



AFCI 1.3/2.0 covariance data

M. Herman, C.M. Mattoon, S. Mughabghab
P. Oblozinsky, M. Pigni

Outline

- Overview of AFCl-1.3 library
- Additions and changes in 1.3
- Quality Assurance
- Plans for AFCl-2.0

1: Overview of the library

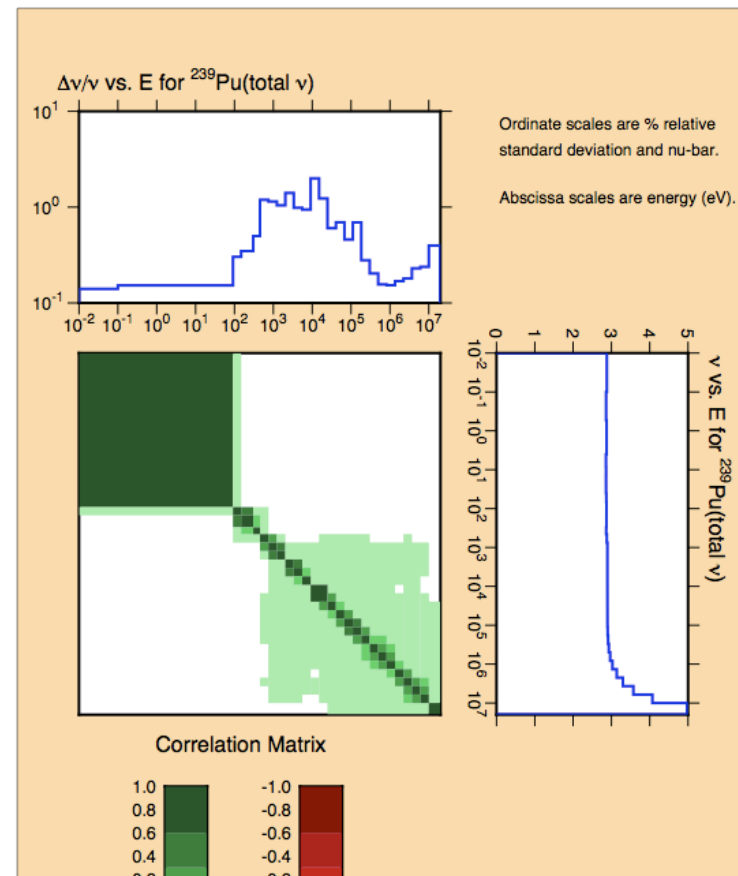
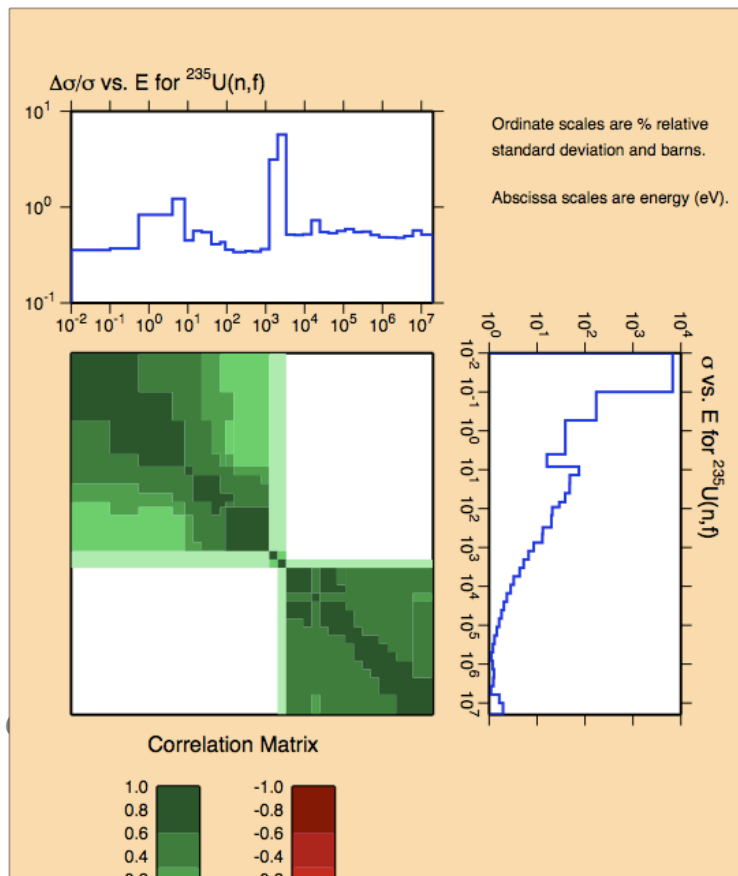
- 110 materials (20 Actinides, 12 Light materials, 78 structural + FP)
- Important materials treated individually at several institutions.
- Bulk of library (approximately 70 of 110 files, FPs and structural) based on the 'low-fidelity' covariance estimates from LANL,ORNL,BNL

Contents of library

- Major Actinides produced by LANL/ORNL
 - ^{232}Th from ENDF/B-VII
 - $^{233,235,238}\text{U}$ and ^{239}Pu from ENDF/A
- Structural materials produced by BNL
 - ^{23}Na , ^{52}Cr , ^{56}Fe , ^{58}Ni
- Light nuclei from LANL (^1H , ^{16}O , ...)
- Minor Actinides partly based on V.Maslov estimates, partly on BNL and LANL efforts
- Fission Products based on low-fidelity covariance estimates

33-group structure

- AFCI is a processed covariance library, using 33 energy bins.
- Group boundaries chosen so that in most cases, $\log(E_2) - \log(E_1) = 0.5$



Key dates for AFCI library

- Initial version (GNEP 1.0) released October 2008
- GNEP 1.1 April 2009, mainly fixes for structural materials
- AFCI 1.2 August 2009, many fixes for minor actinides, structural and fission products
- AFCI 1.3 April 2010, improved structural materials and minor actinides

Overview of library

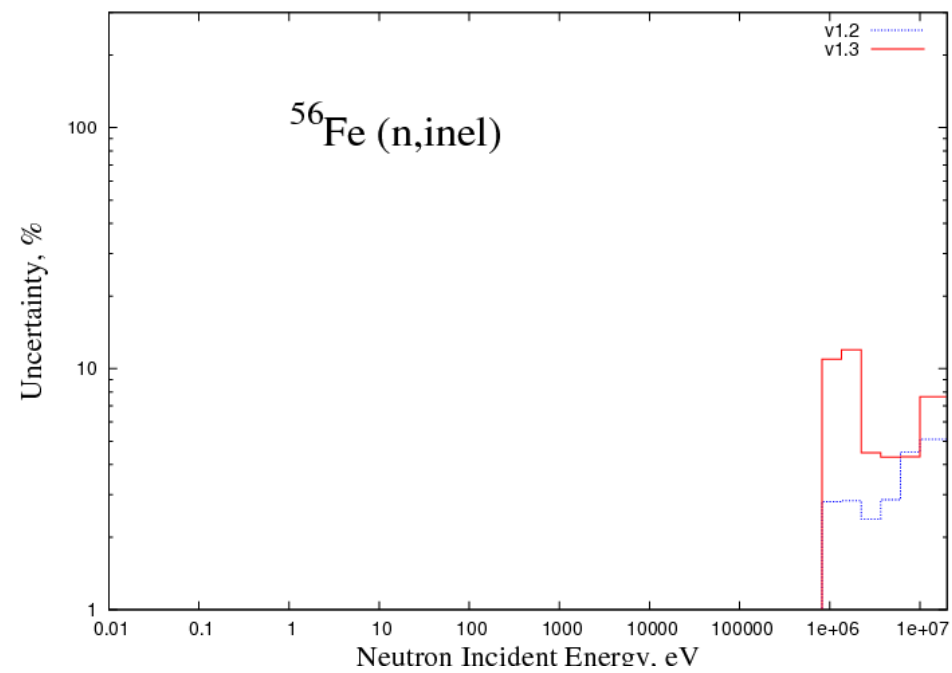
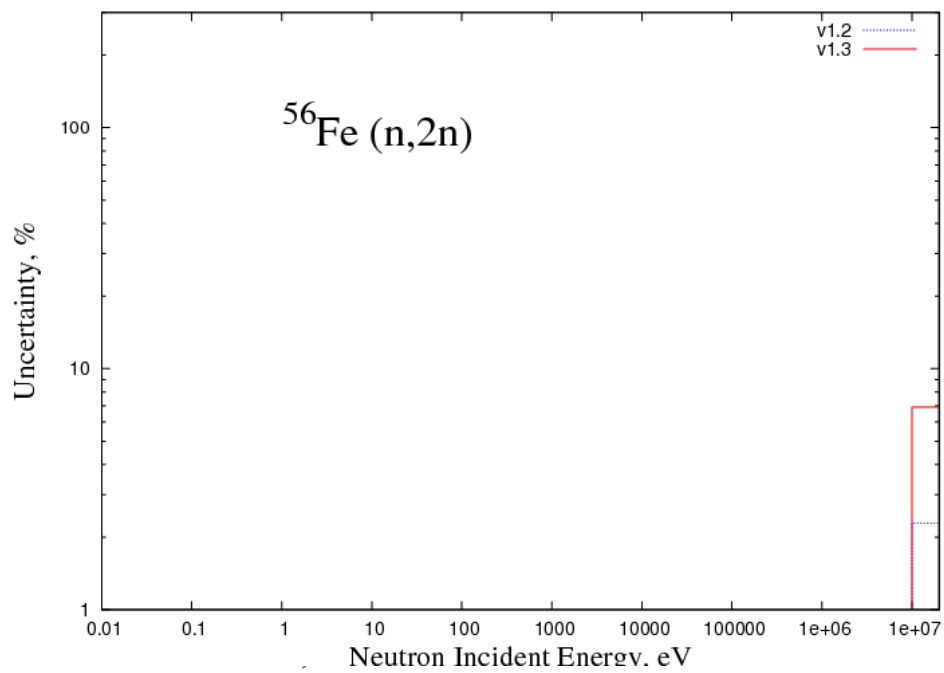
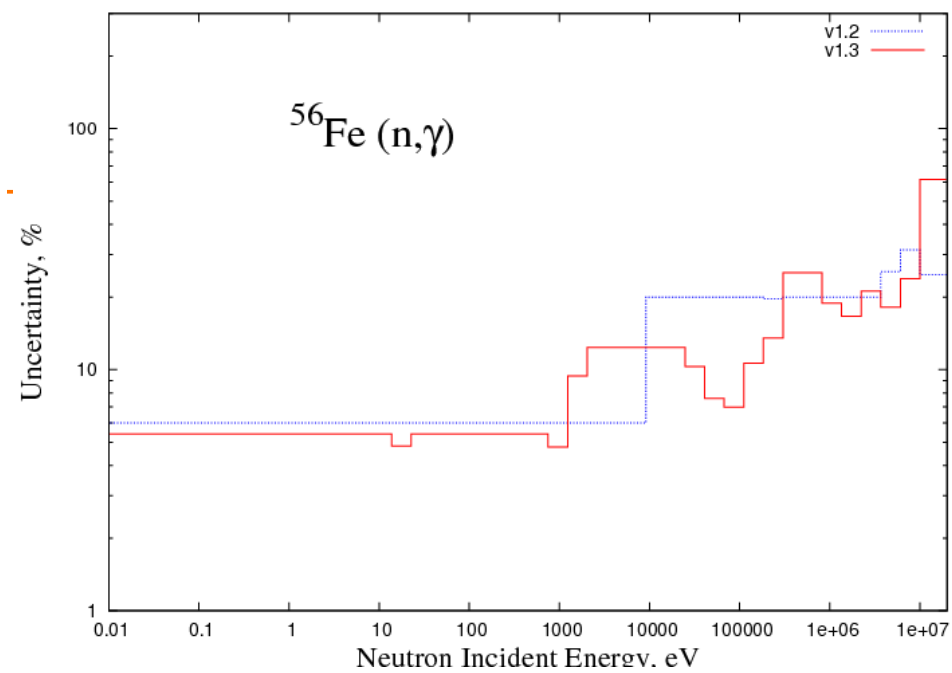
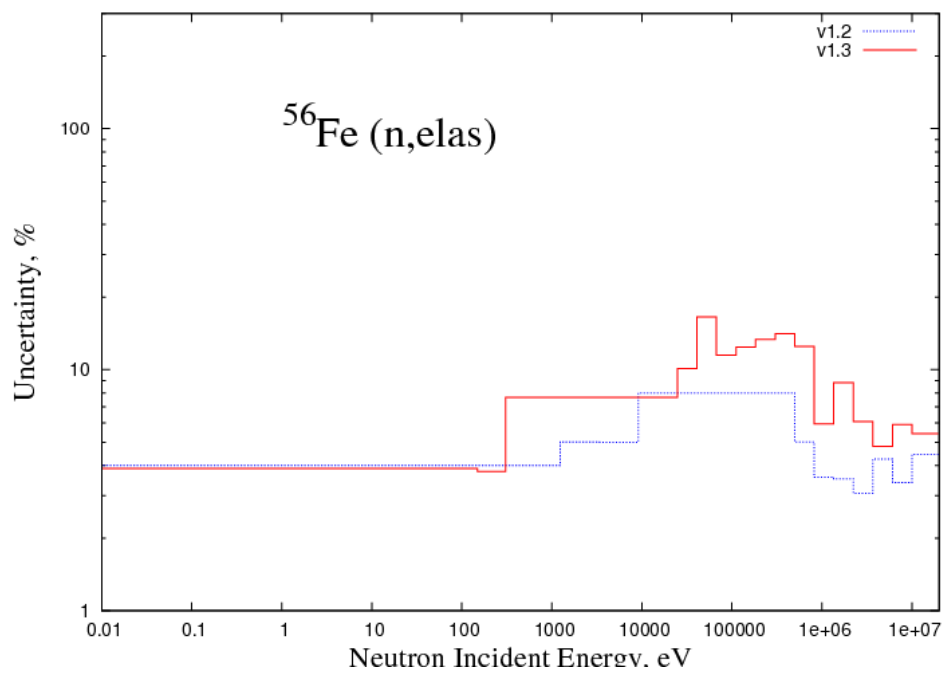
- Active user community (INL and ANL) are providing valuable feedback
- Library is currently available only for testing and development. As the project evolves, a future version will become available for general use

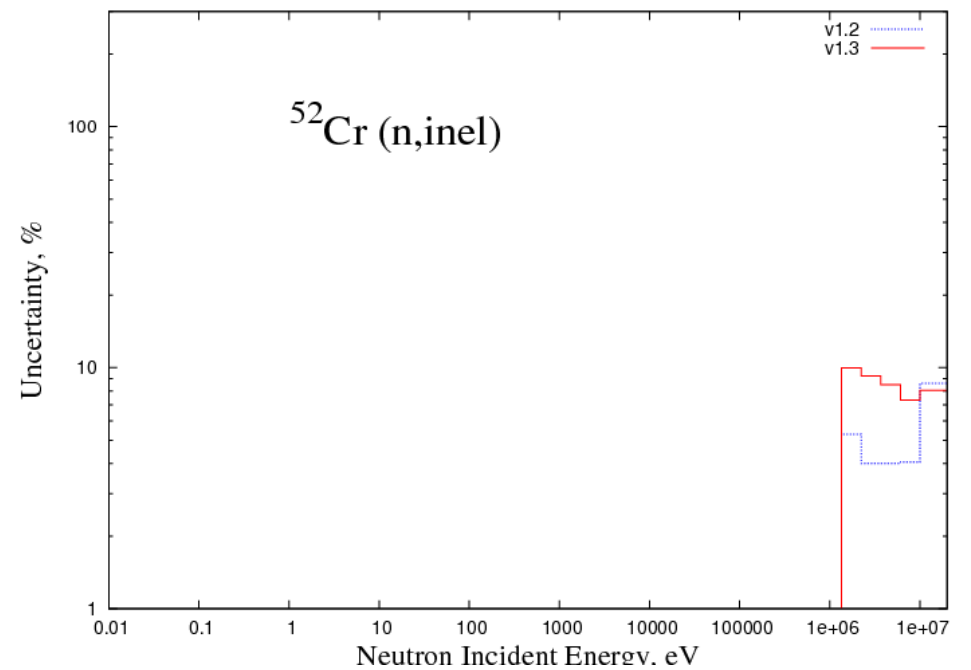
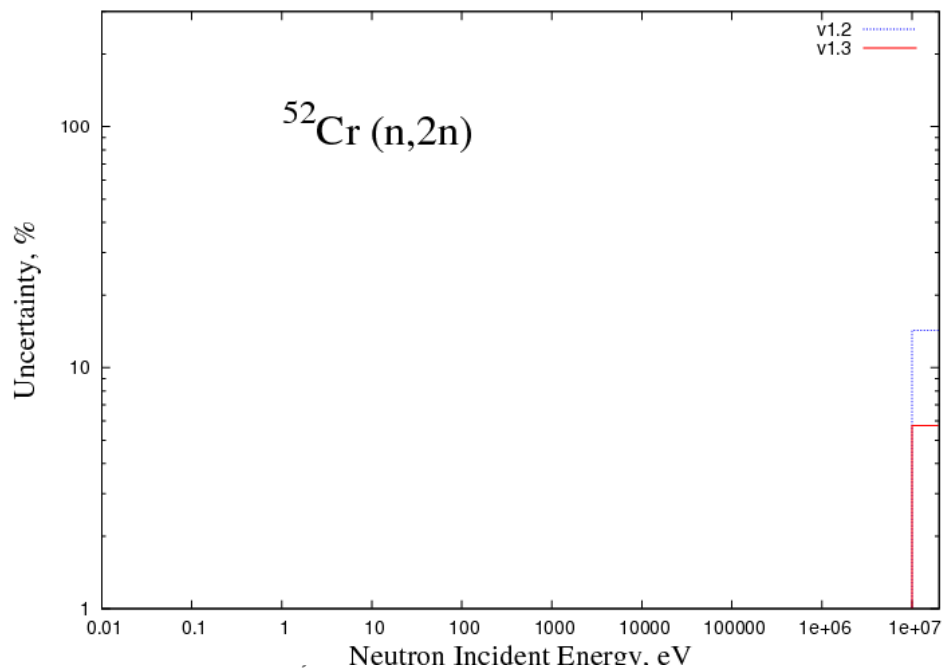
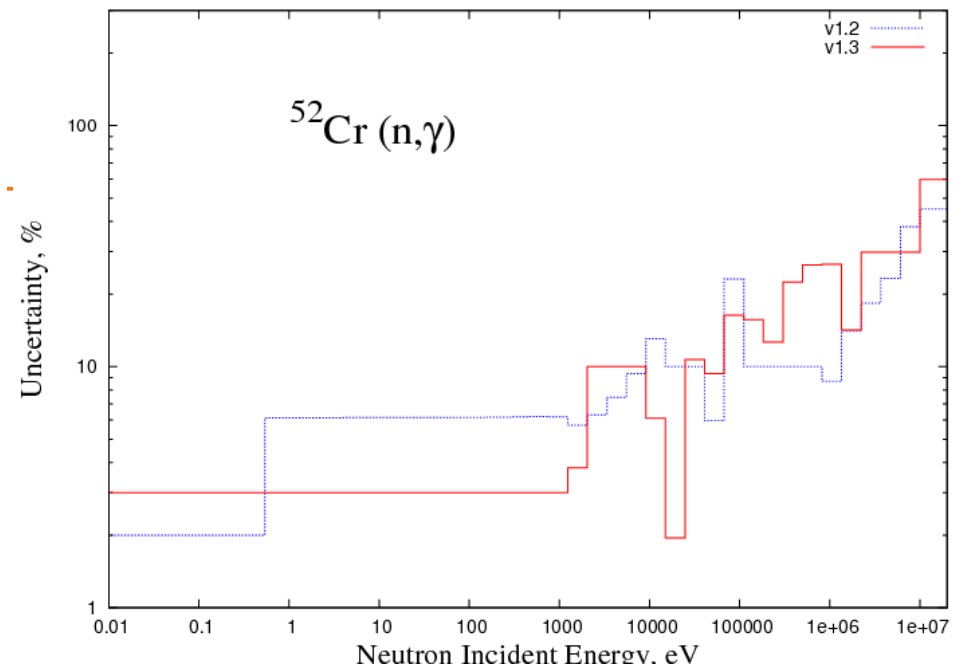
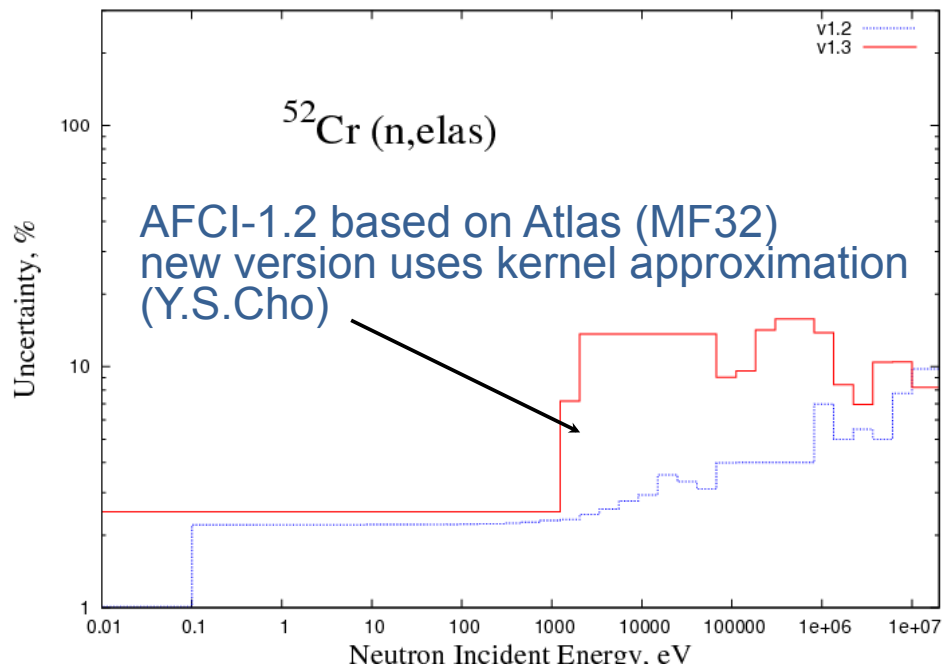
2: Changes for AFCI-1.3

- Structural materials produced at NNDC
 - kernel approximation in RRR
 - Modified VI.8 covariances in fast neutron range
- Improvements for prompt fission neutron spectra
- New content for minor actinides

Changes: Structural Materials

- Structural materials ^{52}Cr , ^{56}Fe and ^{58}Ni : ENDF/B-VI.8 reinstated; inelastic uncertainties increased in the threshold region following dispersion analysis.
- ‘Kernel approximation’ (Y.S.Cho and P.Oblozinsky) used in resonance region:
 - capture kernel defined as $(\Gamma_n \Gamma_\gamma)/\Gamma_{\text{tot}}$
 - for structural materials, $\Gamma_{\text{tot}} \approx \Gamma_n$, so kernel is dominated by capture width and we estimate $\Delta(\text{kernel})$ from capture width uncertainties
 - works very well for (n,γ) , less so for elastic

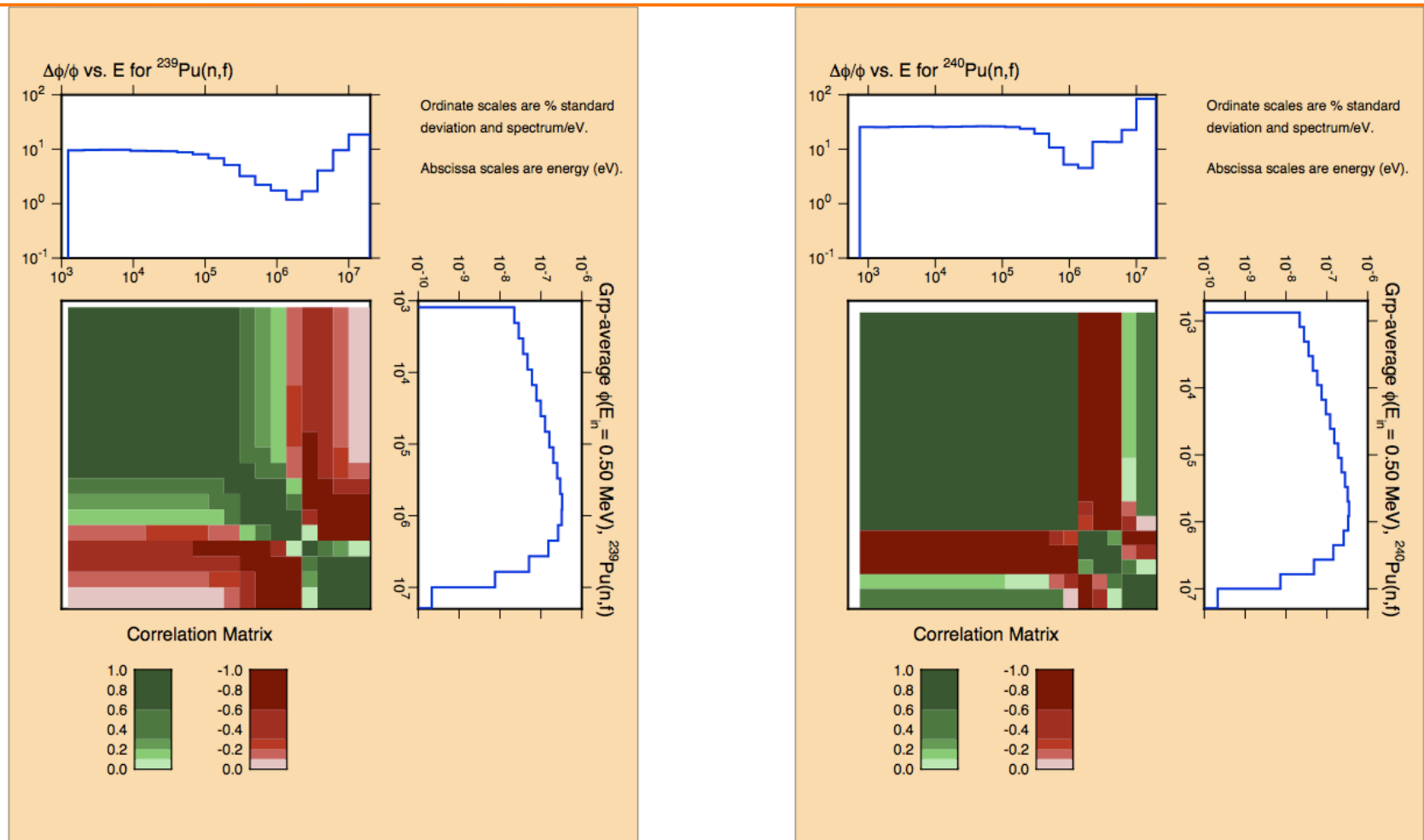




Fission Spectra

- ^{239}Pu PFNS was present in AFCI-1.2
- Problem in v1.2: rows/columns of PFNS did not sum to zero as expected for covariance matrix of normalized distribution
- AFCI-1.3: added ^{240}Pu PFNS, both matrices now obey sum-to-zero condition

239,240Pu PFNS



Fix: PFNS covariance matrices now obey sum-to-zero condition

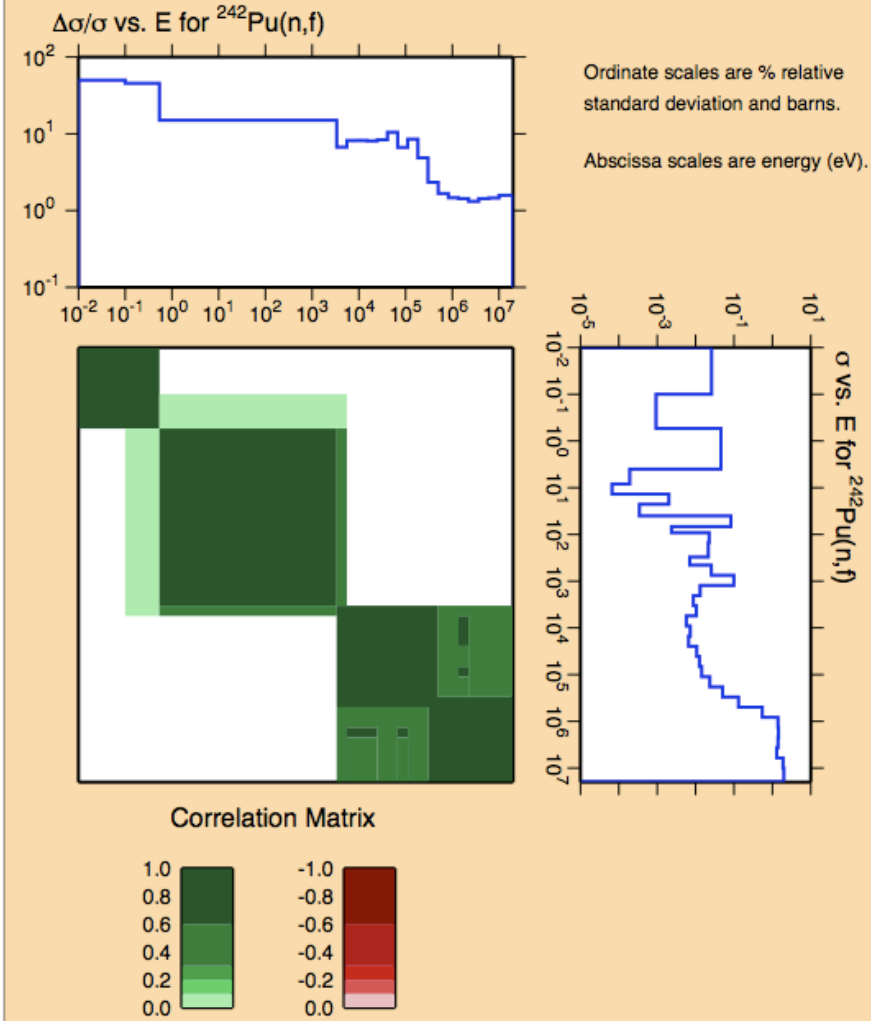
Minor Actinides

- $^{240,241}\text{Pu}$ new files from LANL
- ^{237}Np , ^{242}Pu new files from BNL (EMPIRE/KALMAN)
- These replace older estimates based on V.Maslov recommendations

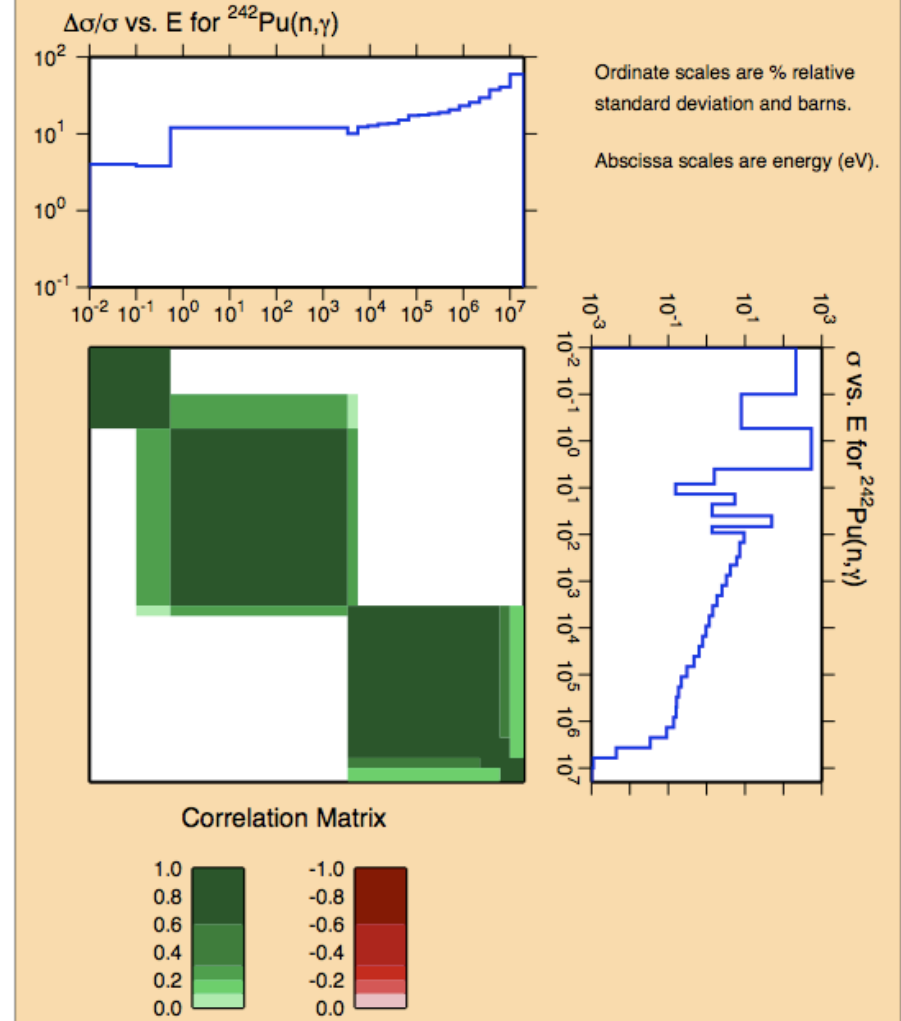
^{242}Pu

- Using new input for EMPIRE (M.Sin), varying fission barrier and optical model parameters
- Experimental data for (n,tot), (n,el), (n,f)
 - For fission, have new data from Tovesson et al (2009)
- Covariances produced with KALMAN filter
- At lower energies, still using 'low-fidelity' values

242Pu (cont.)



C.M. Mattoon, ND2010



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3: Quality Assurance

- Checking covariances visually for major channels
- unCor-1.1 applied to full library, gives warnings for
 - small uncertainties: $(n, \text{tot}) < 1\%$, (n, el) and $(n, \gamma) < 2\%$, etc
 - non-positive-definite matrices
 - PFNS covariance not summing to zero
 - peaks, jumps in uncertainty
- non-positive-definite matrices may be fixed at price of modifying correlations (usually small changes)

Quality Assurance (cont.)

- program 'unCor' checks output of PUFF/NJOY for problems in 'uncertainties' and 'correlations'
- Small uncertainties still appear in v1.3 of library

```
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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4: Plans for AFCI-2.0

- New covariances for the remaining major structural materials (Cr, Fe, Ni) using the same methodology (VI.8 + modified inelastic + kernel approximation in RRR).
- Adopt JENDL Actinoid covariances for the minor actinides (except ^{242}Pu and ^{237}Np done at BNL)
- Covariances for fission spectra for ^{240}Pu (LANL)

Plans for AFCI-2.0 (cont.)

- Replacement of the remaining ‘low-fidelity’ covariances (at least most of them)
 - Adjustment of the RRR upper limit in the ‘low-fidelity’ files from 5 keV to the actual (or more sensible) value.
 - Replacement of the RRR covariances with kernel approximation for most of the cases
 - Replacement of the fast neutron covariances with new estimates based on more advanced EMPIRE calculations
 - CC instead of spherical OM
 - More model parameters varied
 - Use of experimental data

Summary

- AFCI-1.3 covariance library released April 2010
 - New: ^{240}Pu , $^{241}\text{Pu}(n,f)$, ^{237}Np , ^{242}Pu
 - Revised structural materials
- ANL and INL users are providing valuable feedback towards improving the library
- Files are being tested visually and using automatic procedure for quality assurance
- AFCI-2.0 to be completed in August 2010