

Covariances in ENDF/B-VII.1

M. Herman, S. Hoblit & D. Brown

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a passion for discovery



U.S. DEPARTMENT OF
ENERGY

Office of
Science

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



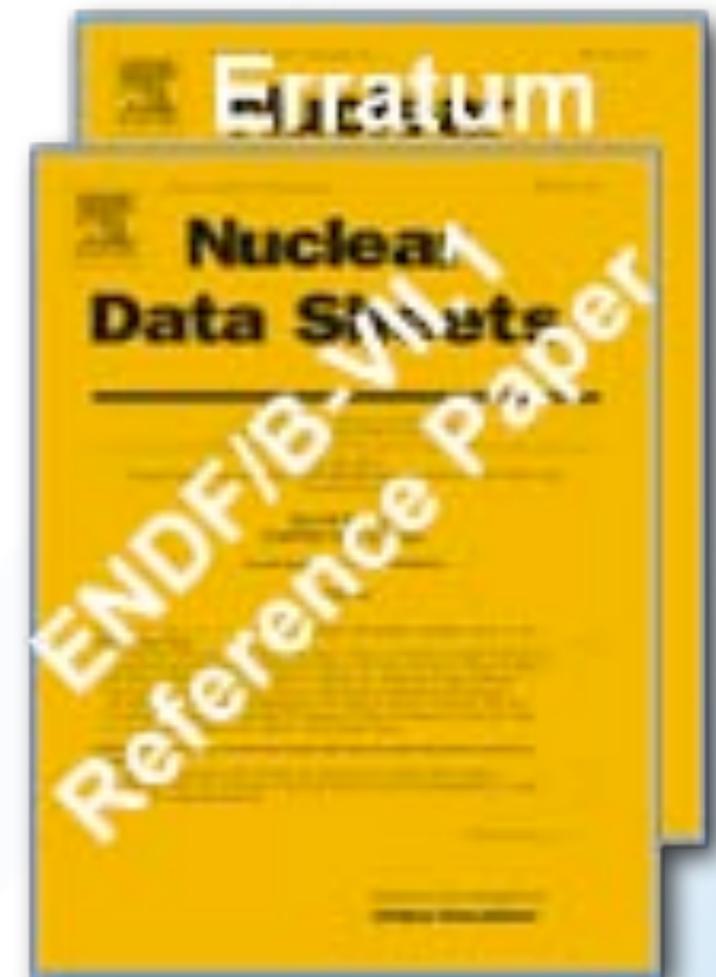
- Many more full evaluations in neutron sublibrary than in any other release
 - ENDF/B-VII.0 contains 393 evaluations
 - ENDF/B-VII.1 contains 423 evaluations

- 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>

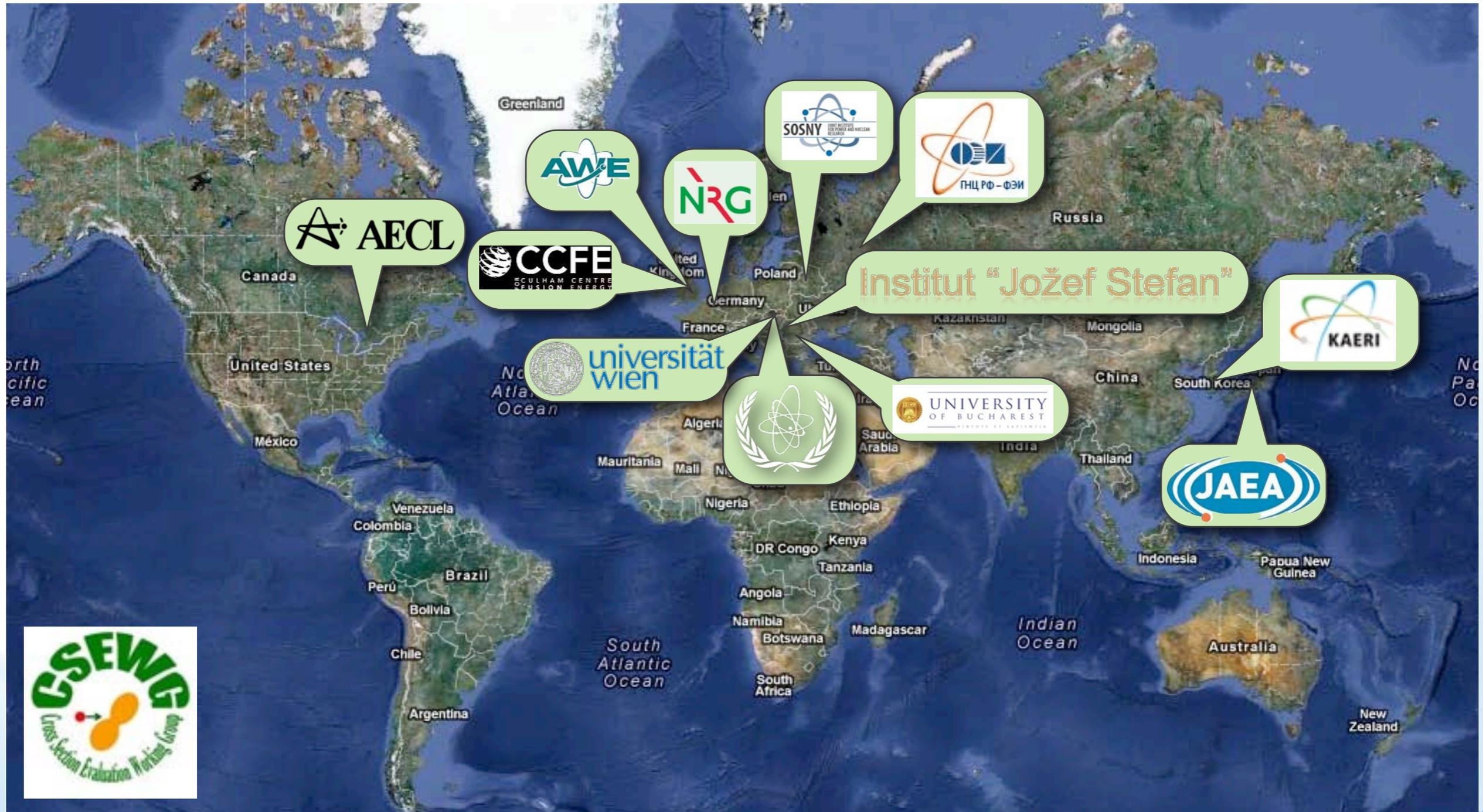


ENDF/B-VII.1 was the combined effort of collaborators from across the US...



... and the world.

ENDF B-VII.1



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



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Nuclear Data Sheets

Evaluated Nuclear Data Covariances: The Journey From ENDF/B-VII.0 to ENDF/B-VII.1

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 (Received 24 June 2011; revised received 23 September 2011; accepted 9 October 2011)

Recent interest from data users on applications that utilize the uncertainties of evaluated nuclear reaction data has stimulated the data evaluation community to focus on producing covariance data to a far greater extent than ever before. Although some uncertainty information has been available in the ENDF/B libraries since the 1970s, this content has been fairly limited in scope, the quality quite variable, and the use of covariance data confined to only a few application areas. Today, covariance data are more widely and extensively utilized than ever before in neutron dosimetry, in advanced fission reactor design studies, in nuclear criticality safety assessments, in national security applications, and even in certain fusion energy applications. The main problem that now faces the ENDF/B evaluator community is that of providing covariances that are adequate both in quantity and quality to meet the requirements of contemporary nuclear data users in a timely manner. In broad terms, the approach pursued during the past several years has been to purge any legacy covariance information contained in ENDF/B-VI.8 that was judged to be subpar, to include in ENDF/B-VII.0 (released in 2006) only those covariance data deemed then to be of reasonable quality for contemporary applications, and to subsequently devote as much effort as the available time and resources allowed to producing additional covariance data of suitable scope and quality for inclusion in ENDF/B-VII.1. Considerable attention has also been devoted during the five years since the release of ENDF/B-VII.0 to examining and improving the methods used to produce covariance data from thermal energies up to the highest energies addressed in the ENDF/B library, to processing these data in a robust fashion so that they can be utilized readily in contemporary nuclear applications, and to developing convenient covariance data visualization capabilities. Other papers included in this issue discuss in considerable detail various aspects of the data producer community's efforts to improve the evaluation methods and to add covariance content to the ENDF/B library. The present paper offers just a brief glimpse of these activities by drawing material from covariance papers presented at meetings, workshops and international conferences during the past five years. Highlighted are: advances in methods for producing and processing covariance data, recently developed covariance visualization capabilities, and the development and implementation of quality assurance (QA) requirements that should be satisfied for covariance data to be included in ENDF/B-VII.1.

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 doi:10.1016/j.nds.2011.11.004

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Nuclear Data Sheets

Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Energy Range

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 (Received 12 July 2011; revised received 4 October 2011; accepted 7 October 2011)

Covariance matrix evaluations in the fast energy range were performed for a large number of actinides, either using low-fidelity techniques or more sophisticated methods that rely on both experimental data as well as model calculations. The latter covariance evaluations included in the ENDF/B-VII.1 library are discussed for each actinide separately.

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 doi:10.1016/j.nds.2011.11.005

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 Nuclear Data Sheets 112 (2011) 3075–3097
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Nuclear Data Sheets

Neutron Cross Section Covariances for Structural Materials and Fission Products

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 (Received 19 September 2011; revised received 3 October 2011; accepted 19 October 2011)

We describe neutron cross section covariances for 78 structural materials and fission products produced for the new US evaluated nuclear reaction library ENDF/B-VII.1. Neutron incident energies cover full range from 10⁻⁵ eV to 20 MeV and covariances are primarily provided for capture, elastic and inelastic scattering as well as (n,2n). The list of materials follows priorities defined by the Advanced Fuel Cycle Initiative, the major application being data adjustment for advanced fast reactor systems. Thus, in addition to 28 structural materials and 49 fission products, the list includes also ²³Na which is important fast reactor coolant. Due to extensive amount of materials, we adopted a variety of methodologies depending on the priority of a specific material. In the resolved resonance region we primarily used resonance parameter uncertainties given in Atlas of Neutron Resonances and either applied the kernel approximation to propagate these uncertainties into cross section uncertainties or resorted to simplified estimates based on integral quantities. For several priority materials we adopted MF32 covariances produced by SAMMY at ORNL, modified by us by adding MF33 covariances to account for systematic uncertainties. In the fast neutron region we resorted to three methods. The most sophisticated was EMPIRE-KALMAN method which combines experimental data from EXFOR library with nuclear reaction modeling and least-squares fitting. The two other methods used simplified estimates, either based on the propagation of nuclear reaction model parameter uncertainties or on a dispersion analysis of central cross section values in recent evaluated data files. All covariances were subject to quality assurance procedures adopted recently by CSEWG. In addition, tools were developed to allow inspection of processed covariances and computed integral quantities, and for comparing these values to data from the Atlas and the astrophysics database KADoNIS.

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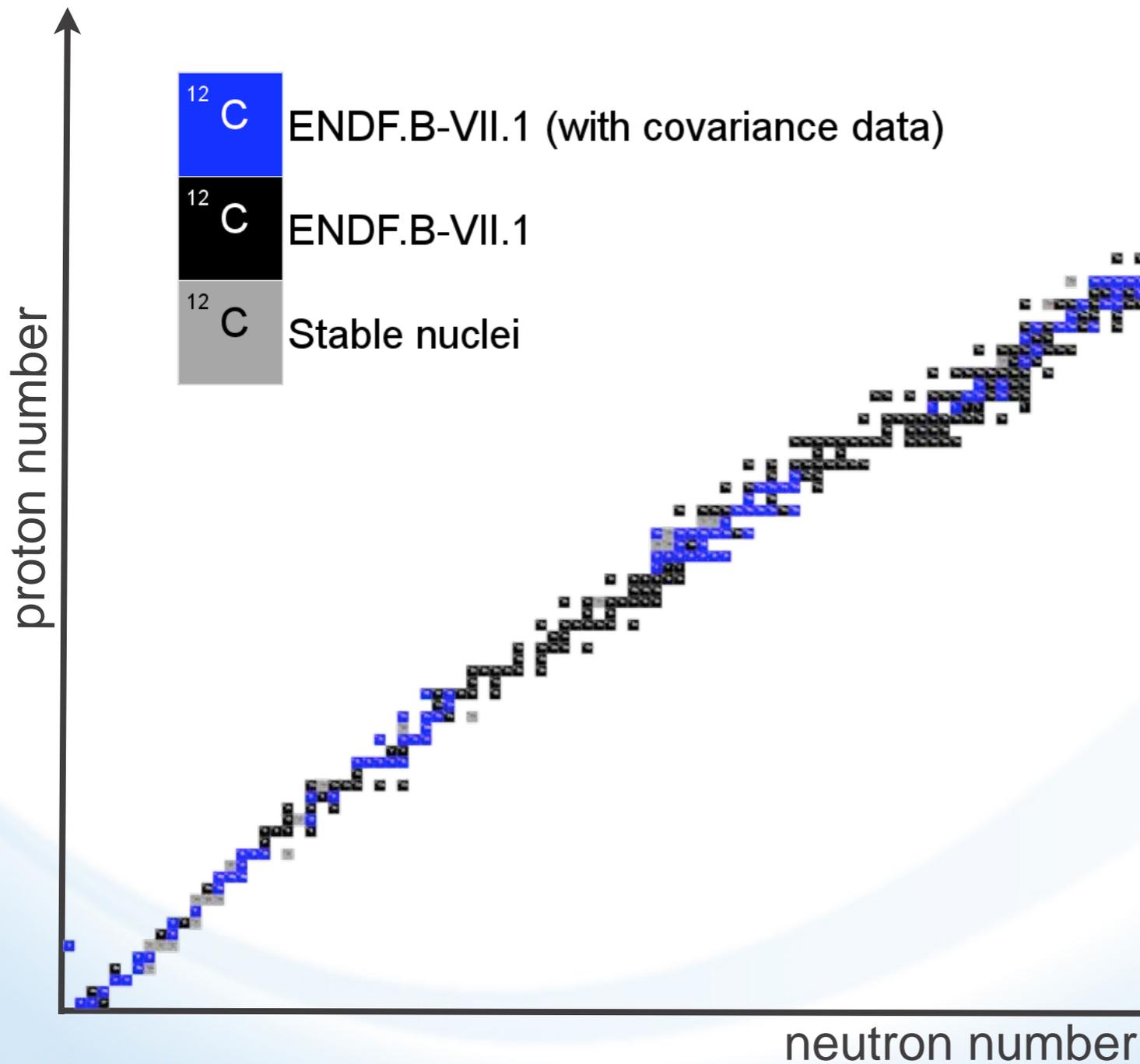
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 0090-3752/\$ - see front matter © 2011 Published by Elsevier Inc.
 doi:10.1016/j.nds.2011.11.006

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

- ^1H , ^2H , ^4He , ^6Li , ^7Li , ^9Be , ^{10}B , ^{11}B , ^{12}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 , $^{242\text{m}1}\text{Am}$, ^{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 , $^{254\text{m}1}\text{Es}$, ^{255}Es , ^{255}Fm

- 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



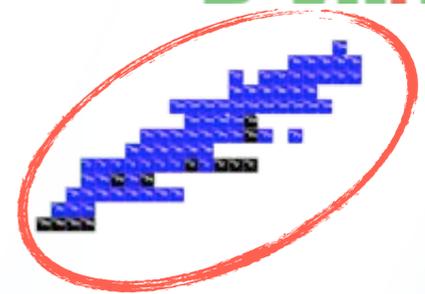
Thermal and Resonance Region

- 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

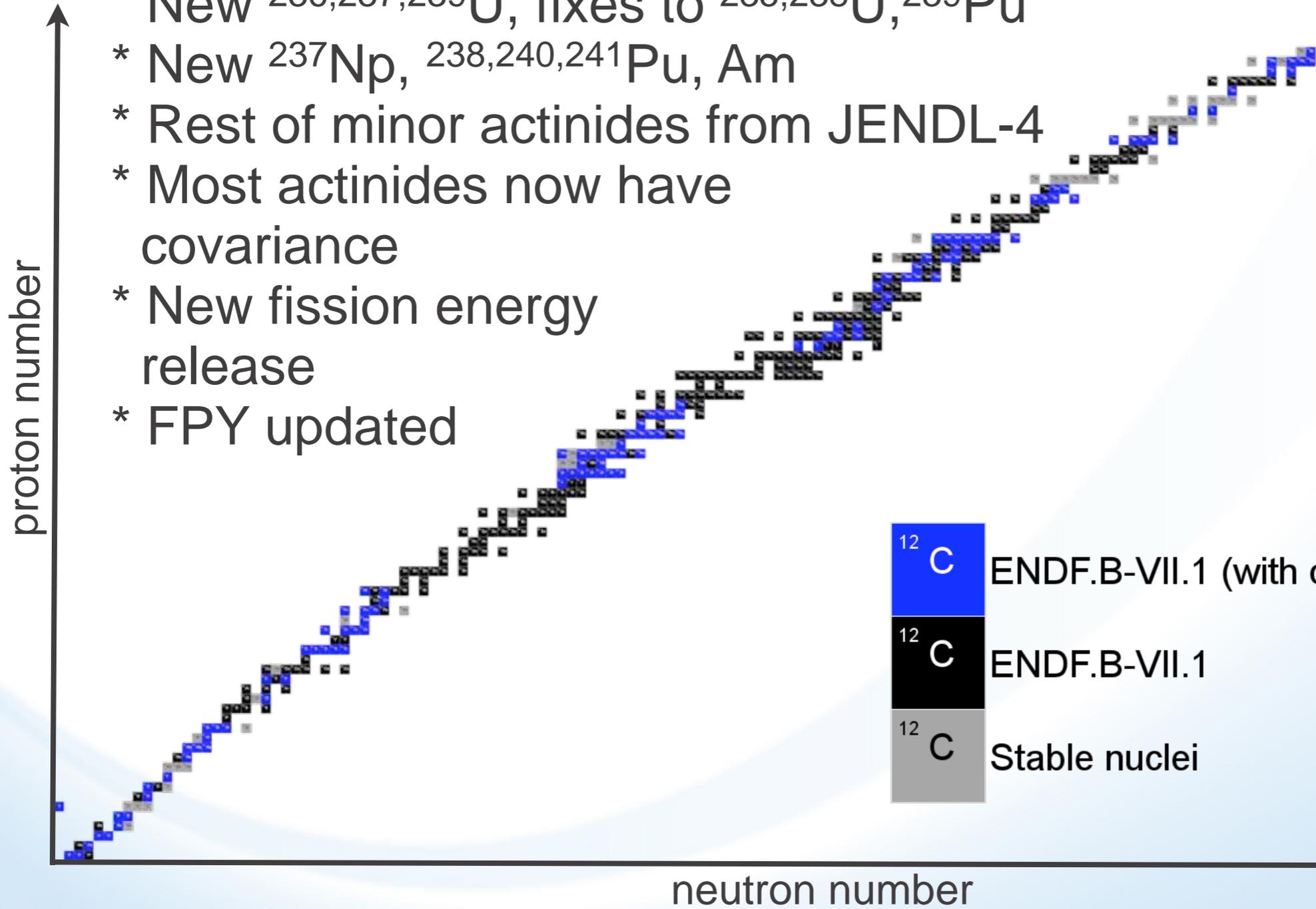
Fast neutron range (MF33)

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



^{12}C	ENDF.B-VII.1 (with covariance data)
^{12}C	ENDF.B-VII.1
^{12}C	Stable nuclei

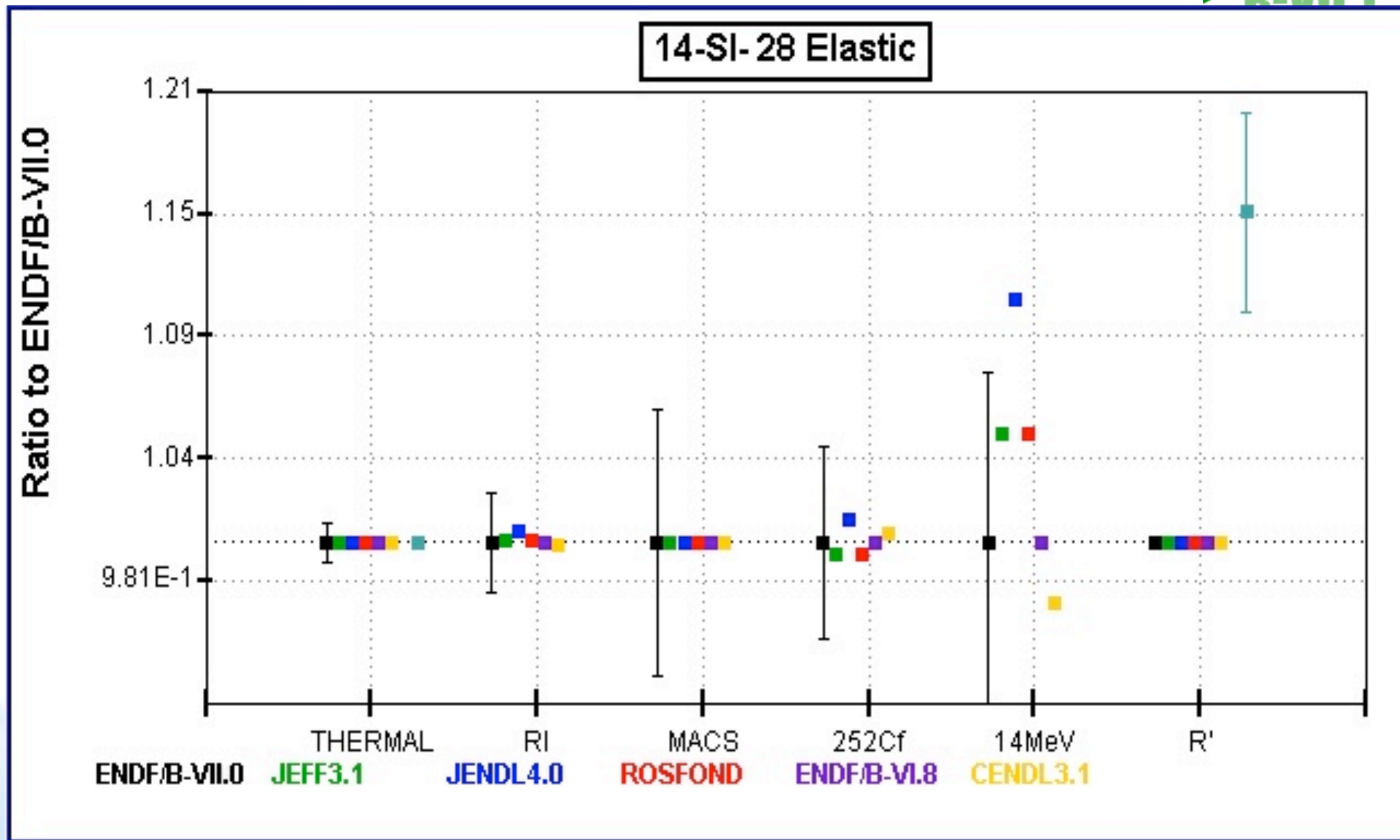
Quality Assurance



- 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 including:
 - small uncertainties: $(n, \text{tot}) < 1\%$, (n, el) and $(n, \gamma) < 2\%$, 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)

ENDF
B-VII.1



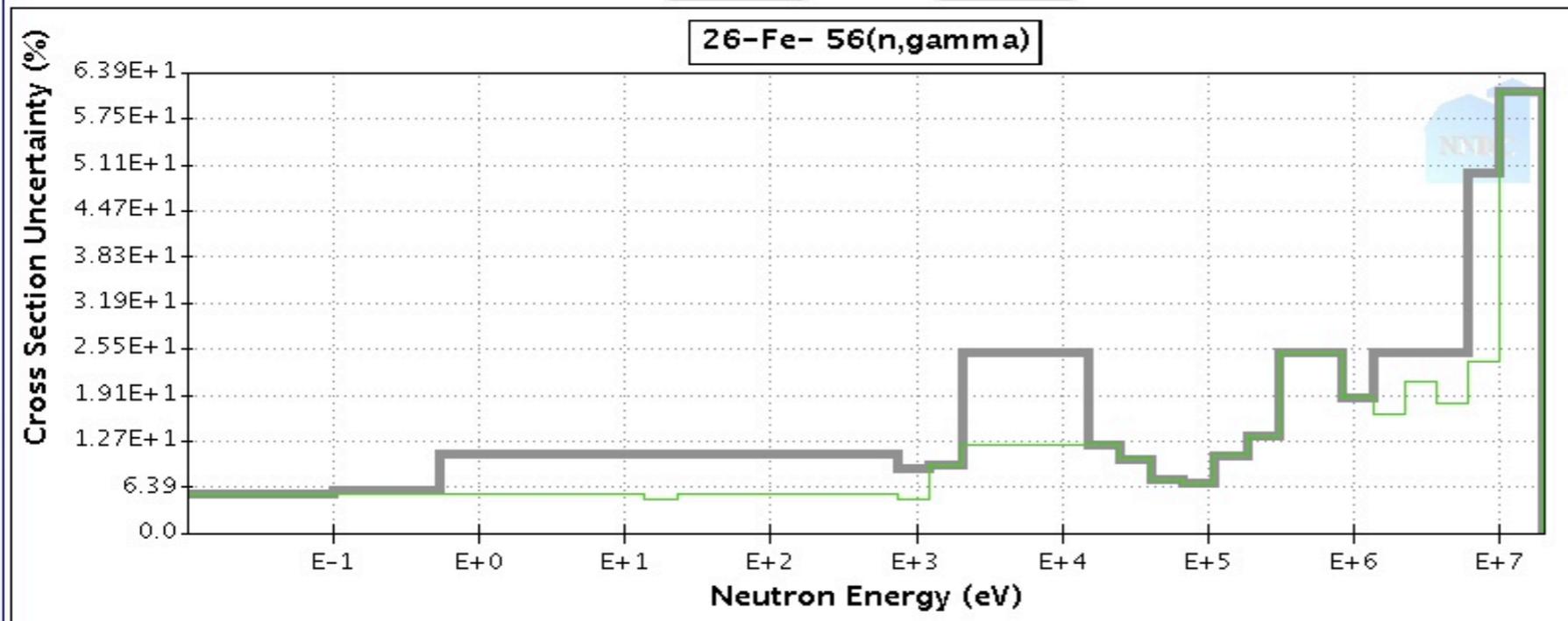
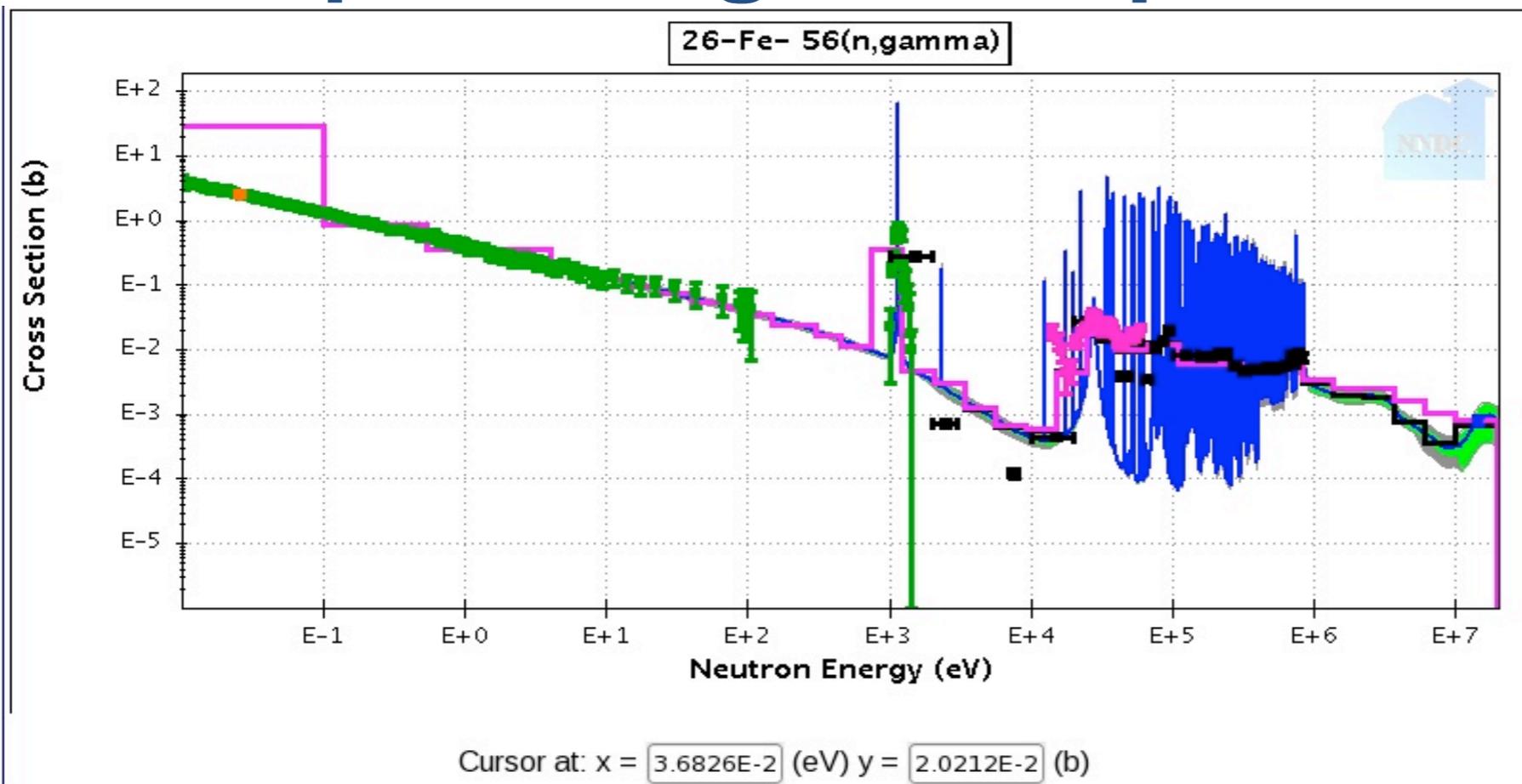
^{28}Si elastic integral quantities from Sigma-QA



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



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](#)

Quality Assurance (continued)



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

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%)
```

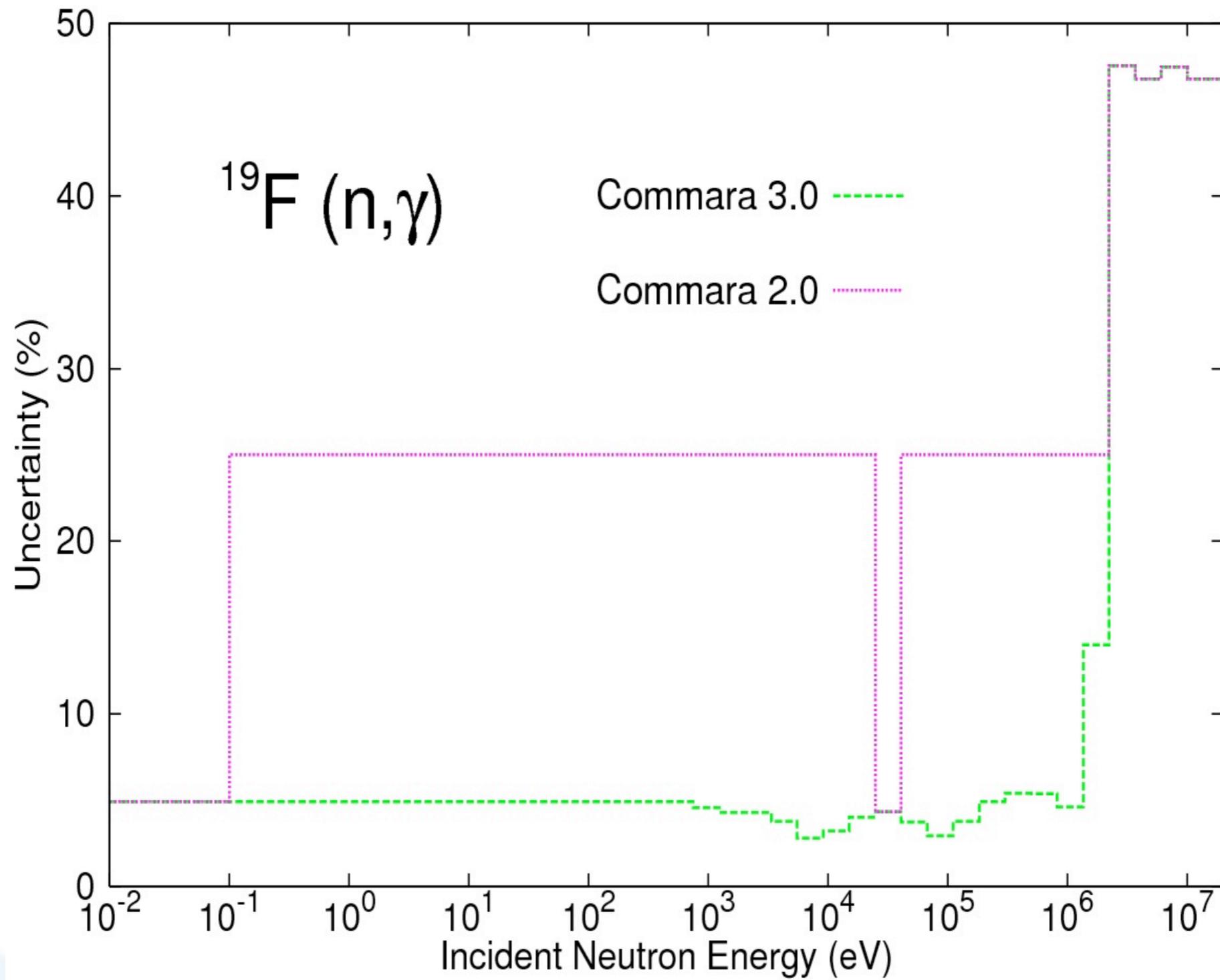
COMMARA-3 (release FY2013)



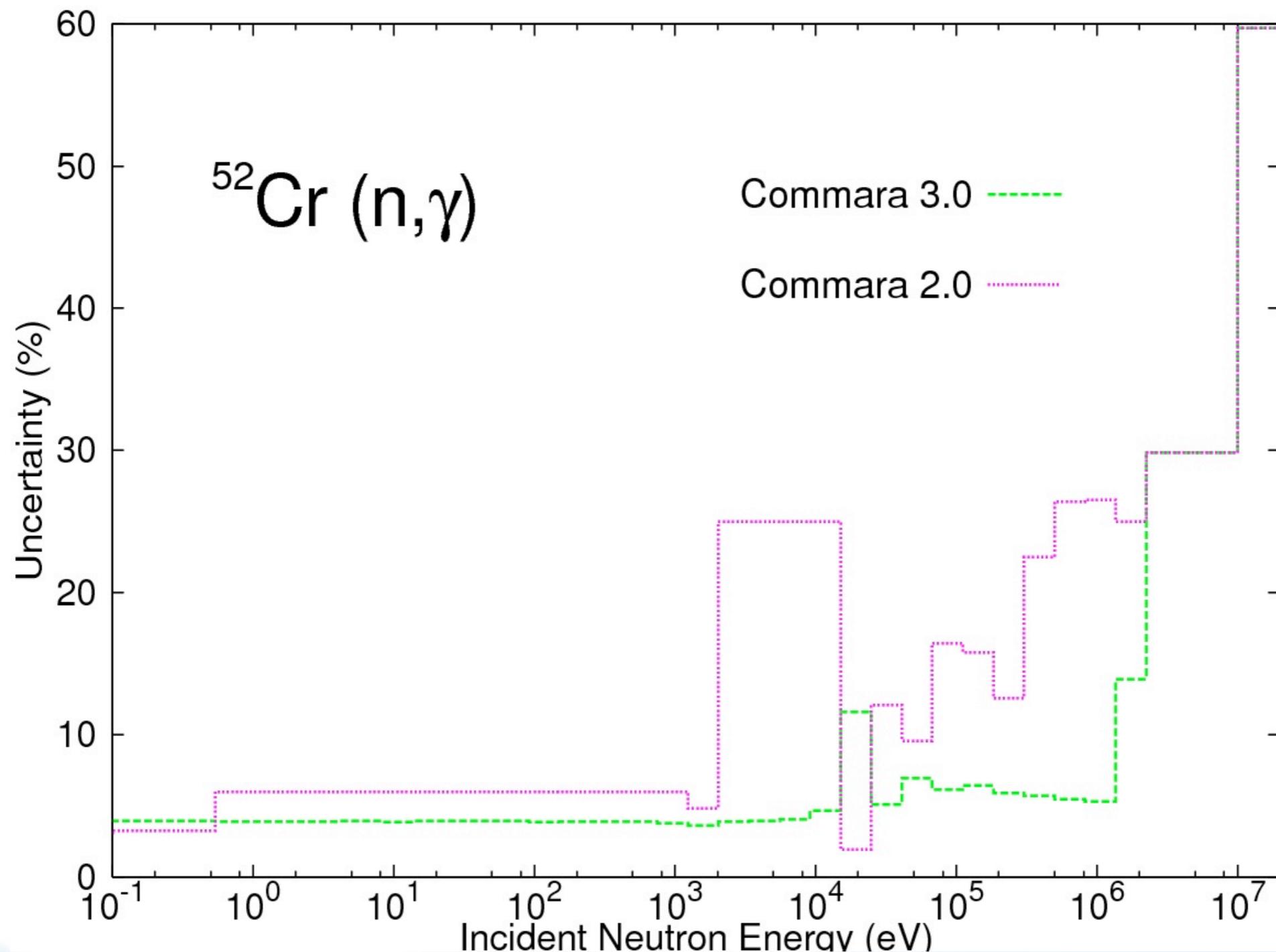
Using new features of EMPIRE will address cross-correlations, PFNS, and mu-bars

- 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

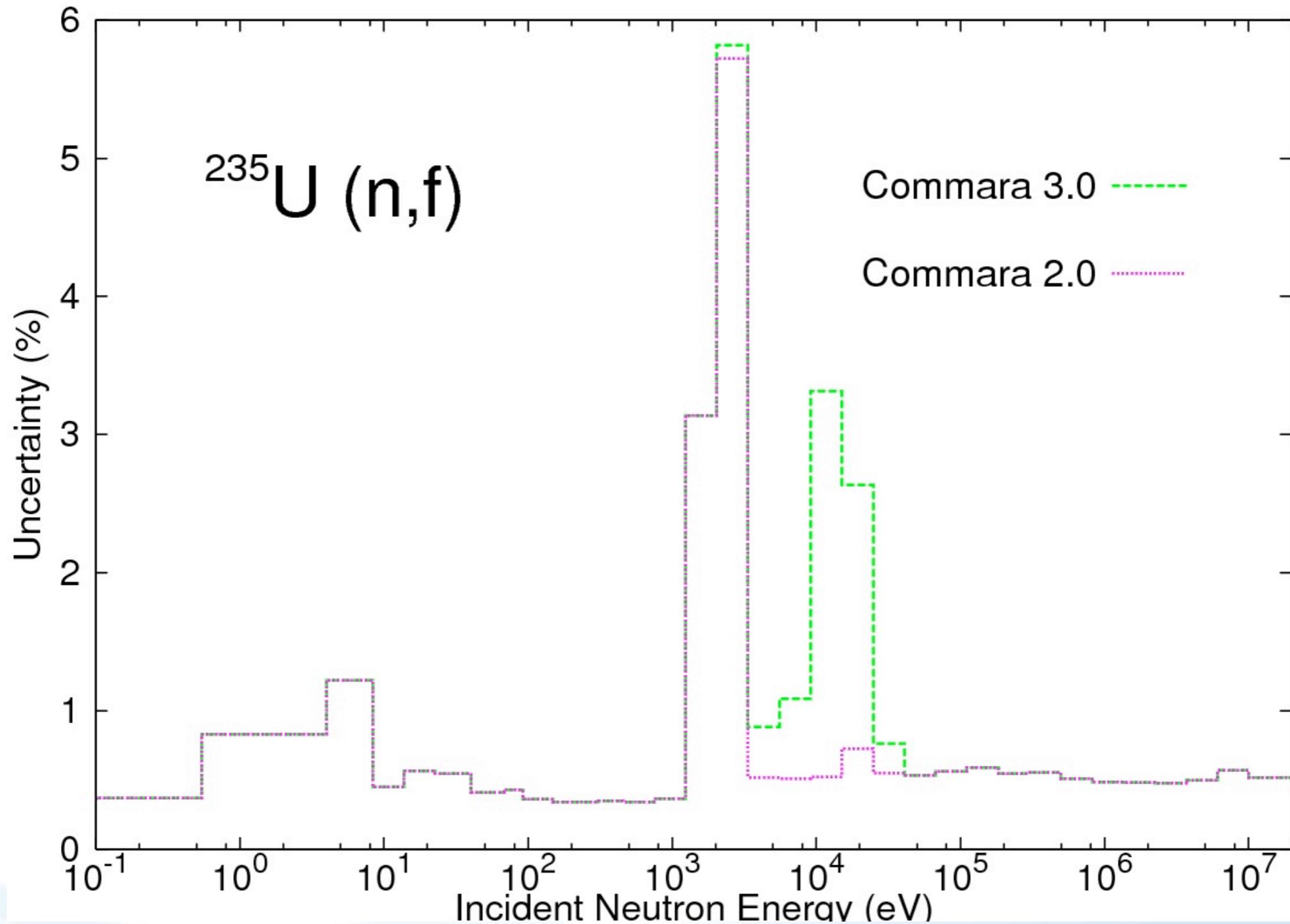
^{19}F (new ORNL evaluation)



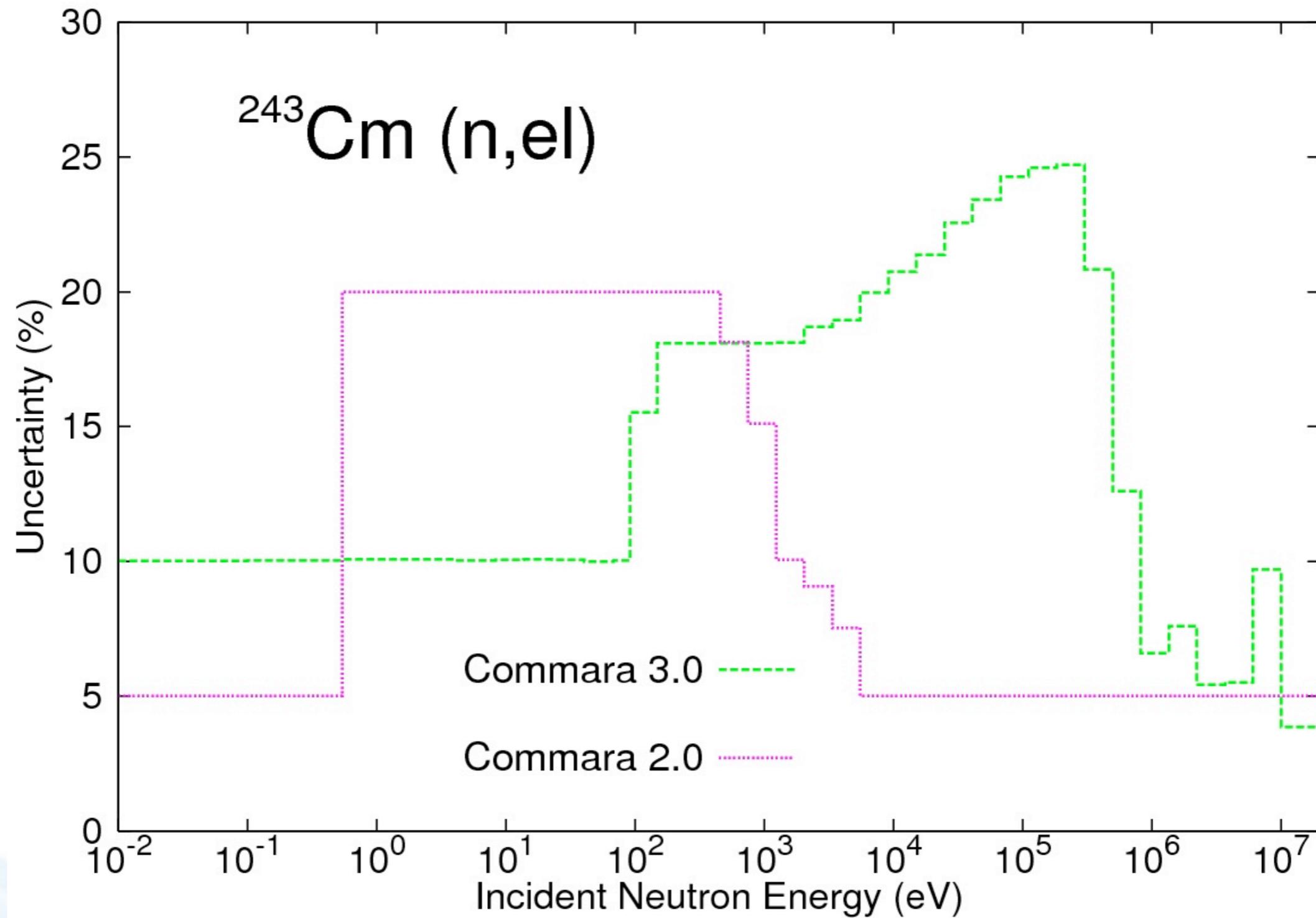
^{52}Cr (New ORNL RRR evaluation)



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

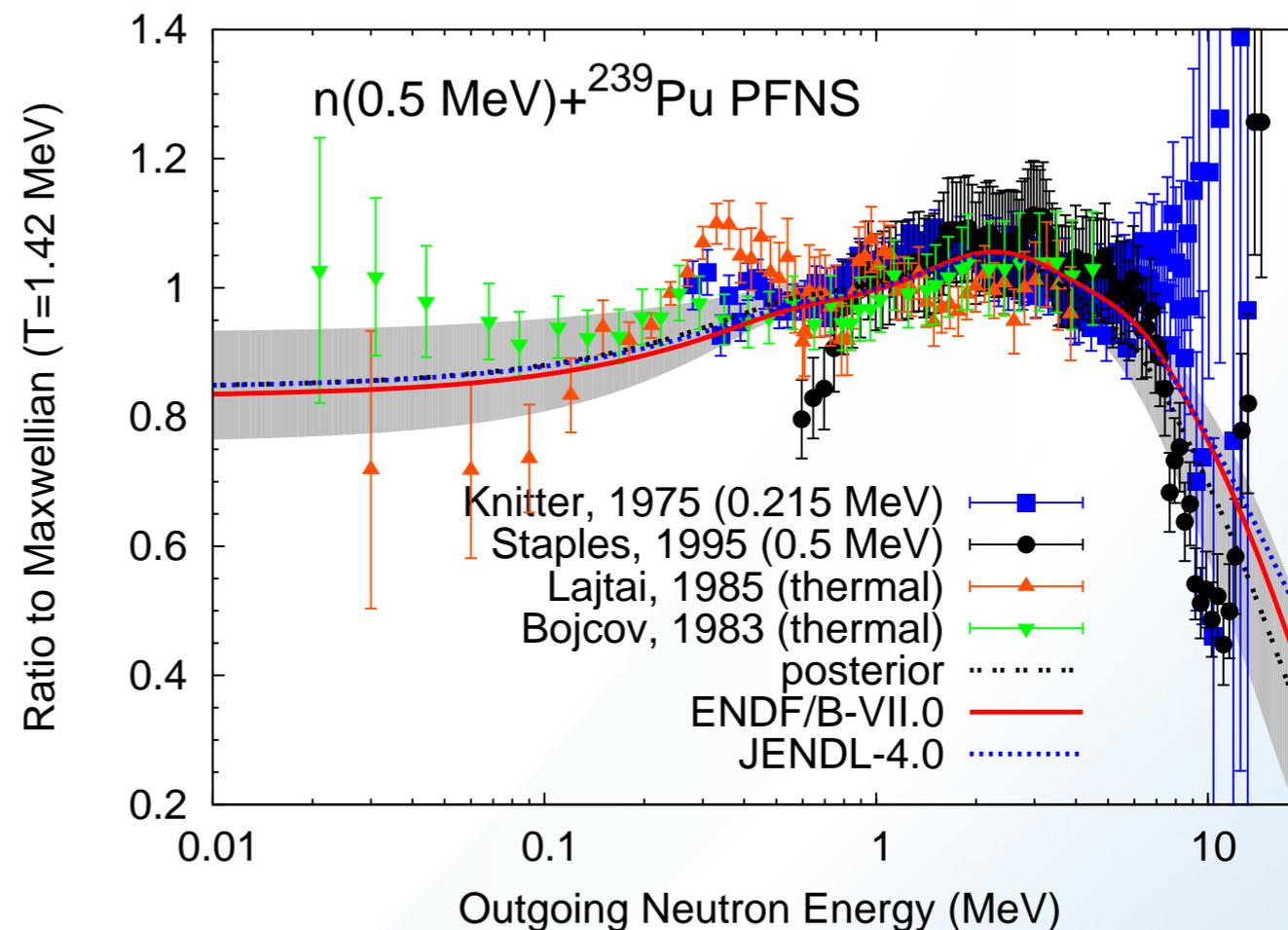
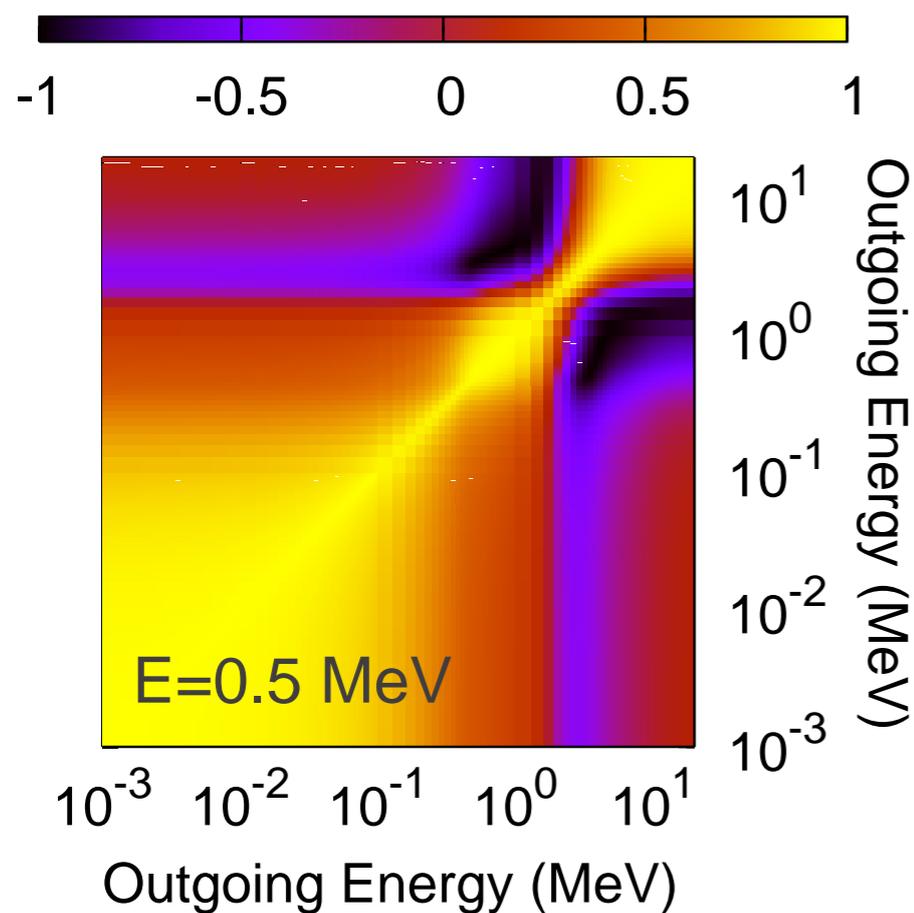


^{243}Cm (from JENDL-4)



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

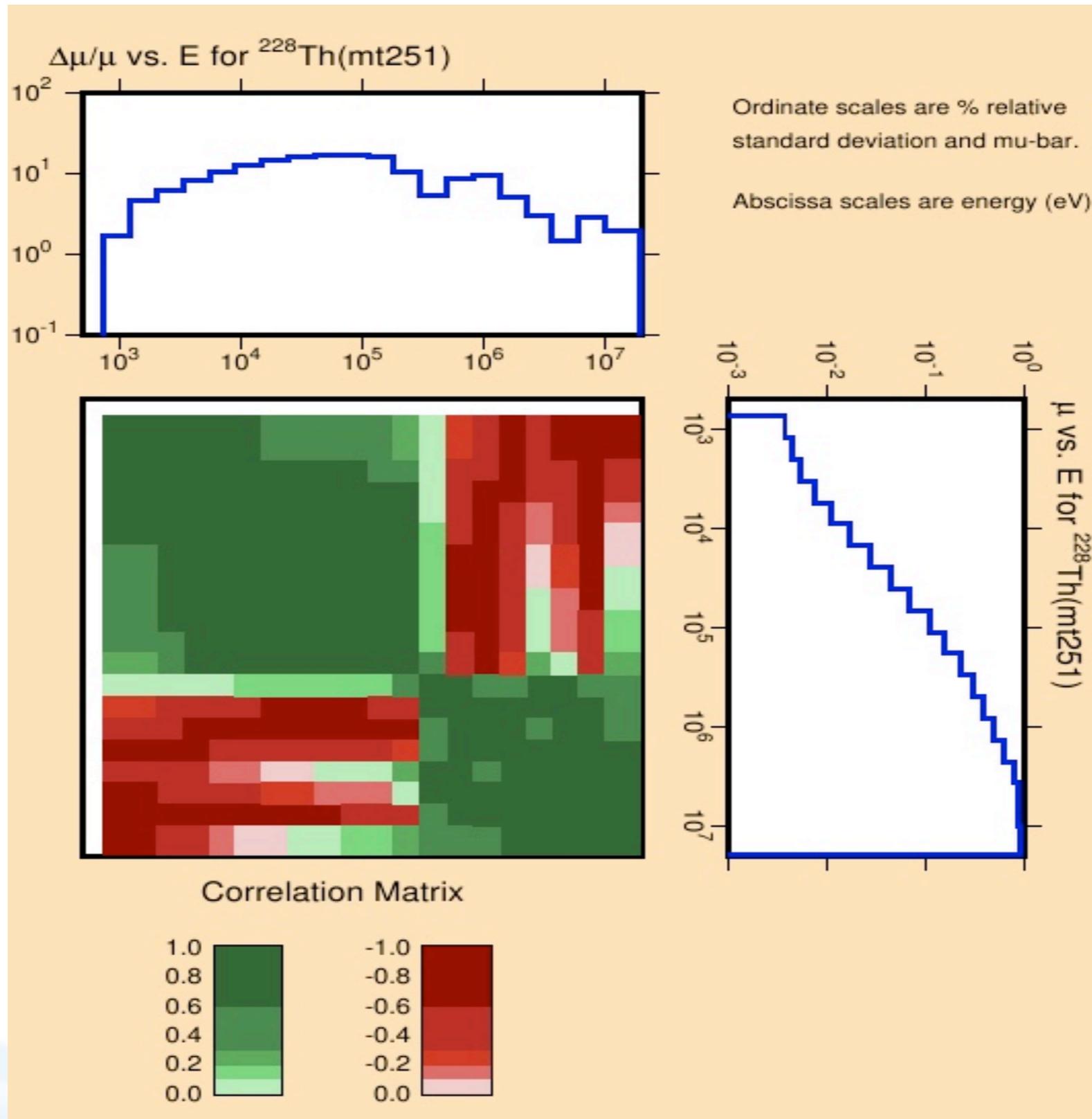
ENDF
B-VII.1



- 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)

ENDF
B-VII.1



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), ^{232}Th , W, ^{55}Mn (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 :)