainties reproduced through correlations (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

An overview of the library

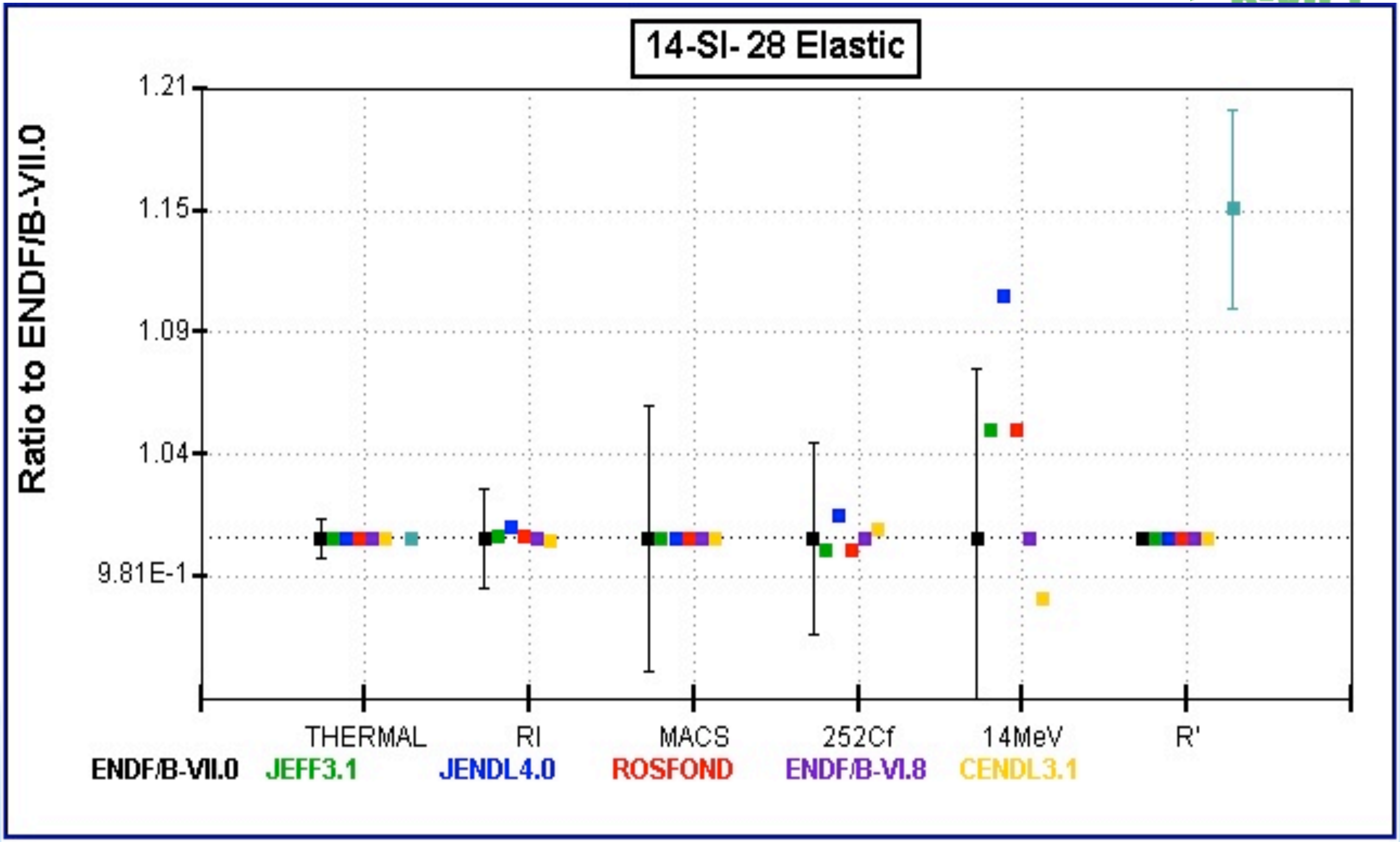
* Major actinides essentially unchanged,
* New $^{236,237,239}U$, fixes to $^{235,238}U$, ^{239}Pu
* New ^{237}Np, $^{238,240,241}Pu$, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated



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)

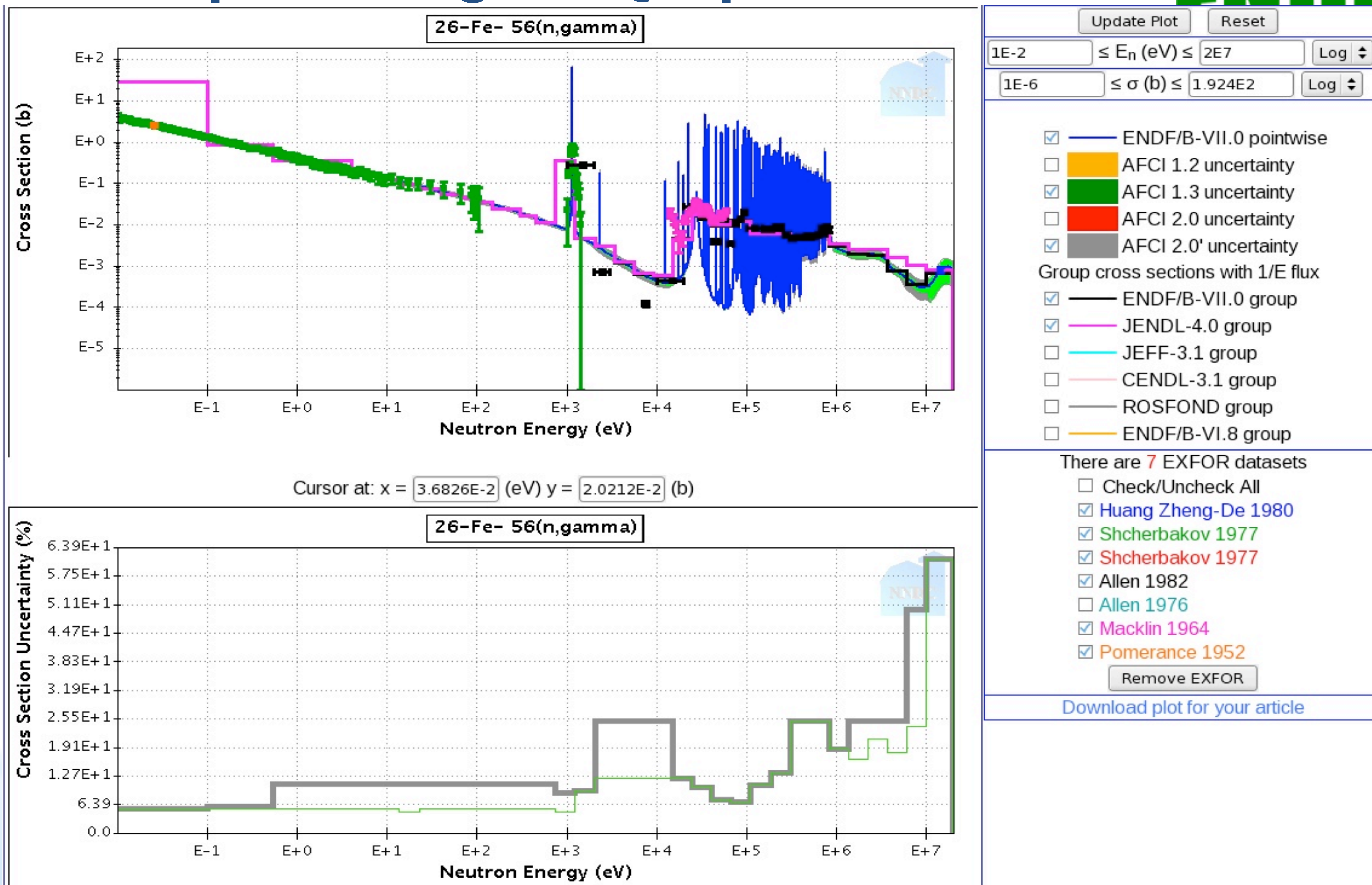


^{28}Si elastic integral quantities from Sigma-QA

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%

Example of Sigma-QA plot

ENDF



Quality Assurance (continued)

ENDF B-VII.1

- Code ‘**unCor**’, (Mattoon, Oblozinsky) checks the library for possible problems in uncertainties and/or correlations

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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%)
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%)
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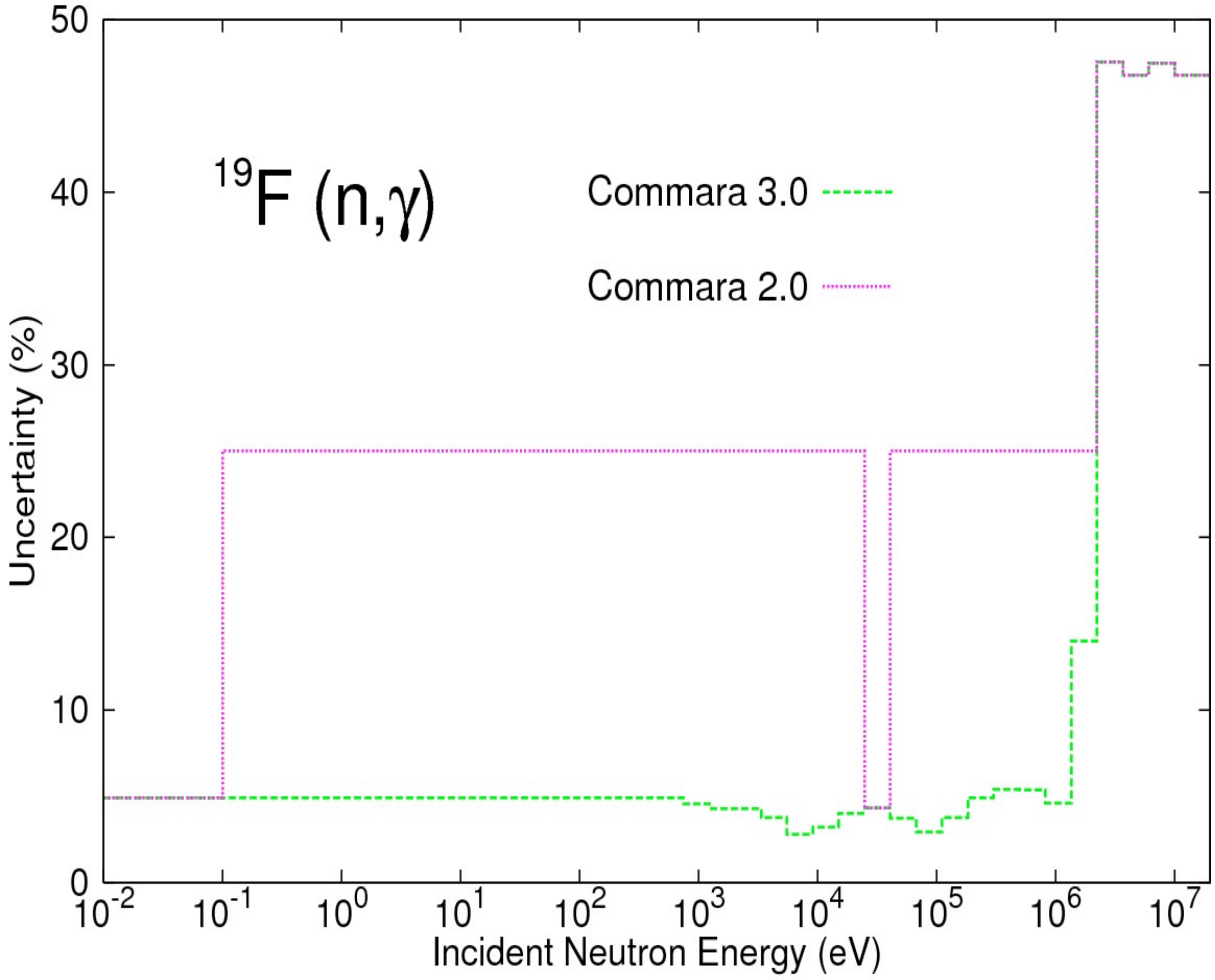
COMMARA-3 (release FY2013)

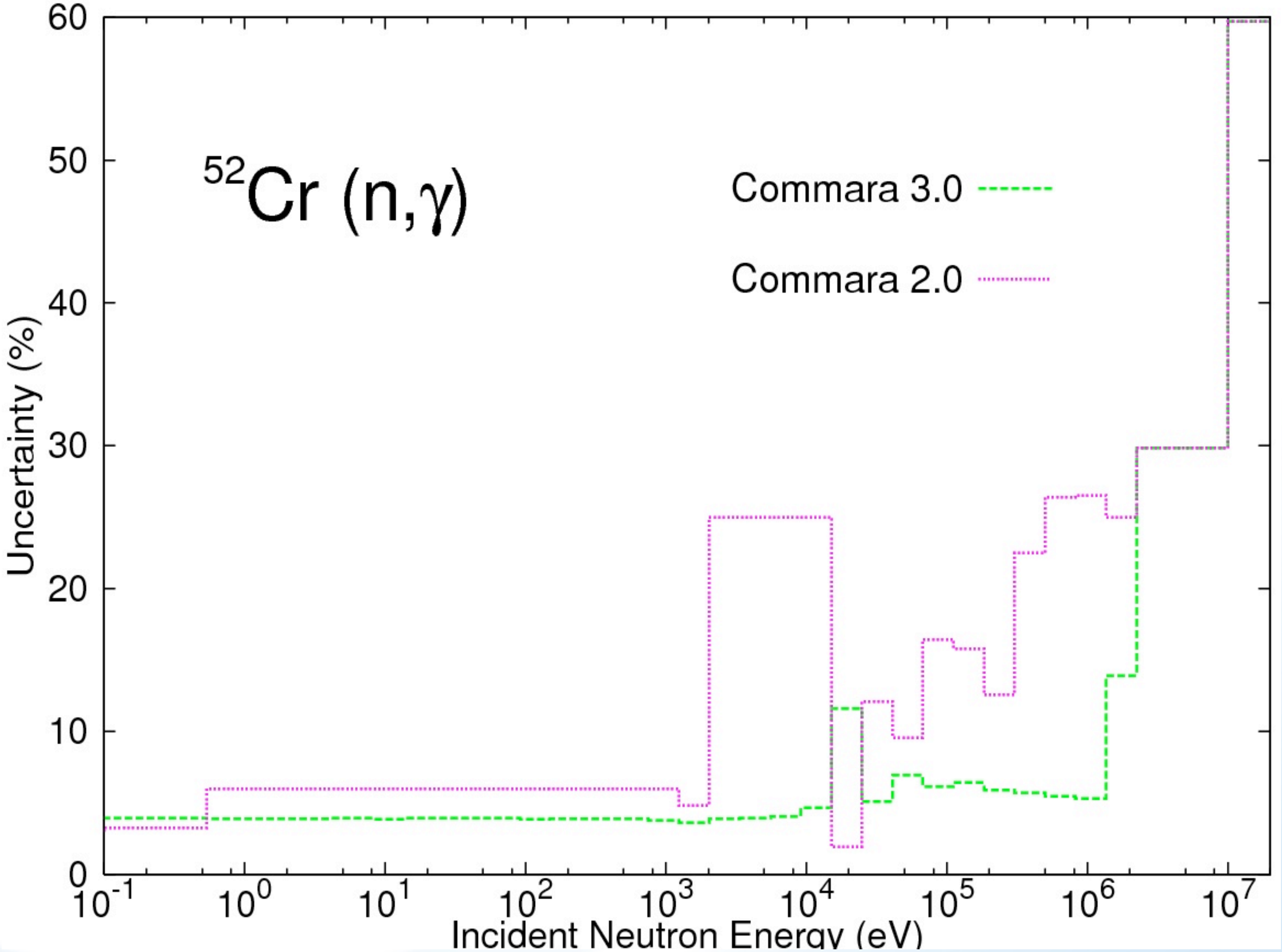
Using new features of EMPIRE will address cross-correlations, PFNS, and mu-bars

- 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

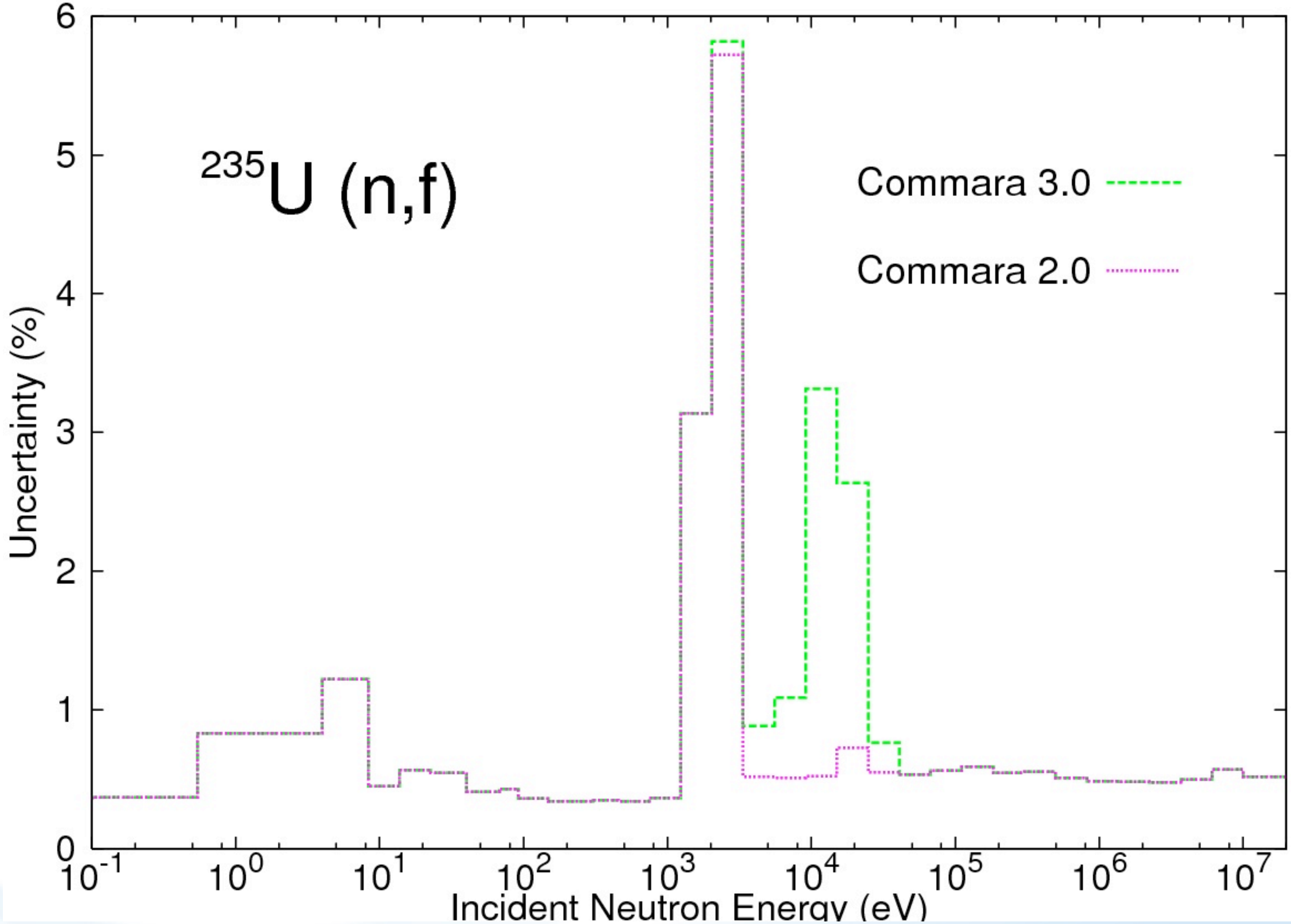
^{19}F (new ORNL evaluation)



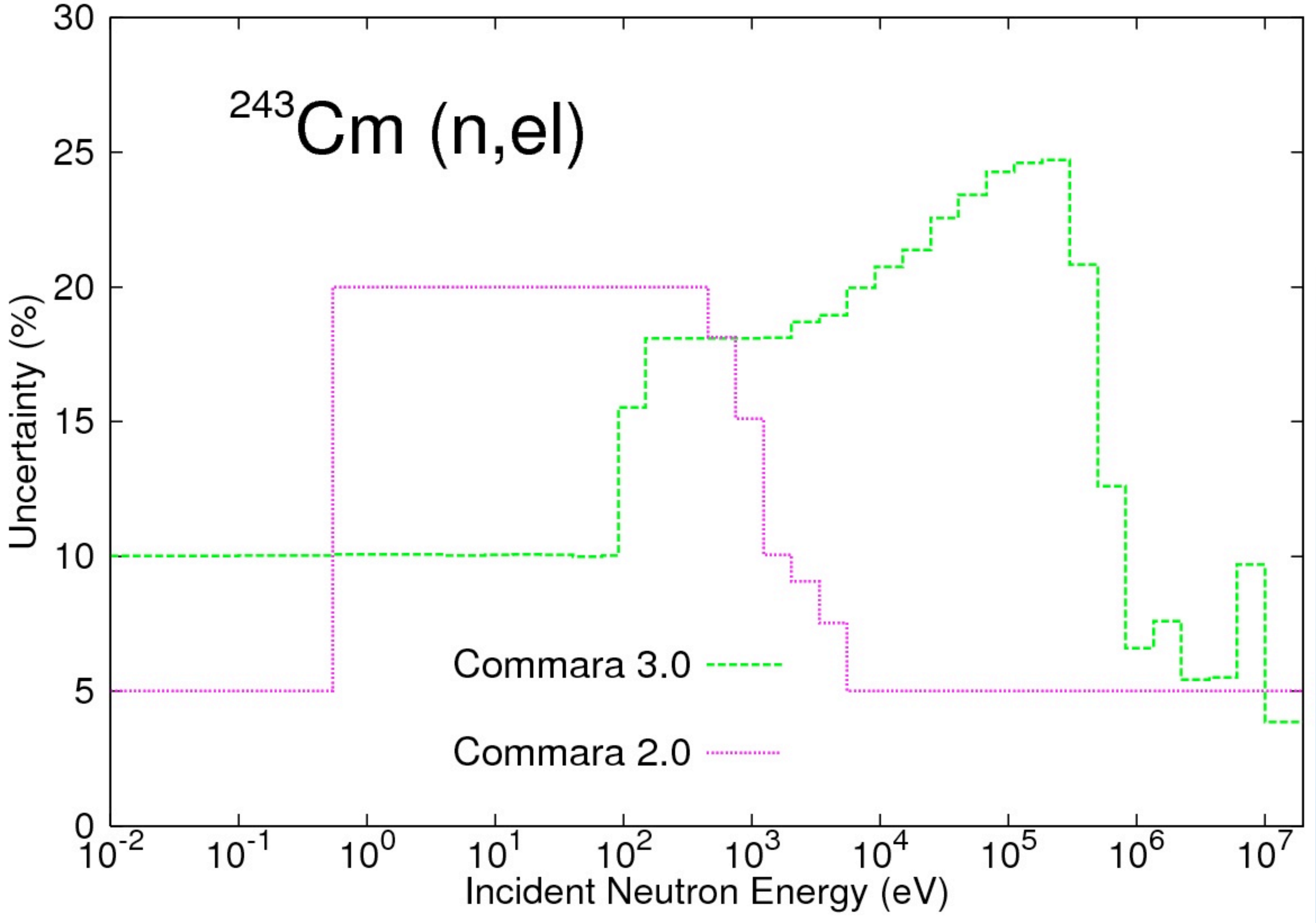
^{52}Cr (New ORNL RRR evaluation)



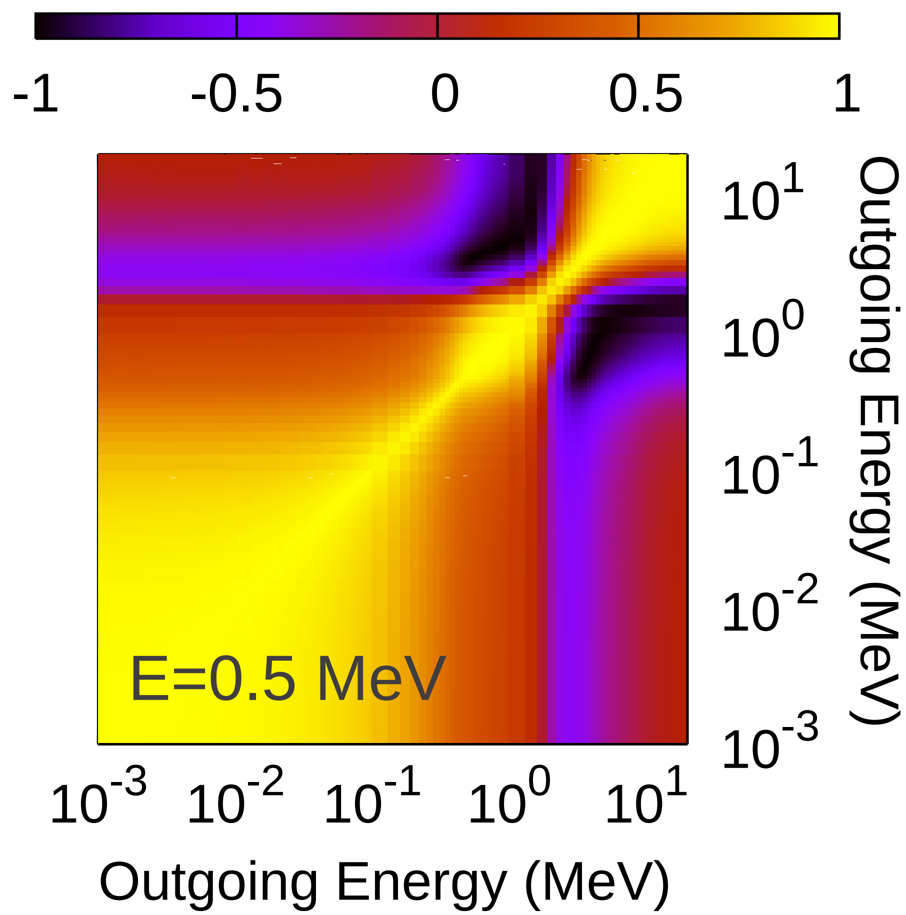
^{235}U (New MF33 eval by LANL/ORNL)

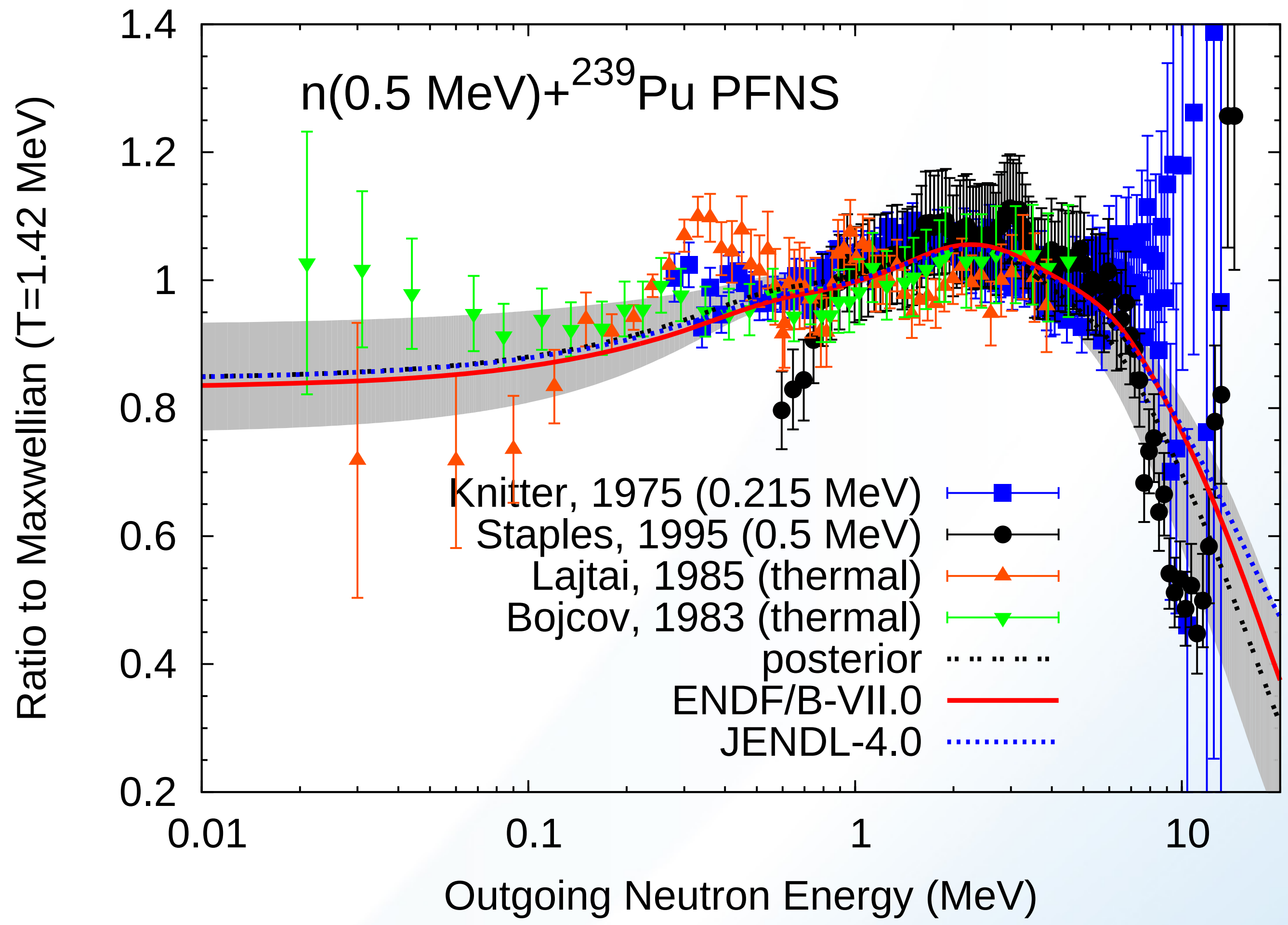


^{243}Cm (from JENDL-4)



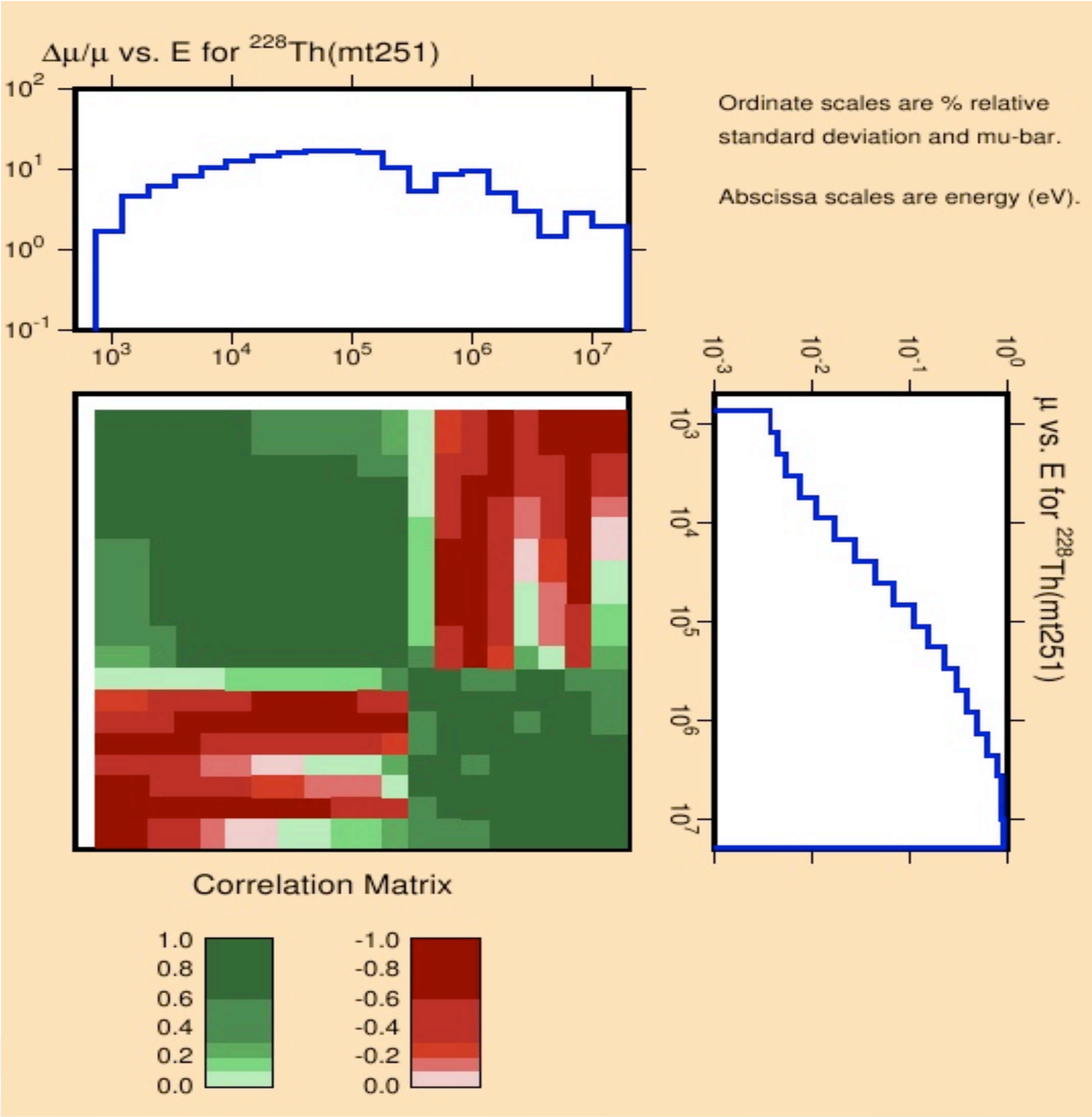
Only substantial change to ^{239}Pu: addition of prompt fission neutron spectrum covariance





- Talou et al (LANL) retrofitted using Madland-Nix model
- Valuable contribution enabling full QMU studies in Pu systems (previously only nubar and cross section covariance available)

^{228}Th mu-bar covariance (JENDL-4)



Conclusions

- ENDF/B-VII.1 contains covariances for 190 materials (184 basically complete)
- Several of "High Fidelity" (3 major actinides and 6 R-matrix light nuclei (LANL), 232Th, W, 55Mn (IAEA), RR in recent ORNL evaluations)
- 40 "Medium Fidelity" (fission products and structural materials, coolants)
- Many "Low Fidelity" for low priority materials
- JENDL-4 for minor Actinides (59)
- These covariances are supposed to be at least reasonable :)