



COMMARA-2.0

Release to SG33 participants

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Name of the Library

GNEP => AFCI => COMMARA

- **GNEP-1.1** - initial version under Global Nuclear Energy Partnership (GNEP) released Oct 2008
- **AFCI-1.2** - name changed to Advanced Fuel Cycle Initiative (AFCI) at version 1.2
- **AFCI-1.3** - release in Apr 2010 included many improved structural & actinide evaluations
- **AFCI-2.0 β** release in Oct 2010
- **AFCI-2.0** prepared Jan 2011, bringing in LANL actinide covariances
- **COMMARA-2.0** - renamed for final release (**C**ovariance **M**ultigroup **M**atrix for **A**dvanced **R**eactor **A**pplications)

Goals

- Provide reasonable set of covariances in support of fast reactor R&D
 - data adjustment
 - defining target accuracies
- Provide core of neutron covariances in ENDF/B-VII.1
- Advance covariance methodology
 - thermal and resonance range
 - fast neutron range
 - covariance processing
 - Quality Assurance

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 nubar, s,
 - 3 PFNS,
 - 2 mubar, s

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

Scope

- Associated with neutron cross sections from ENDF/B-VII.0
- Multigroup (processed) covariances with uniform lethargy energy groups (33 groups, 1/E flux)
- Reaction channels:
 - (n,el), (n,inl), (n,2n), (n, γ)
 - (n,f) & nubar
 - prompt fission neutron spectra (PFNS, 238,239,240Pu by LANL)
 - mubar (23Na and 56Fe only)

Methodology

- Covariance evaluation methodology determined by priorities:
 - Most important materials (~30) treated individually
 - Medium importance materials (~40) treated with simplified methods
 - Low priority materials (~40, mostly fission products) treated with low-fidelity type approach

- Existing resources
 - ENDF/B-VI.8
 - ENDF/B-VII.0
 - ENDF/B-VII.1 new evaluations
 - ‘Low-Fidelity’ project
 - WPEC SG23

Methodology (cont.)

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)

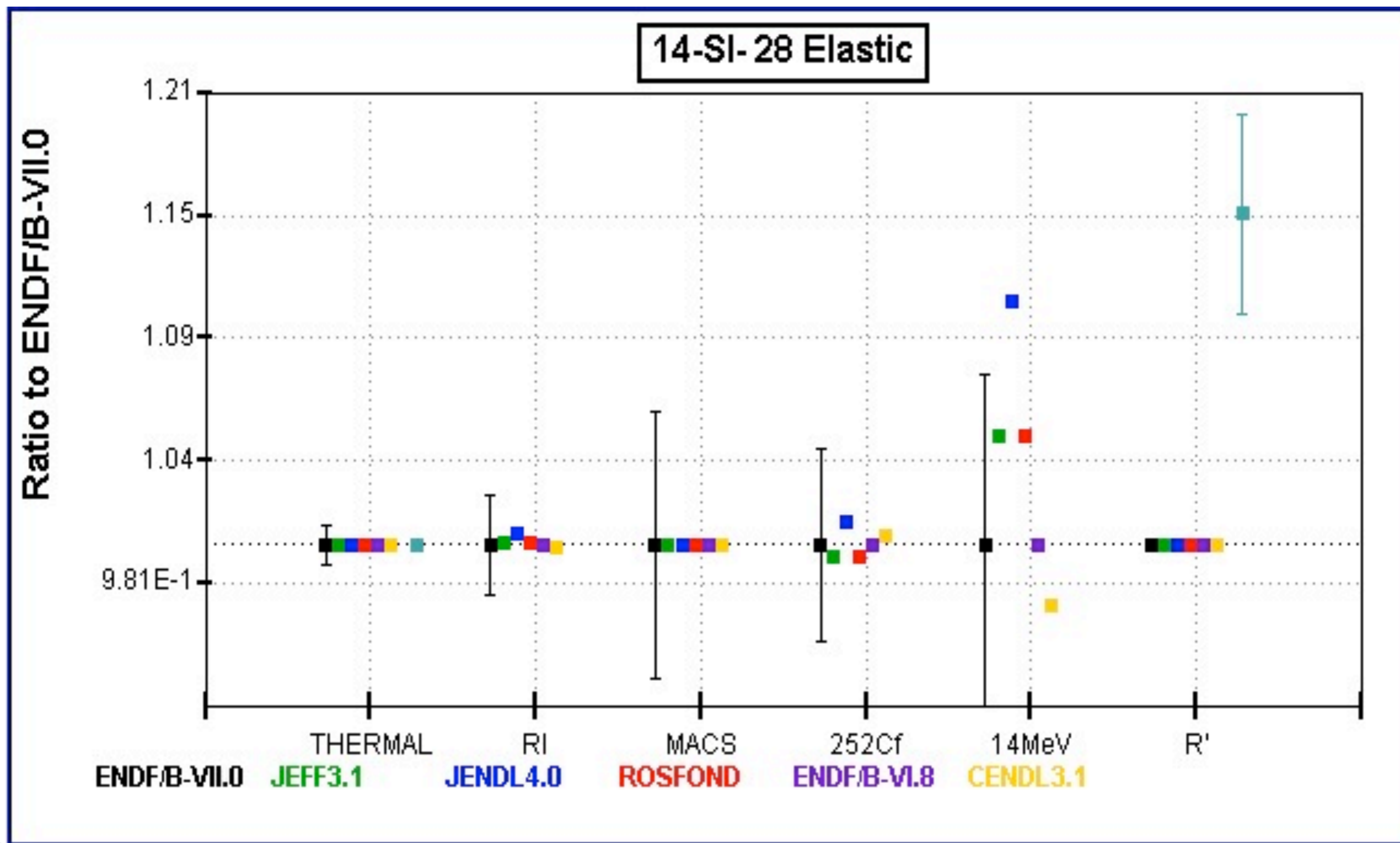
- EMPIRE/KALMAN considering experimental data
- Least Square fitting of experimental data (SOK code)
- EMPIRE/KALMAN without experimental data (Low-Fidelity)
- Dispersion analysis - differences among evaluations (and exp. data)
- Reconsider previous work (ENDF/B-VI.8, Low-Fidelity)
- Visual analysis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

Goal: provide consistent and reasonable set of covariances for nuclei relevant to AFCI (extensive checking)

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: $(n,tot) < 1\%$, (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)



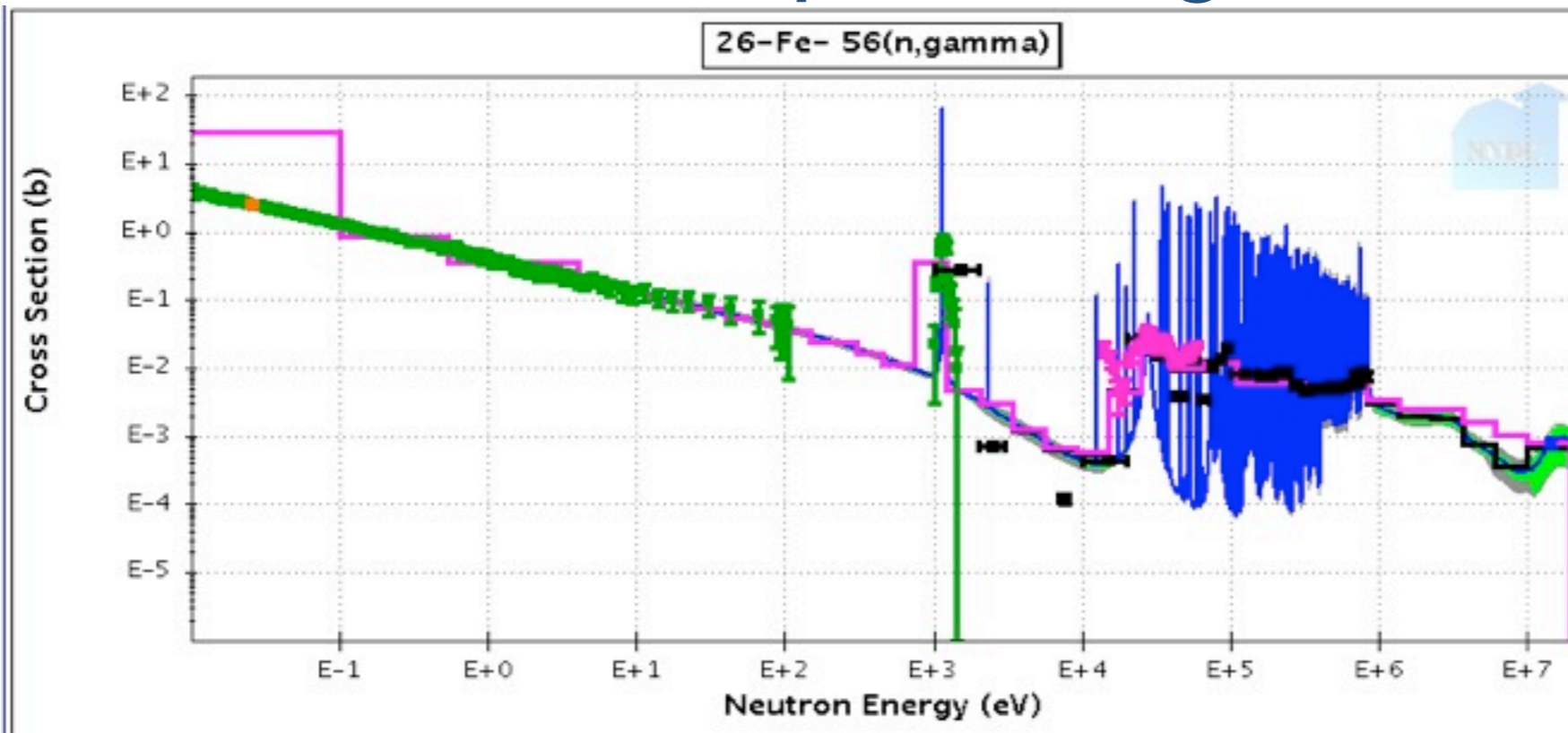
^{28}Si elastic integral quantities from Sigma-QA

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%

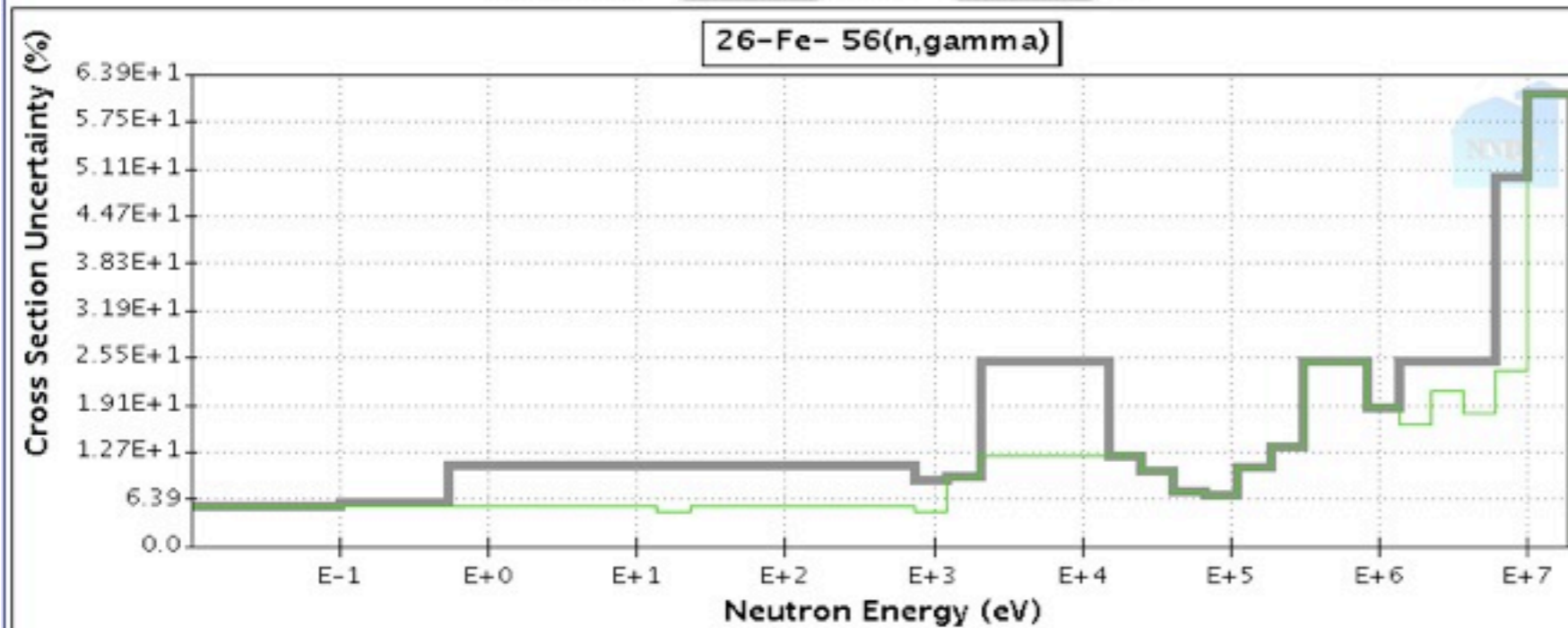
^{60}Ni capture integral quantities from Sigma-QA

Library	Capture				
	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](#)

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%)
```

Summary

- COMMARA-2.0 released - distributed to SG33 members by NEA Data Bank (e-mail?).
- Files tested using Sigma-QA and UnCor procedures for Quality Assurance
- Active user community (mainly ANL and INL) provided valuable feedback; feedback also expected from WPEC-SG33
- COMMARA -2.0 covariance files constitute core of covariances in ENDF/B-VII.1