Neutron Cross Section Covariances for the ENDF/B-VII Library

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U.S. DEPARTMENT OF ENERGY | Office of Science

Scope of the project

Respond to needs of Advanced Fuel Cycle Initiative

- Address issues in the covariance methodology in the resonance as well as fast neutron region
- Develop new methods and codes to evaluate covariances of prompt fission neutron spectra and neutron multiplicities (LANL).
- Produce covariances in the whole energy range up to 20 MeV for 110 nuclei to be included in ENDF/B-VII.1 to be released in December 2011.

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 nubars,
  - 3 PFNS,
  - 2 mubars

Synergy with the NE funded AFCI project - **multi-group** covariance library COMMARA-2 serving as a reference

^{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**

FY2010 milestones (BNL)

Q1: Develop improved **covariance module** in the nuclear reaction code EMPIRE

Q2: Develop initial version of **Quality Assurance** procedures for covariance data

Q3: Produce **covariance evaluations** for several priority materials (Fe, Cr, Ni)

Q4: Produce covariance estimates for lower priority materials

FY2011 milestones (BNL)

Q1: Complete covariance evaluations for about 25 structural materials

Q2: Complete covariance evaluations for about 40 fission products

Q3: Update Quality Assurance procedures based on the accumulated experience; assemble files; perform basic testing; submit to ENDF/B-VII.1 beta1

Q4: Update covariance files as necessary, **perform quality assurance**, submit to ENDF/B-VII.1 beta2 for another round of CSEWG testing

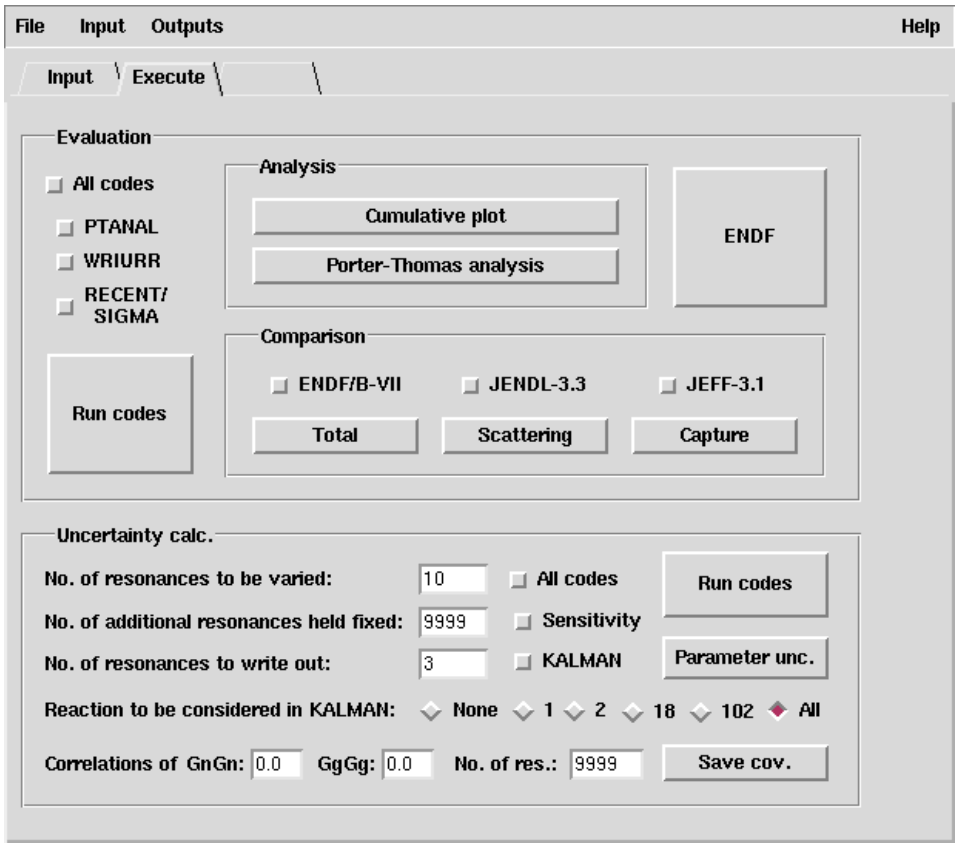
FY2013 milestones (BNL)

Q1: Release of about 100 covariance files as part of the **ENDF/B-VII.1 library**

Q2: Produce report describing the work done under this project

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)
- "Kernel Approximation" (MF33, ANR)
- EMPIRE Resonance Module (MF32, ANR, scattering radius and thermal point uncertainties reproduced through correlations
- MF32 with systematic uncertainties in MF33
- 'low-fidelity' (Mark Williams)



Resonance module of EMPIRE

Methodology
Fast neutron range (MF33)

- R-matrix analysis (LANL, light nuclei)
- EMPIRE/KALMAN considering experimental data (BNL)
- GNASH/KALMAN considering experimental data (LANL)
- Least Square fitting of experimental data (LANL, SOK code)
- Dispersion analysis - differences among evaluations (BNL)
- Reconsider previous work - ENDF/B-VI.8, Low-Fidelity (BNL)
- Visual analysis of experimental data
- Assimilation (BNL)

Methodology: EMPIRE code
Complete system for nuclear data evaluation

- A few mouse clicks
  - calculate cross sections, spectra, angular distributions, energy-angle correlated distributions
  - read and format neutron resonances
  - plot comparison with experimental data
  - format ENDF-6 file
  - run checking codes
  - run processing code (NJOY)
- Covariances need more clicks

The Battle of Lodi (May 10, 1796)

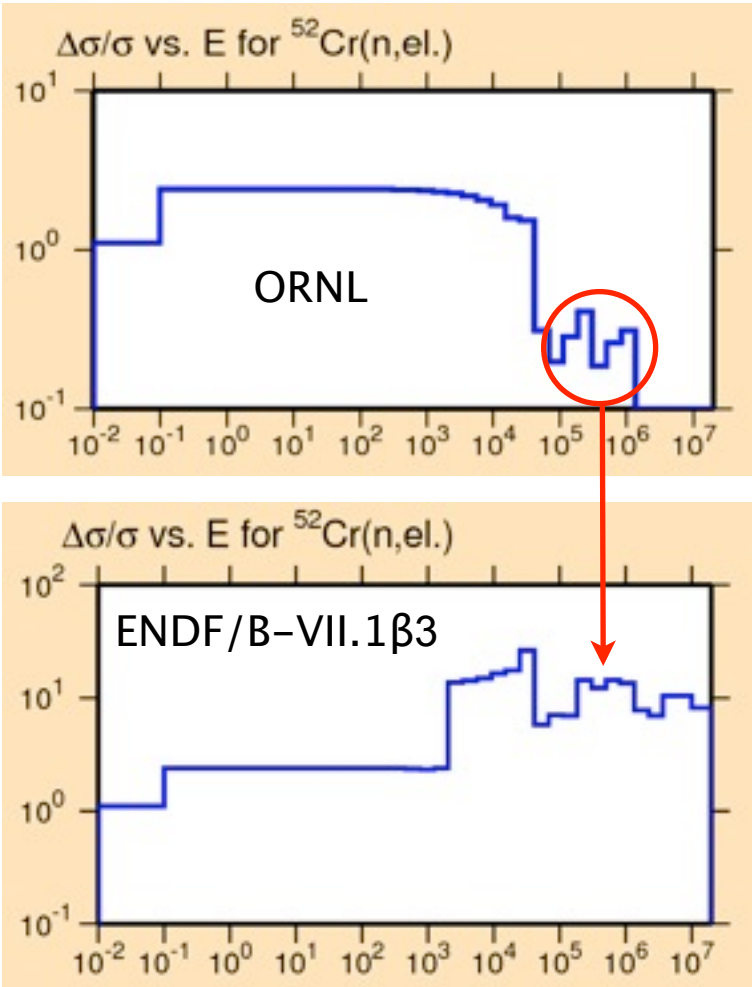
- EMPIRE contains:
  - state of the art modeling
  - RIPL-3 database of input parameters
  - Atlas of neutron resonances
  - Kalman filter

EMPIRE
Nuclear Reaction Model Code

^{50,52,53}Cr & ^{60}Ni

Merging ORNL RR evaluation with COMMARA

- COMMARA covariance data adopted in the fast region.
- Additional section added to ORNL elastic to account for the uncertainty in the scattering radius R'
- For ^{50,52}Cr and ^{58}Ni additional MF33 sections added to capture to match COMMARA uncertainties.

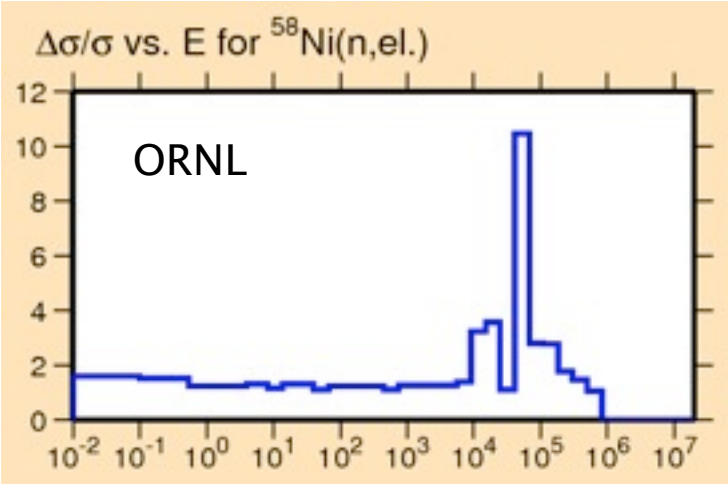


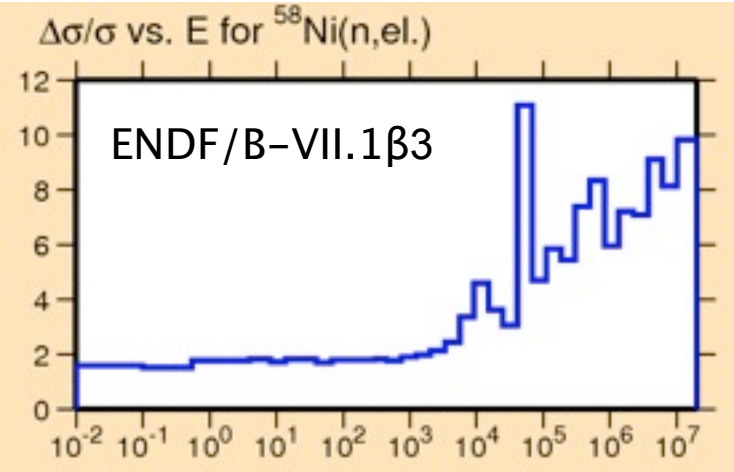
^{58}Ni

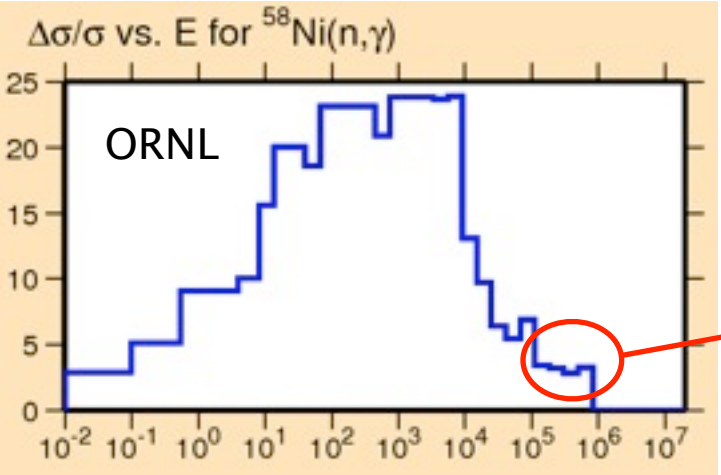
Extension of the ORNL evaluation

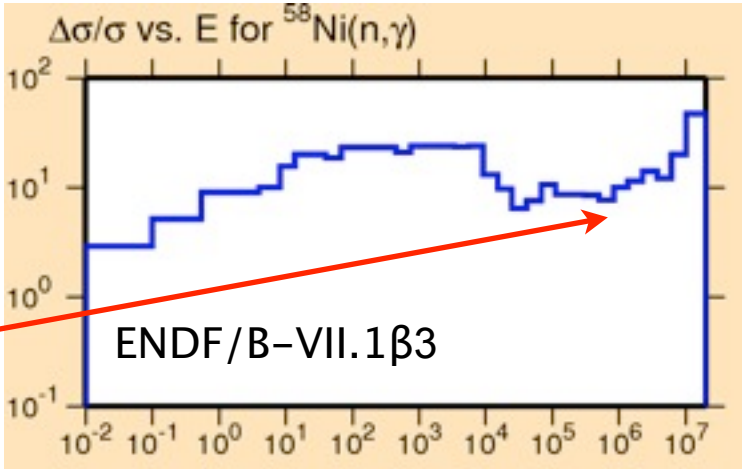
MF32 Resonance region only

MF32 + fast neutron range



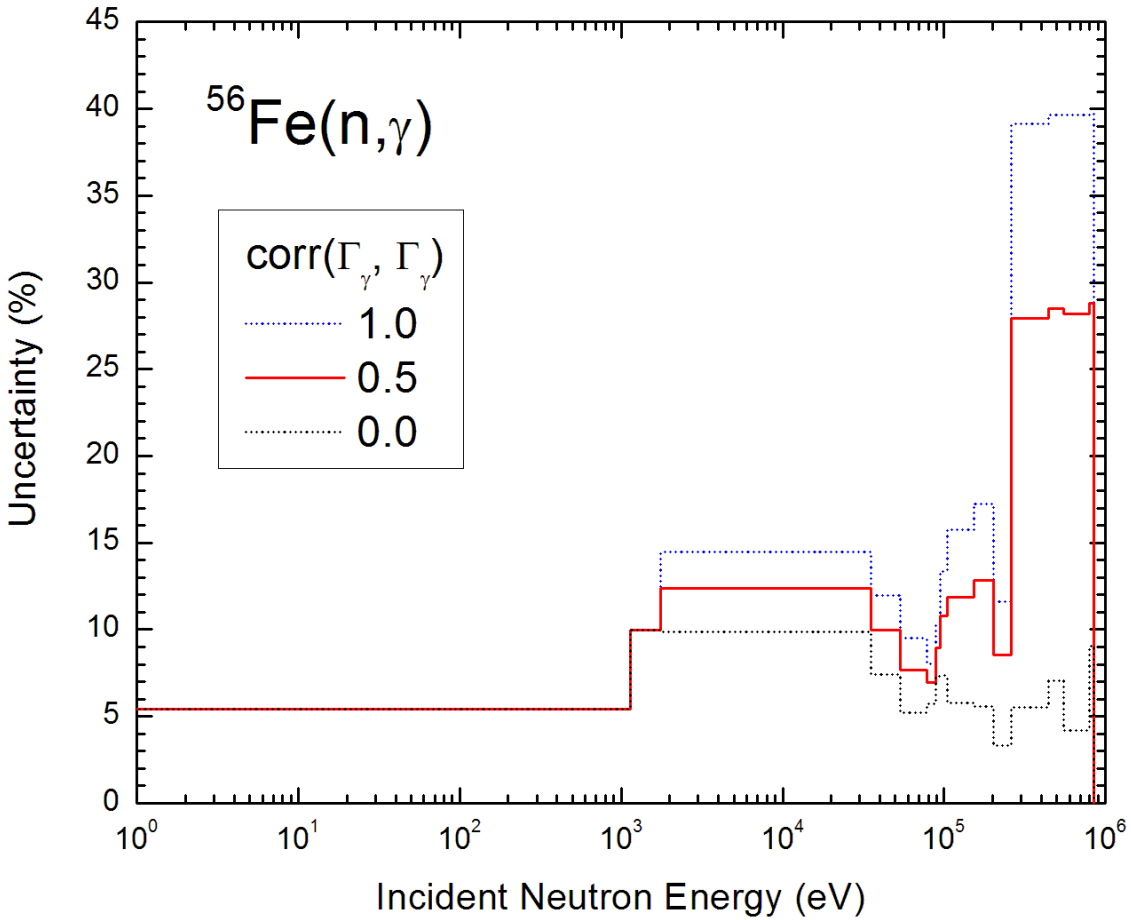






^{56}Fe(n,g)

Role of correlations among gamma widths



Kernel method in resonance region

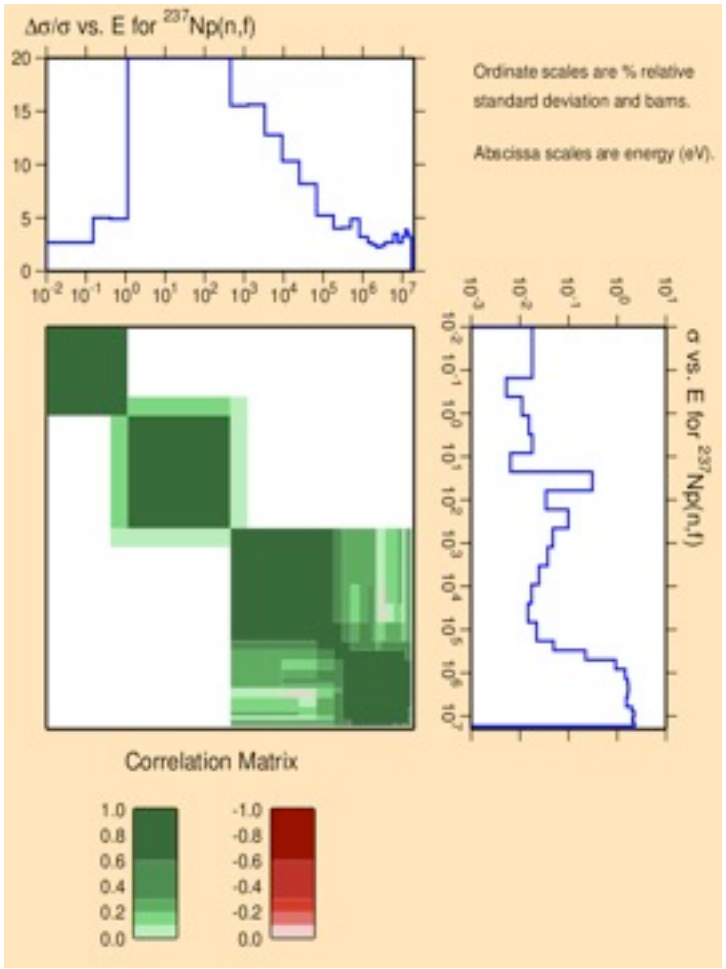
Correlations among gamma widths change capture uncertainty by an order of magnitude!

They are usually not available in the experimental papers (not provided in Atlas!)

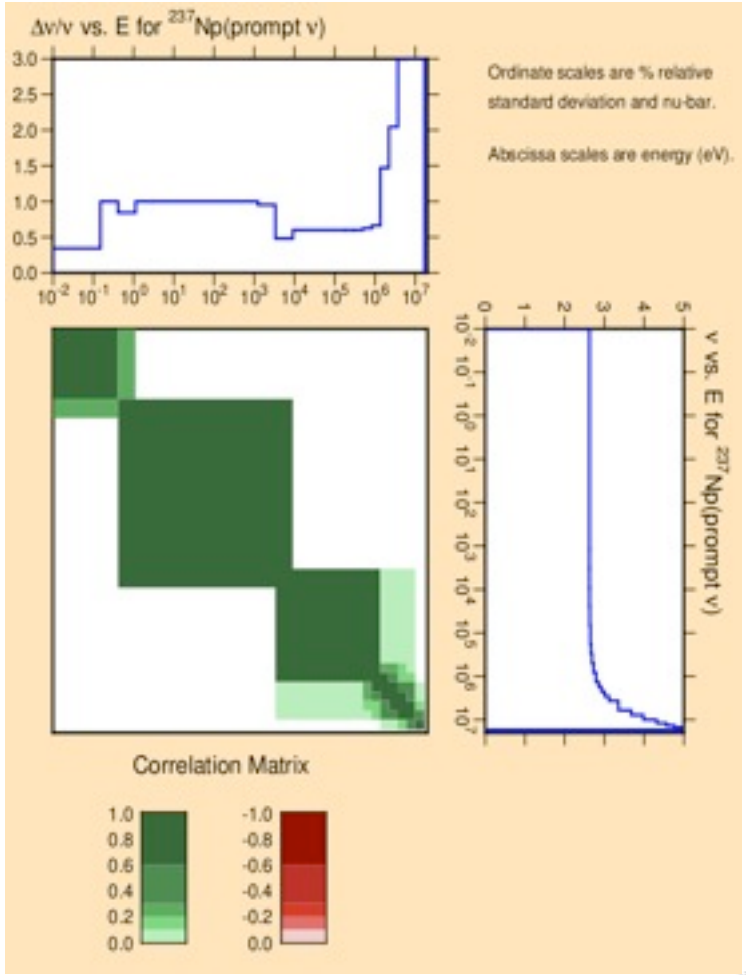
^{237}Np(n,f)

Revised 'low-fidelity' in RR; EMPIRE/KALMAN in fast n

Fission cross section covariances



nu-bar covariances (dispersion analysis)

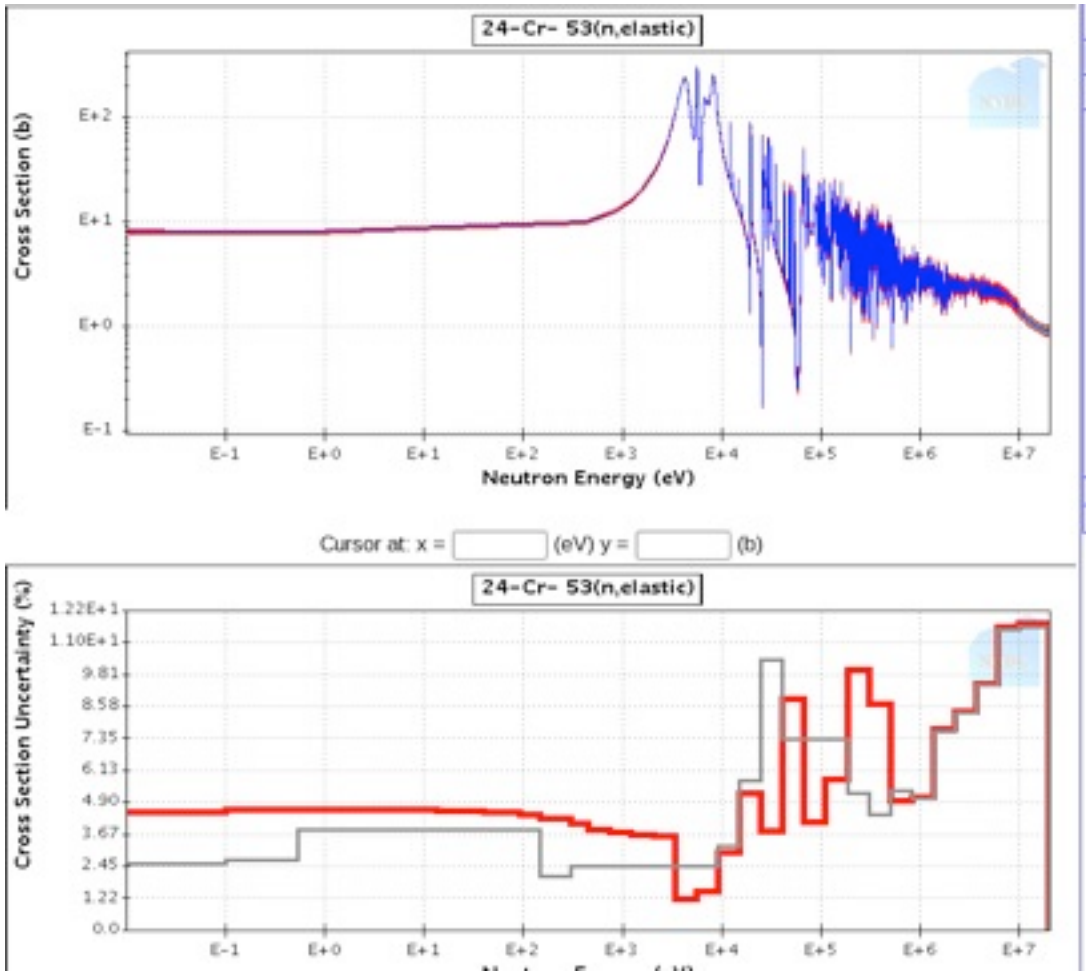


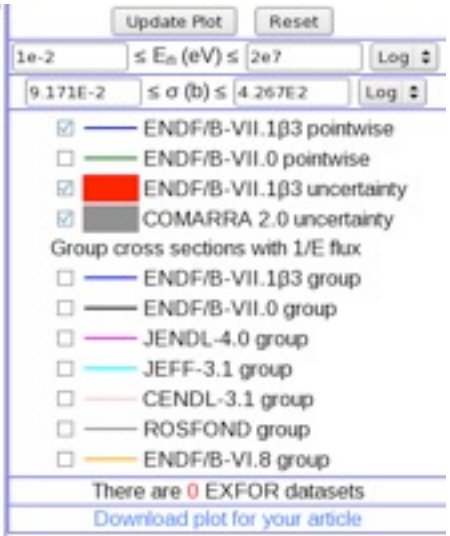
Quality Assurance

- Web-based Sigma-QA allows visual and 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,γ)<2%, etc.
  - non-positive-definite matrices
  - PFNS covariance not summing to zero

Web based QA system

Differential uncertainties 53-Cr(n,el)





Acceptable agreement between COMMARA-2.0 and ENDF/B-VII.1b3

Summary of total expenditures (LANL)

ID #	Item/Activity	Baseline Total Cost (AY$)	Costed & Committed (AY$)	Estimate To Complete (AY$)	Estimated Total Cost (AY$)
1	Prompt Fission Neutron Spectrum (PFNS) Covariance Evaluations	**188K**	**140K**	**48K**	**188K**
1.1	Method and code developments	50K	50K	0	50K
1.2	PFNS covariance evaluations for a suite of actinides	138K	90K	48K	138K
2	R-matrix covariance evaluations for light nuclei	**208K**	**110K**	**98K**	**208K**
2.1	O-16 Evaluation	30K	30K	0	30K
2.2	He-4 Evaluation	50K	50K	0	50K
2.3	Others (TBD)	128K	30K	98K	128K
3	Covariance evaluations for actinides	**458K**	**180K**	**278K**	**458K**
3.1	Pu-238, Pu-240, Pu-241 fission	50K	50K	0	50K
3.2	Am isotopes	50K	50K	0	50K
3.3	Others (TBD)	358K	80K	278K	358K
4	Quality Assurance tests of evaluated covariance evaluations + NJOY improvements	**146K**	**50K**	**96K**	**146K**
4.1	Identify suite of critical assemblies	20K	15K	5K	20K
4.2	Propagate uncertainties in transport simulations	76K	10K	66K	76K
4.3	NJOY improvements	50K	25K	20K	50K
Totals:		**1,000K**	**480K**	**520K**	**1,000K**

Summary of total expenditures (BNL)

WBS or ID #	Item/Activity	Baseline Total Cost (AY$)	Costed & Committed (AY$)	Estimate To Complete (AY$)	Estimated Total Cost (AY$)
1	Development of improved covariance module in EMPIRE	160K	160K	0	160K
2	Development of covariance quality assurance procedures	130K	140K	20K	160K
3	Production of covariances for priority materials	420K	410K	10K	420K
4	Production of covariances for materials of lower priority	390K	40K	350K	390K
5	QA of covariances	170K	20K	150K	170K
6	Assembly and release of ENDF/B-VII.1 library	100K	60K	40K	100K
Totals:		**1,400K**	**830K**	**570K**	**1,400K**

Summary of expenditures by FY (BNL)

BNL	FY 2010	FY 2011	FY 2012
a) Funds allocated	$450K	$574K	$350K
b) Costs accrued	$476K	$468K	0
c) Uncosted commitments	0	0	0
d) Uncommitted funds (d=a-b-c)	-$26K	$106K	$350K

LANL	FY 2010	FY 2011	FY 2012
a) Funds allocated			
b) Costs accrued	$290K	$190K	
c) Uncosted commitments	0	0	0
d) Uncommitted funds (d=a-b-c)			

Training of new staff

- Newly trained evaluators:
  - Marco Pigni (currently at ORNL)
  - Caleb Mattoon (currently at LLNL)
  - Samuel Hoblit (BNL)
- New evaluators being trained:
  - Gustavo Nobre (postdoc, BNL)
  - Annalia Palumbo (postdoc, BNL)

Summary

- Covariance methodology advanced
  - kernel approximation
  - role of correlations
  - resonance module in EMPIRE
  - coupling of Kalman filter to GANSH and EMPIRE
  - marginalization technique (systematic uncertainties and model defects)
  - covariances for PFNS
- QA procedures established and made available
- Covariance evaluations prepared for 110 materials
  - ENDF/B-VII.1β3 released May 24 - covariances for 186 materials (including 110 ANS&T supported)

Summary

- Covariance evaluations prepared for 110 materials
  - ENDF/B-VII.1β3 released May 24 - covariances for 186 materials (including 110 ANS&T supported)
  - QA currently being performed
  - ENDF/B-VII.1β4 to be released in September
  - ENDF/B-VII.1 to be released in December after QA
- Two extensive papers (BNL & LANL) being prepared for Nuclear Data Sheets (to be published in Dec. 2011)

Project is proceeding according to the schedule

Are we done yet?

- **Great Milestone: COMMARA-2.0**
  - First science-based covariance library for application
- **UQ Evaluations in ENDF/B-VII.1… First Generation**

- **How do we go beyond?**
  - Develop better Data Assimilation tools
  - Develop better Experimental Covariance Matrices
  - Move toward more physical and predictive models (with really physical model parameters)
  - Include cross-correlations among isotopes, reactions, experiments
  - Propagate all uncertainties in complicated transport simulations