Calculations of Nuclear Astrophysics and Californium Neutron Cross Section Uncertainties using ENDF/B-VII.1, JEFF-3.1.2, JENDL-4.0 and Low-Fidelity Covariances

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s-process

- Slow neutron capture takes place in Red Giants and AGB stars, where neutron temperature (*kT*) varies from 8 to 90 keV.
- The capture time of the *s*-process is ~1 year.
- ENDF/B-VII.0 release.

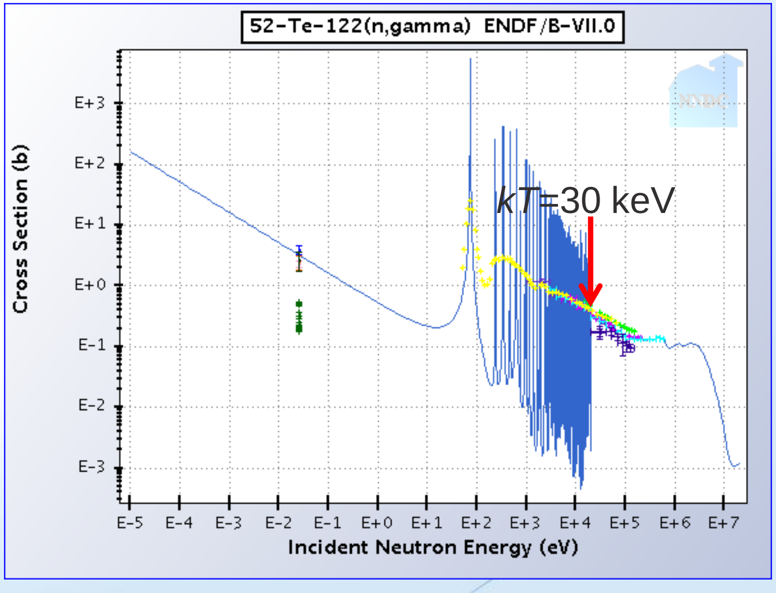
Maxwelian-averaged Cross Sections

- *s*-process nucleosynthesis Maxwellian-averaged cross sections (MACS) can be expressed as

$$\sigma^{Maxw}(kT) = \frac{2}{\sqrt{\pi}} \frac{(m_1/(m_1+m_2))^2}{(kT)^2} \int_0^\infty \sigma(E_n^L) E_n^L \exp(-\frac{aE_n^L}{kT}) dE_n^L$$

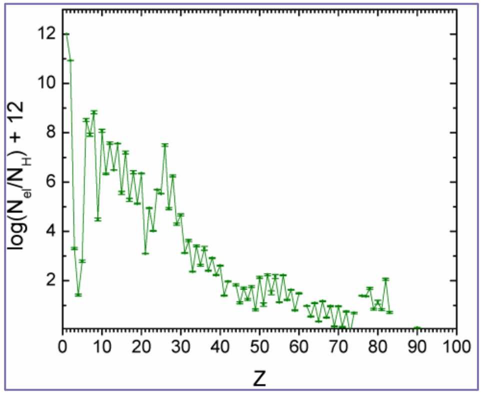
where k and T are the Boltzmann constant and temperature of the system.

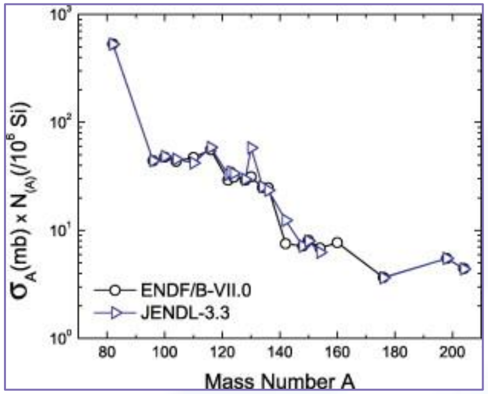
- Commonly accepted: kT = 30 keV.

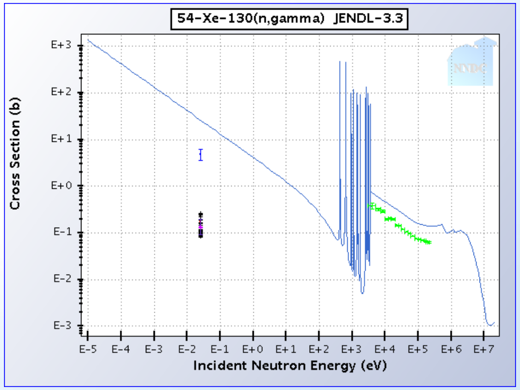


Stellar Nucleosynthesis

- Solar system abundances.
- $\sigma_A N_{(A)} = \sigma_{A\text{-}1} N_{(A\text{-}1)} = constant.$
- B. Pritychenko et *al*., ADNDT **96**, 645 (2010).

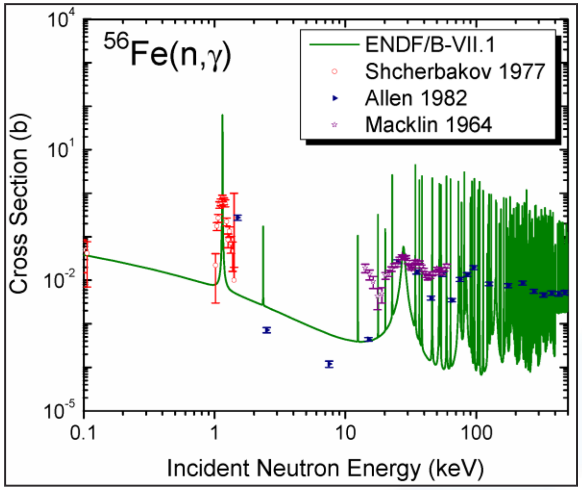




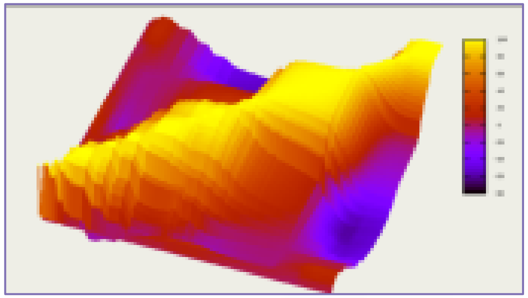


Evaluated Nuclear Data File (ENDF)

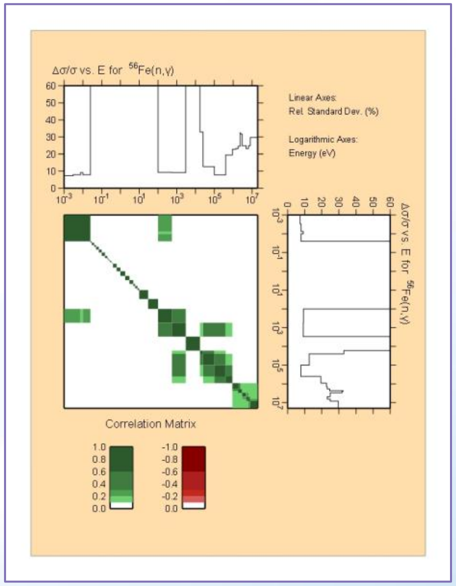
- First nuclear database in direct response to nuclear industry data needs: theory + experiment (resonance parameters).
- 423 neutron materials (isotopes) in ENDF/B-VII.1.



Nuclear Data Covariances

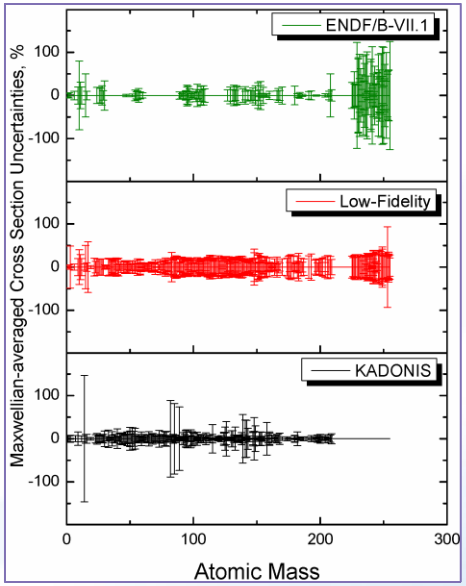


- Wikipedia: In probability theory and statistics, covariance is a measure how two random variables change together.
- Nuclear data covariance plots are very beautiful.
- What are physics implications of nuclear data covariances???
- Cross section uncertainties can be extracted using the error propagation formalism.



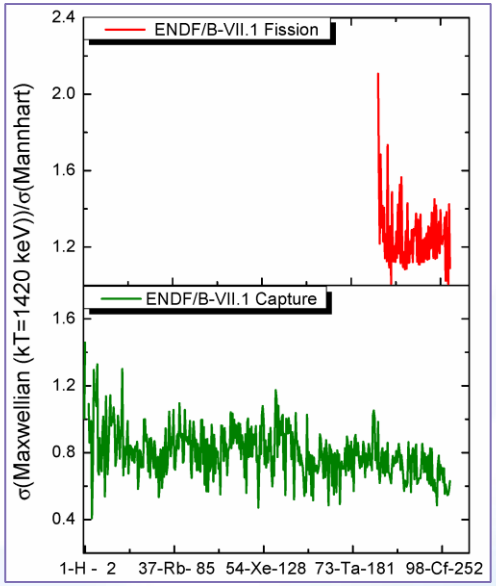
Maxwellian-Averaged Cross Section Uncertainties

- Further interactions with the fundamental and applied science communities have initiated work on the extended list of integral values and their uncertainties.
- Maxwellian-averaged neutron capture cross section, *kT*=30 keV, uncertainties for ENDF/B-VII.1 library, Low-Fidelity project and KADoNiS database.
- B. Pritychenko & S.F. Mughabghab, NDS 113, 3120 (2012).



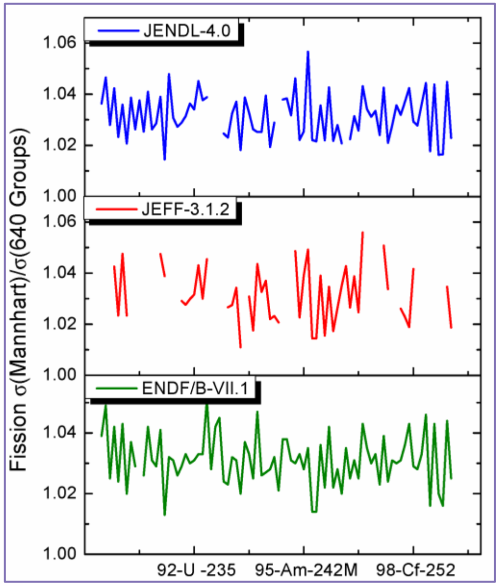
^{252}Cf Spectrum Neutron Cross Sections

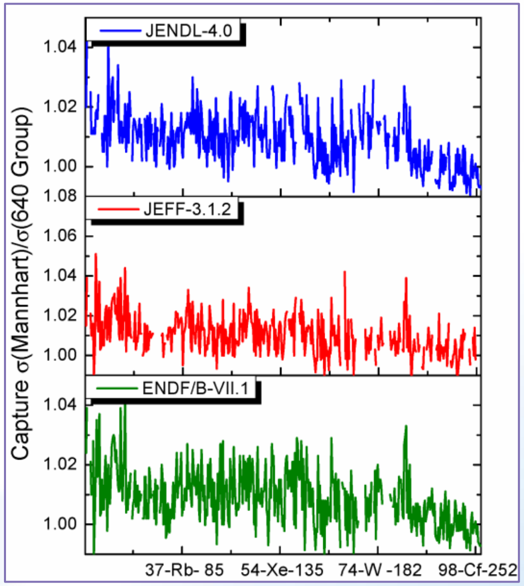
- We have to extend the scope to the MeV region using ^{252}Cf spectrum.
- The ratio of calculated ENDF/B-VII.1 californium spectrum neutron cross sections using Maxwellian, kT=1420 keV, and Mannhart spectra.
- Mannhart spectra should be used instead of Maxwellian.



^{252}Cf Spectrum Neutron Cross Sections

- Presently, the original and 640-group representations of Mannhart evaluation are frequently considered.
- Doppler-broadened linear files at T=293.6 K result in slightly different cross section values.





^{252}Cf Spectrum Neutron Cross Section and their Uncertainties

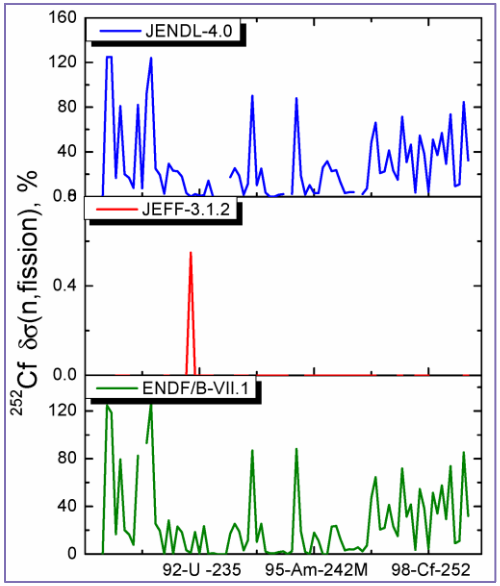
- Following the nuclear dosimetry example, ^{252}Cf spectrum, cross sections for major evaluated libraries: ENDF/B-VII.1, JEFF-3.1.2, and JENDL-4.0 have been produced using the 640-group format.
- These values are in agreement with CIELO: M.B. Chadwick et *al*., NDS **118**, 1 (2014) and EXFOR data.

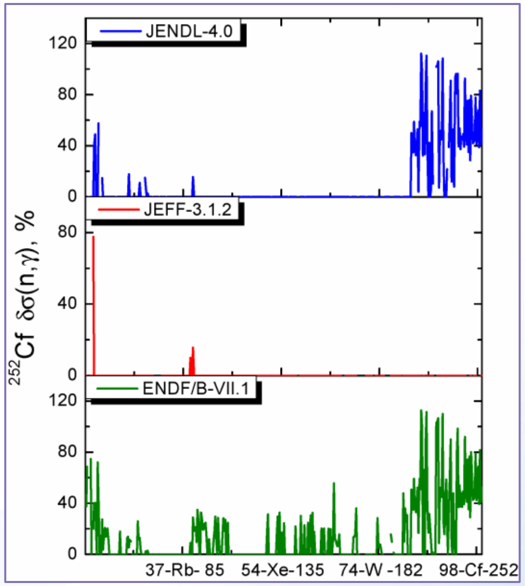
TABLE I: 640-group californium spectrum neutron fission cross sections for ENDF, JEFF, and JENDL major evaluated libraries, and EXFOR (experimental nuclear reaction) data (kT~1.42 MeV) [2, 11-13].

Material	ENDF/B-VII.1 (barns)	JEFF-3.1.2 (barns)	JENDL-4.0 (barns)	EXFOR (barns)
88-Ra-223	5.485E-2±8.293E-4	5.485E-2±8.293E-4	5.485E-2±8.293E-4	
88-Ra-224				
88-Ra-225				
88-Ra-226	3.741E-4±5.990E-6	3.741E-4±5.990E-6	3.740E-4±5.988E-6	
89-Ac-225	3.505E-2±4.369E-2		3.503E-2±4.379E-2	
89-Ac-226	3.478E-2±4.126E-2		3.472E-2±4.337E-2	
89-Ac-227	1.253E-2±2.089E-3	1.316E-2±1.755E-4	1.252E-2±2.082E-3	
90-Th-227	2.968E-1±2.358E-1	4.747E-1±7.820E-3	2.966E-1±2.402E-1	
90-Th-228	3.768E-1±7.536E-2	1.073E-1±1.443E-3	3.757E-1±7.561E-2	
90-Th-229	3.433E-1±5.660E-2	4.747E-1±7.819E-3	3.431E-1±5.780E-2	
90-Th-230	2.044E-1±1.592E-2		2.042E-1±1.594E-2	
90-Th-231	1.977E-1±1.630E-1		1.977E-1±1.623E-1	
90-Th-232	7.582E-2±1.824E-3		8.170E-2±6.032E-3	8.470E-2±4.900E-3
90-Th-233	9.916E-2±9.237E-2	1.084E-1±1.850E-3	9.918E-2±9.174E-2	
90-Th-234	3.542E-2±4.487E-2		3.541E-2±4.396E-2	
91-Pa-229	1.939E+0±4.916E-1		1.938E+0±4.862E-1	
91-Pa-230	1.782E+0±3.484E-1		1.781E+0±3.463E-1	
91-Pa-231	7.667E-1±1.031E-2	9.843E-1±1.330E-2	8.442E-1±2.385E-2	9.700E-1±4.500E-2
91-Pa-232	9.581E-1±2.711E-1	1.082E+0±1.739E-2	9.572E-1±2.804E-1	
91-Pa-233	2.384E-1±3.065E-3		2.463E-1±5.697E-2	
92-U -230	2.377E+0±5.504E-1		2.375E+0±5.416E-1	
92-U -231	2.162E+0±3.938E-1		2.161E+0±3.900E-1	
92-U -232	2.038E+0±6.916E-2	2.442E+0±3.590E-2	2.038E+0±6.916E-2	
92-U -233	1.867E+0±3.478E-2	1.883E+0±3.130E-2	1.879E+0±2.949E-2	1.947E+0±3.100E-2
92-U -234	1.186E+0±2.199E-1	1.171E+0±1.591E-2	1.211E+0±3.167E-2	
92-U -235	1.209E+0±2.000E-2	1.203E+0±1.913E-2	1.202E+0±2.162E-2	1.266E+0±1.823E-2
92-U -236	5.873E-1±1.371E-1	6.059E-1±7.922E-3	5.801E-1±9.429E-3	
92-U -237	6.320E-1±9.515E-3	8.719E-1±1.339E-2	5.874E-1±8.340E-2	
92-U -238	3.117E-1±4.753E-3	3.102E-1±4.006E-3	3.094E-1±4.815E-3	3.109E-1±1.400E-2
92-U -239	3.730E-1±5.929E-3			
92-U -240	1.953E-1±2.549E-3			
92-U -241	1.881E-1±2.812E-3			
93-Np-234	2.436E+0±4.196E-1		2.436E+0±4.243E-1	
93-Np-235	2.173E+0±5.521E-1	1.878E+0±2.709E-2	2.173E+0±5.495E-1	
93-Np-236	2.062E+0±3.925E-1	1.891E+0±2.975E-2	2.062E+0±3.888E-1	
93-Np-237	1.339E+0±4.624E-2	1.313E+0±1.773E-2	1.322E+0±2.803E-2	1.442E+0±2.300E-2
93-Np-238	1.431E+0±1.659E-1	1.453E+0±2.560E-2	1.430E+0±1.645E-1	
93-Np-239	5.923E-1±5.151E-1		5.916E-1±5.341E-1	
94-Pu-236	2.324E+0±2.389E-1	2.075E+0±3.180E-2	2.324E+0±2.390E-1	
94-Pu-237	2.399E+0±6.080E-1	2.954E+0±4.526E-2	2.400E+0±6.024E-1	
94-Pu-238	1.925E+0±4.890E-2	1.973E+0±2.816E-2	1.944E+0±7.337E-2	
94-Pu-239	1.774E+0±2.865E-2	1.774E+0±2.653E-2	1.777E+0±2.654E-2	1.947E+0±3.100E-2

^{252}Cf Cross Section Uncertainties Analysis

- The ENDF, JEFF, and JENDL calculated californium spectrum neutron fission and capture cross section uncertainties using the 640-group Mannhart spectrum.





ENDF/B-VII.1 Maxwellian and ^{252}Cf Cross Section Uncertainties

- The summary of reanalysis of the previous Maxwellian data (*kT*=30 keV) and analysis of the current Mannhart spectrum uncertainties for ENDF/B-VII.1 library.

TABLE II. The summary of the ENDF/B-VII.1 library cross section uncertainties analysis.

Reaction	Maxwellian spectrum, kT=30 keV		Mannhart spectrum [10]	
	Uncertainty <1%	Uncertainty >100%	Uncertainty <1%	Uncertainty >100%
(n,fission)	^{235}U, ^{239,240}Pu	^{225,226}Ac, ^{233}Th, ^{229}Pa, ^{235}Np, ^{246}Pu, ^{250}Cm, ^{247,250}Bk, ^{246,248,250,254}Cf, ^{251,253,255}Es	^{235,238}U, ^{239,240}Pu	^{225,226}Ac, ^{234}Th
(n,γ)		^{229}Pa, ^{237}Pu, ^{249}Cm, ^{250}Bk, ^{255}Fm	^{52}Cr	^{229}Pa, ^{231}U, ^{234,235,236}Np, ^{237}Pu

Cross Section Uncertainties Recommendations

- Absolute cross section values for linearized files are sensitive to the changes of Mannhart evaluation group structure. Calculated values are model dependent and may vary within 1-5%.
- Nuclear astrophysics and energy applications require covariances for all ENDF materials.
- Realistic covariances are needed:
  - Covariance matrices that result in >100% cross section uncertainties should be avoided, such large uncertainties are not very useful for application development.
  - Covariance matrices that result in <1% cross section uncertainties are not realistic; strong contradiction with the best experiments.
  - Presently, covariance matrices produce wide variations of cross section uncertainties within 0.5-120% range. This spread should be kept within 3-50% range.
- Multiple MF=33 covariance matrices can be confusing.

CIELO/EXFOR Cooperation

- NRDC 2014 Meeting, May 6-9, 2014.
- What EXFOR community can do for CIELO and covariances ???
- How both communities can interact ???

Conclusion & Outlook

- Covariances are important for application development.
- Maxwellian-averaged cross section uncertainties have been re-analyzed.
- ^{252}Cf cross sections and their uncertainties have been calculated.
- ^{252}Cf cross section uncertainties have been analyzed.
- Recommendations for covariances have been produced using the application development requirements.
- Further work may needed a stronger interaction with EXFOR and experimental communities.

s-process in Tellurium

- $\sigma_A N_{(A)} = \sigma_A N_{(A)}$ product ratios for neutron capture in $^{122,123,124}Te$ isotopes, B. Pritychenko et *al*., ADNDT **96**, 645 (2010).

Data source	Ratio of $^{122,123,124}Te$ products
ENDF/B-VII.0	0.943:1.119:1
JENDL-3.3	0.972:1.035:1
Atlas of Neutron Resonances	0.985 ± 0.0352:0.994 ± 0.0364:1
Classical model, Wisshak et al.	0.984 ± 0.012:1.003 ± 0.012:1
Low mass stars, Wisshak et al.	0.91 ± 0.01:0.94 ± 0.01:1
Bao et al.	1.031 ± 0.0105:1.003 ± 0.0097:1