PROGRESS REPORT OF CENDL PROJECT 2016-2017

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OUTLINE

I. Situation of CENDL Project

II. Covariance Evaluation of CENDL 3.2β0

III. Benchmark Testing of CENDL 3.2β0

IV. Other Information Related to CENDL Project

Ⅰ. Situation of CENDL Project

A view of the CENDL Project

CENDL Project contains following aspects:

1) Nuclear data evaluation activities and nuclear data , and the main output is CENDL library.
2) Nuclear data measurements, which provided some important experimental information for the nuclear data evaluation of CENDL library, are performed by Chinese scholars with experimental facilities in China and oversea. (Prof. Ruan' s report)
3) Methodology studies of data measurement, evaluation, theory, processing and benchmark/testing etc.
4) Provide proposals(capability building, research plan) for government base on the requirements of nuclear data from Chinese users, and according the development tendency of nuclear data technology in the world.
5) Coordinate the nuclear data activities in China (Nuclear Data Coordination Network-CNDCN and more than 10 institutions and universities are involved.).

Progress of CENDL-3.2b0

CENDL-3.2b0 will be the updated library as the main fruit of the CENDL project recent years.

Various kinds of nuclear data are involved in CENDL library, which mainly include the complete set of neutron data, activation data, decay data, fission yield data files.

Therefore, the massive activities are carried out and going on to develop our methodologies of nuclear data evaluation to fulfill the mission, including microscopic nuclear model, covariance evaluation scheme, theory of fission product… …

Nucl.	*Content of Nuclei in CENDL-3.2b0 （250）*
Light Elements	$^{1-3}$H, ^{3,4}He, ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12}C, ^{14}N, ^{16}O, ^{19}F
Structural Materials	^{23}Na, $^{24-26}$Mg, ^{27}Al, $^{28-30}$Si, ^{31}P, ^{32,33,34,36}S, ^{0}Cl, ^{0}K, ^{40}Ca, $^{46-50}$Ti, ^{0}V, $^{50,52-54}$Cr, ^{55}Mn, $^{54,56-58}$Fe, ^{59}Co, $^{58,60-62,64}$Ni, ^{0,63,65}Cu, ^{0}Zn, ^{0}Ge, $^{90-92,94,96}$Zr, $^{92,94-98,100}$Mo, ^{0,107,109}Ag, ^{0}Cd, ^{0}Sn, $^{174,176-180}$Hf, ^{181}Ta, ^{180,182,183,184,186}W, ^{197}Au, ^{0}Hg, ^{0}Tl, $^{204,206-208}$Pb, ^{209}Bi
Fission Products & Medium Elements	^{69,71}Ga, $^{70-78}$Ge, ^{75,77,79}As, ^{83,84,85,86,87}Kr, ^{85,87}Rb, $^{88-90}$Sr, ^{89,91}Y, ^{93,95}Zr ^{93,95}Nb, ^{99}Tc, $^{99-105}$Ru, ^{103,105}Rh, ^{105,108}Pd, ^{113}Cd, ^{113,115}In, $^{112,114-120,122,124}$Sn, ^{121,123,125}Sb, ^{130}Te, ^{127,129,135}I $^{123,124,129,131,132,133,134-136}$Xe, $^{133-135,137}$Cs, $^{130,132,134-138}$Ba, ^{139}La $^{136,138,140-142,144}$Ce, ^{141}Pr, $^{142-148,150}$Nd, ^{147,148,148m,149}Pm $^{144,147-152,154}$Sm, $^{151,153-155}$Eu, $^{152,153,154-158,160}$Gd, ^{164}Dy
Actinides	^{232}Th, $^{232-240,241}$U, $^{236-239}$Np, $^{236-246}$Pu, $^{240-244,242m}$Am, ^{249}Bk, ^{249}Cf

Nucl.	New evaluated and updated nuclei in CENDL-3.2b0 (57)	
Light Elements	^{1}H, ^{6,7}Li	3
Structural Materials	^{23}Na, ^{32,33,34,36}S, ^{27}Al, ^{40}Ca, ^{56}Fe, ^{58}Ni, ^{181}Ta, ^{180,182,183,184,186}W	15
Fission Products	^{87,88}Kr, ^{93}Nb, ^{125}Sb, ^{123,124,129,131,133,134,135}Xe, ^{140,141,142}Ce, ^{152,153,154,155,156,157,158,160}Gd	22
Actinides	^{232}Th, ^{233,235,236,237,239,240}U, ^{236,237,238,239}Np, ^{237,238,241}Pu, ^{241}Am	15

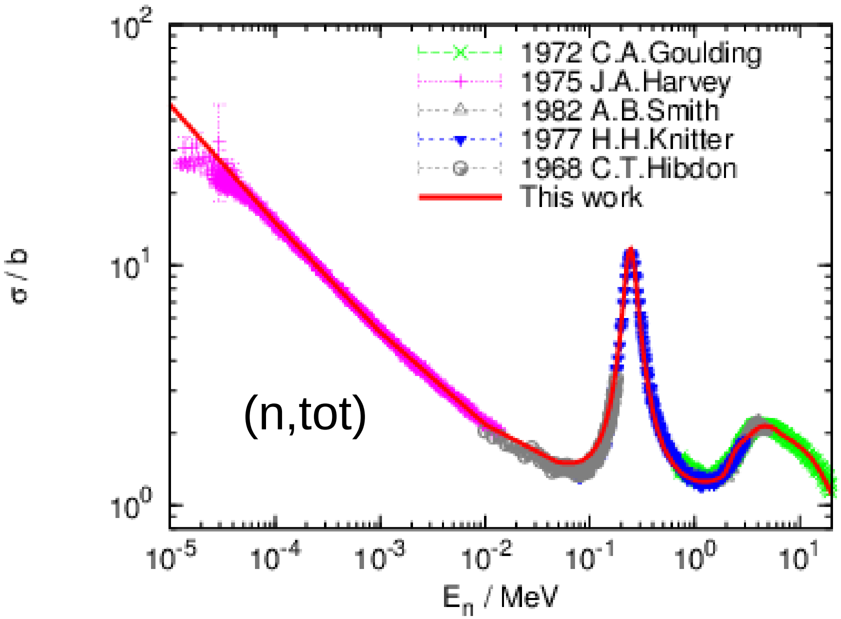
1、The total materials of CENDL3.2b0 is 250 (240 in CENDL3.1);

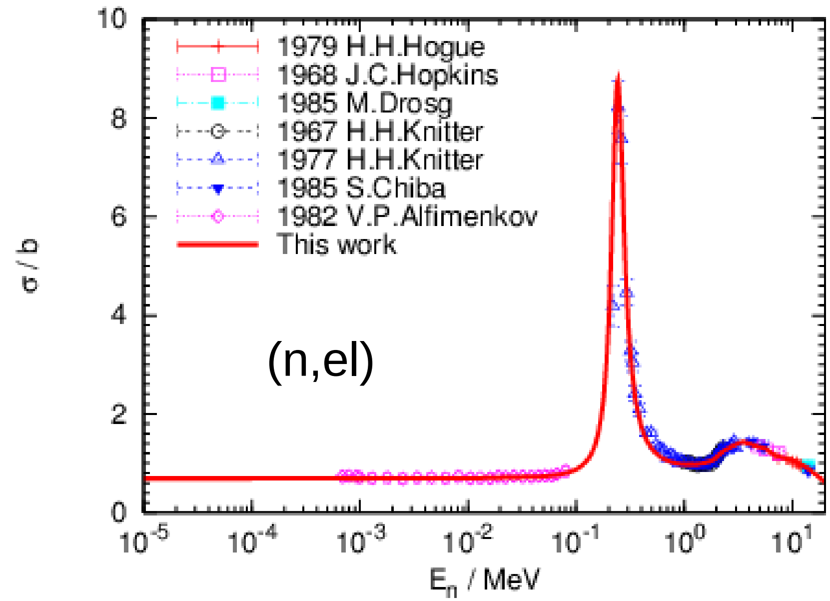
- 56 nuclides are newly evaluated and updated in CENDL3.2b0;
- 14 nuclides are new members in CENDL3.2b0;
- 42 nuclides are revised based on CENDL3.1;
- Covariance for 16 nuclides (^{2,3}H, ^{3}He, ^{19}F, ^{40}Ca, ^{48}Ti, ^{55}Mn, ^{63,65,0}Cu, ^{90,91,92,93,94,95,96}Zr, ^{180,182,183,184,186}W, ^{233,235}U) with high fidelity based on CENDL3.1

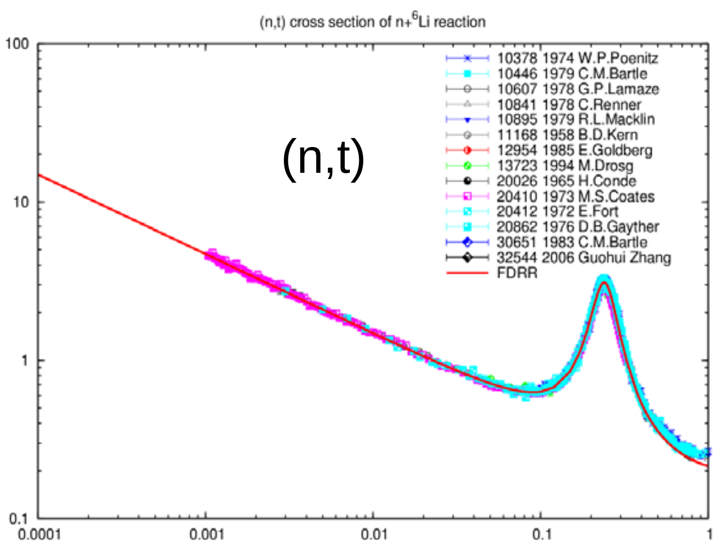
2、The incident neutron energy $E_n \leq 20$MeV;

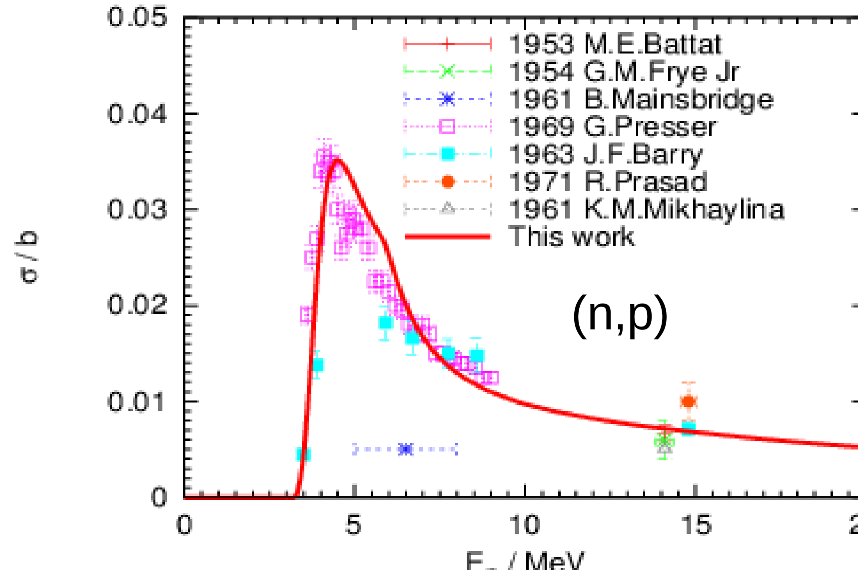
3、MF = 1, 3, 4, 5, 6, 12, 14, 15, 33.

1-Light Nuclei

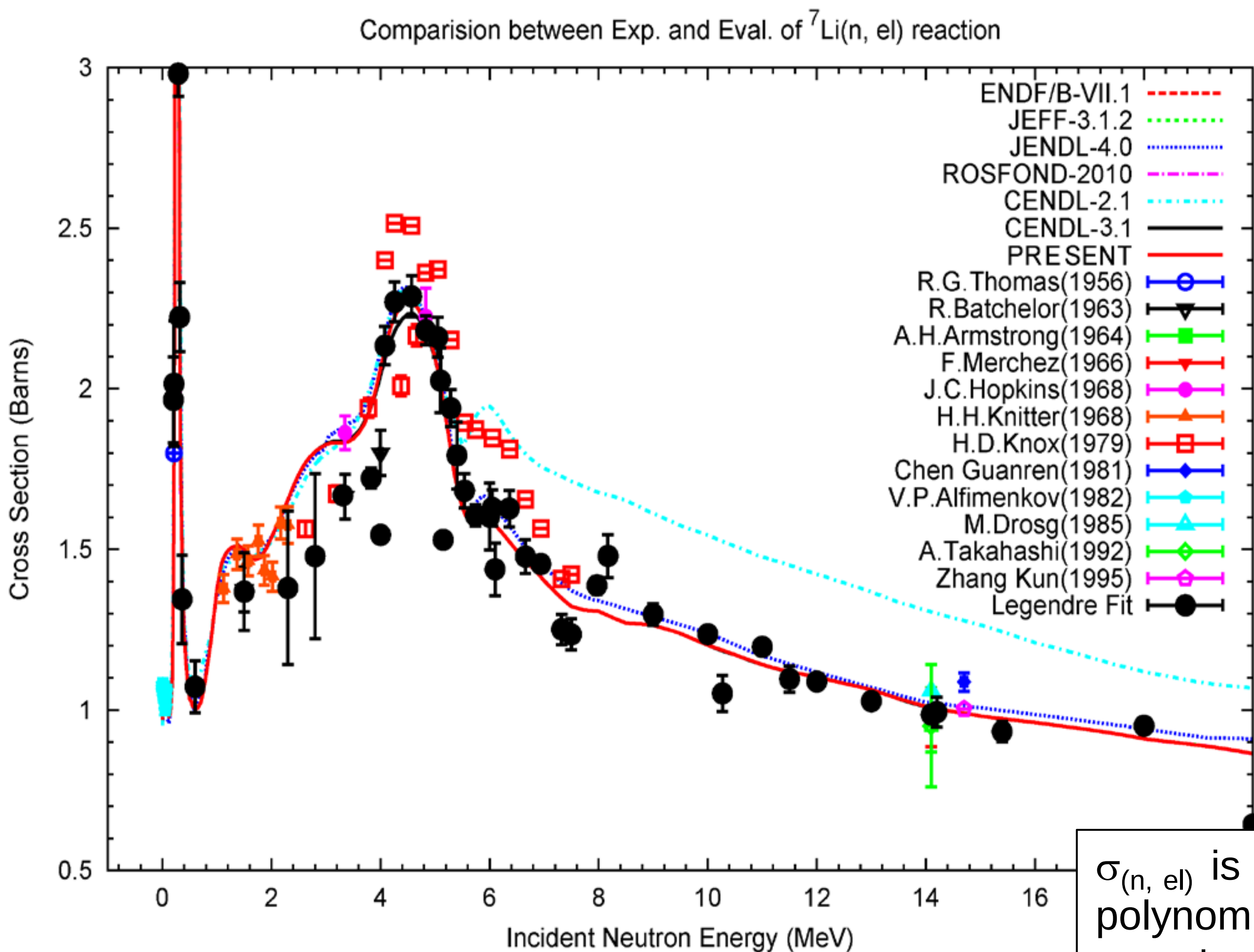








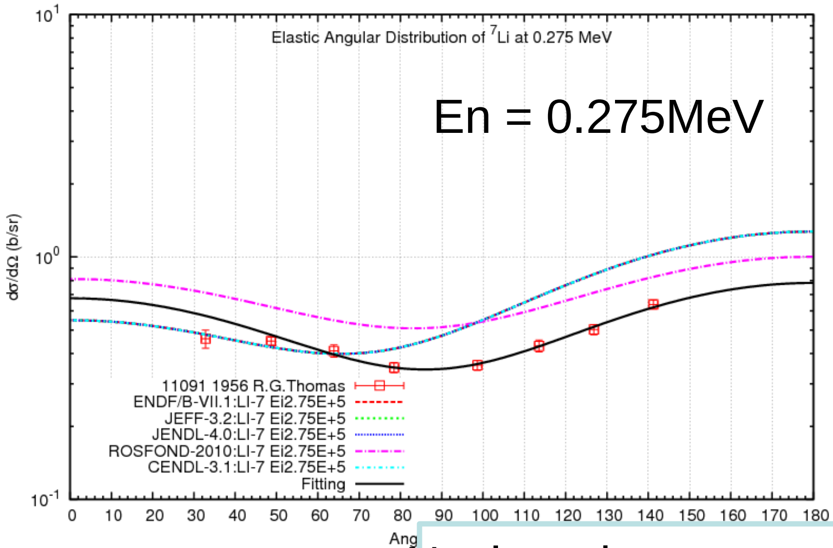
Experimental data evaluation are performed, and some reaction cross sections and angular distributions of neutron elastic scattering of $^{6,7}Li$ are updated.

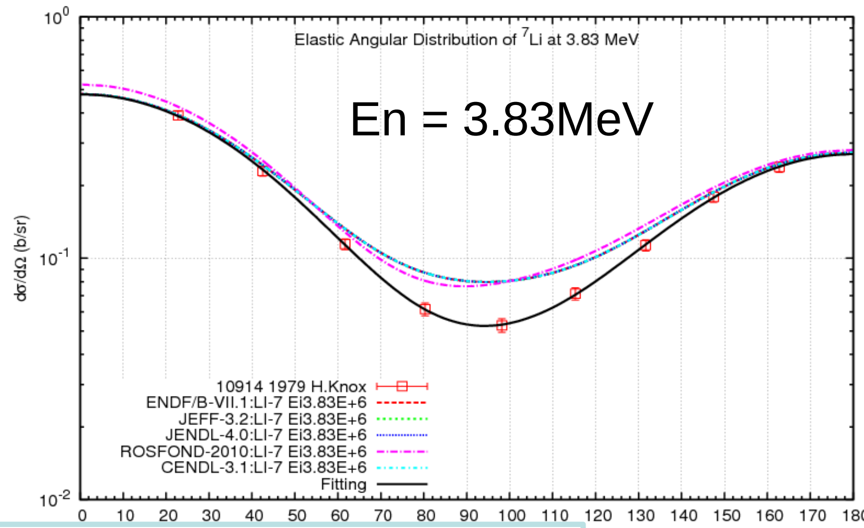


Channels	Q values
$\gamma+{}^{8}Li$	2.033
$n'+{}^{7}Li^{*}$	-0.4776
$d+{}^{6}He$	-7.750
$t+{}^{5}He$	-3.3362
$2n+{}^{6}Li$	-7.2490
$n,p+{}^{6}He$	-9.9740
$n,d+{}^{5}He$	-9.618
$n+t+\alpha$	-2.476
$2n,p+{}^{5}He$	-11.842
$2n+d+\alpha$	-8.724

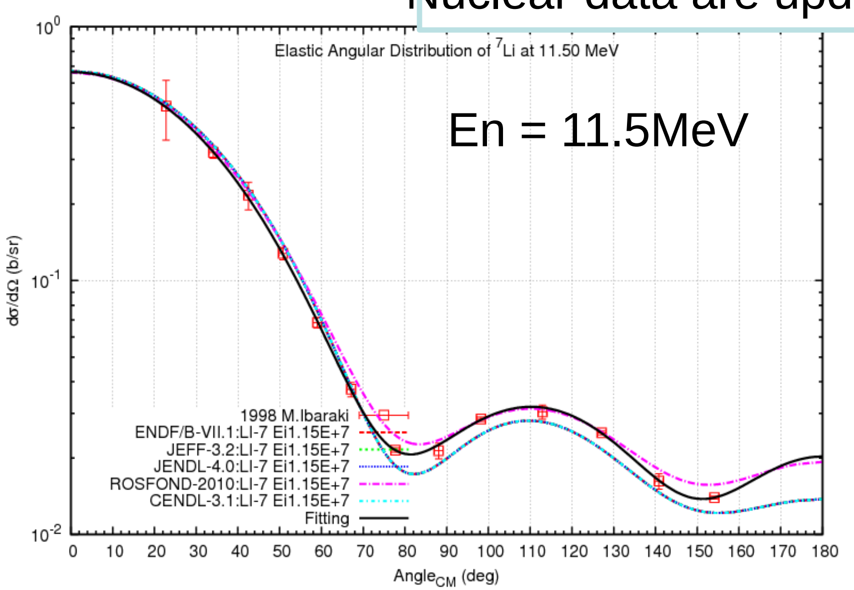
$\sigma_{(n,\ el)}$ is derived through Legendre polynomial function fitting to the experimental data of $d\sigma/d\omega$.

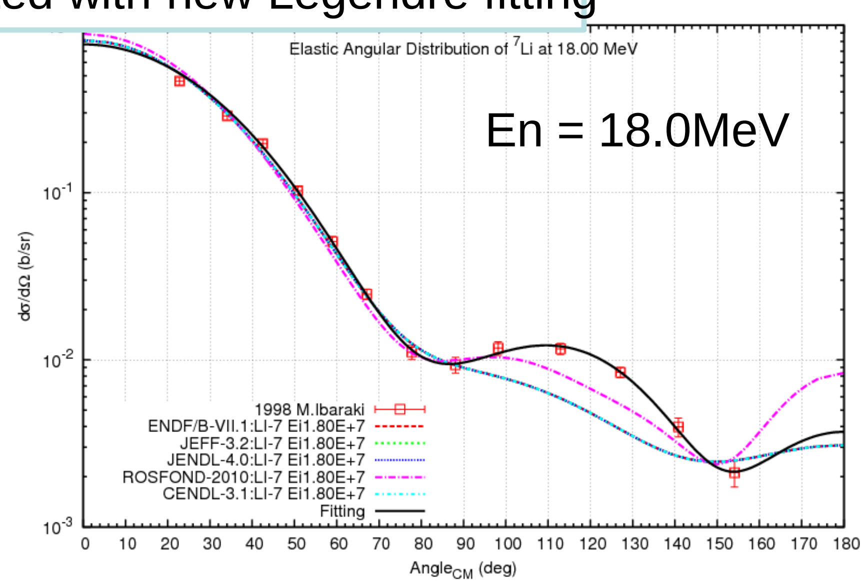
Angular distribution of elastic scattering of ^{7}Li

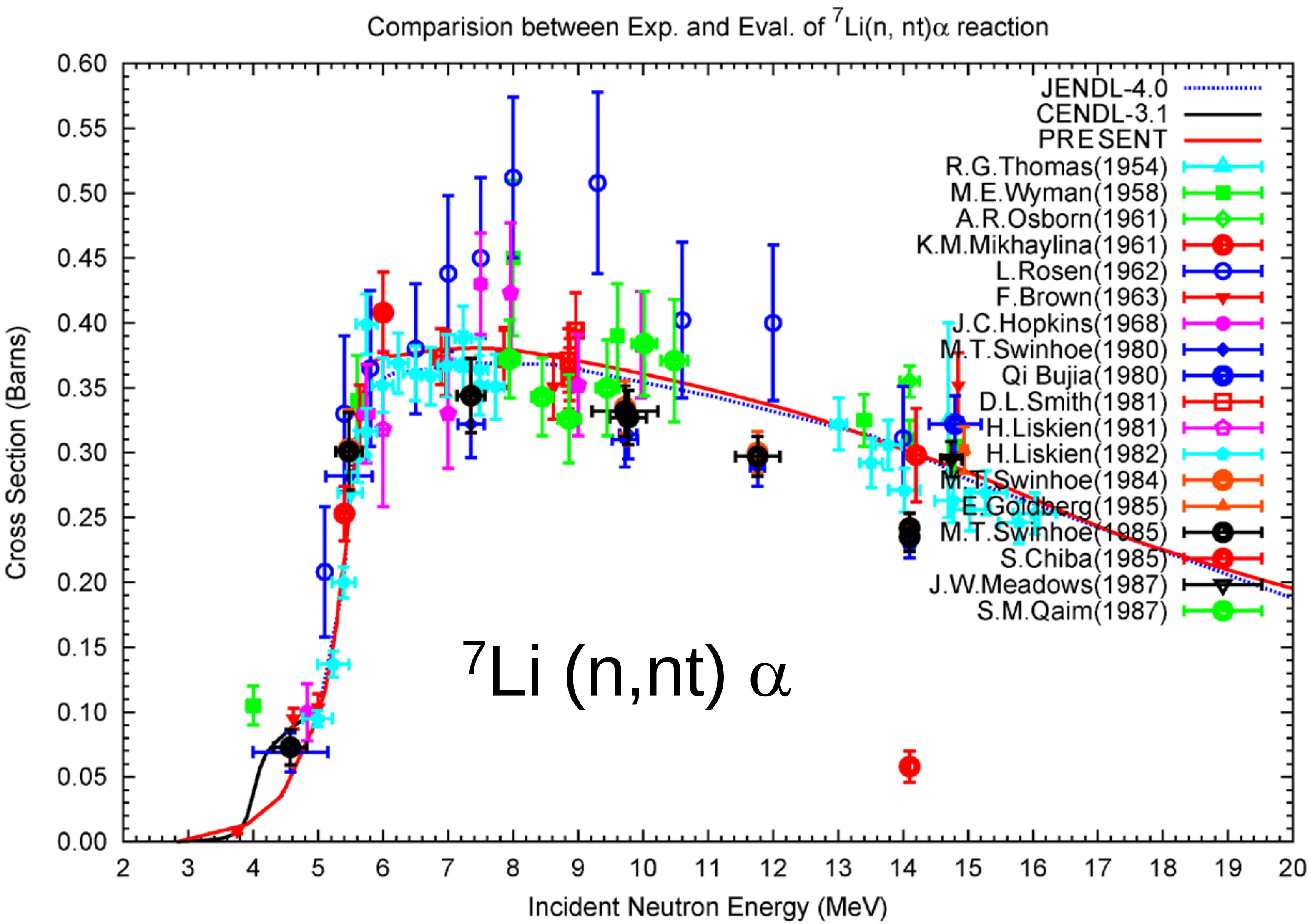




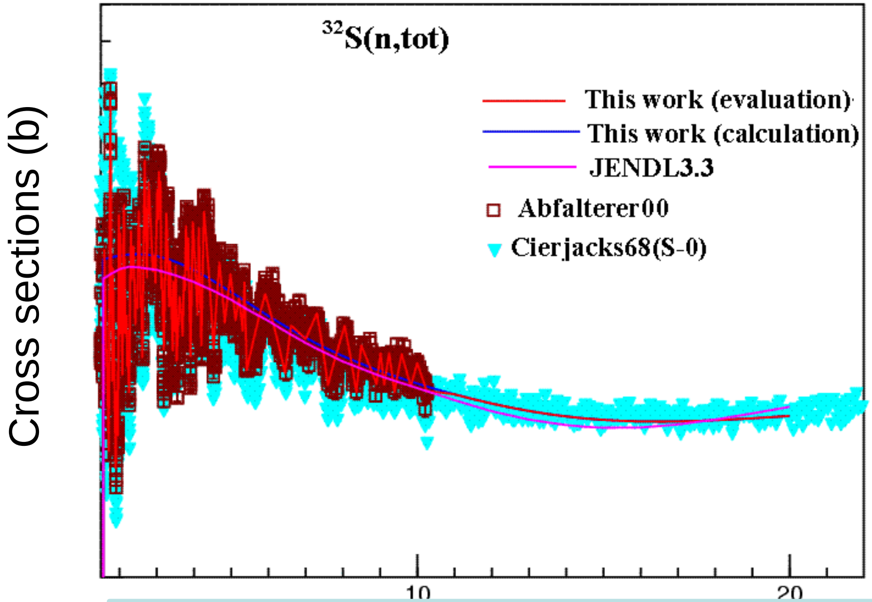
Nuclear data are updated with new Legendre fitting

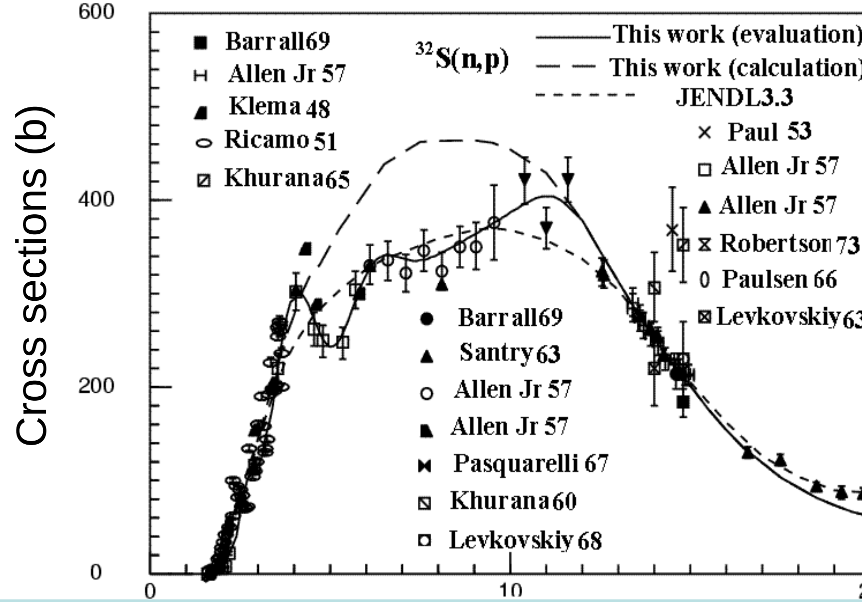




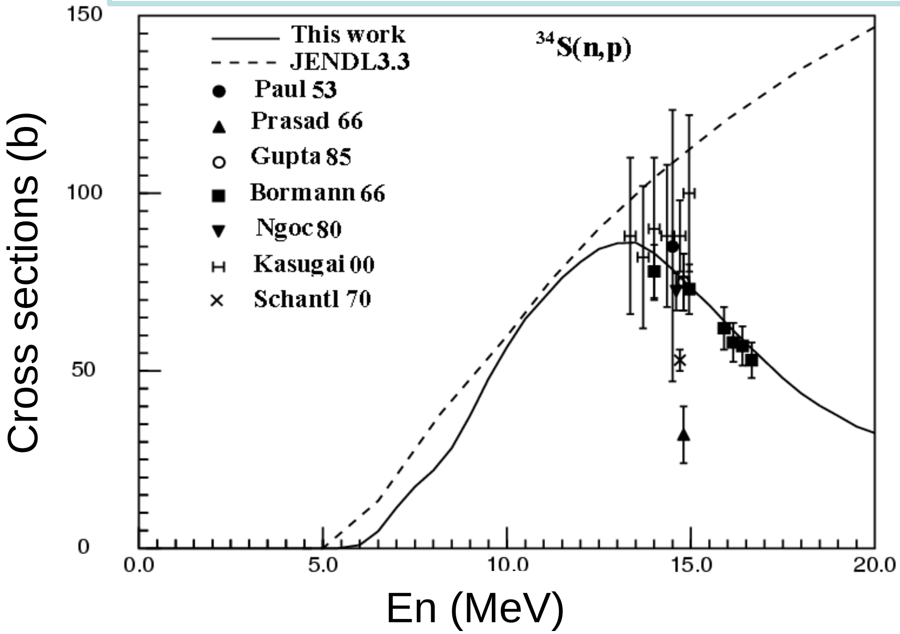

Comparision between Exp. and Eval. of 7Li(n, nt)α reaction
Cross Section (Barns)
Incident Neutron Energy (MeV)
JENDL-4.0
CENDL-3.1
PRESENT
R.G.Thomas(1954)
M.E.Wyman(1958)
A.R.Osborn(1961)
K.M.Mikhaylina(1961)
L.Rosen(1962)
F.Brown(1963)
J.C.Hopkins(1968)
M.T.Swinhoe(1980)
Qi Bujia(1980)
D.L.Smith(1981)
H.Liskien(1981)
H.Liskien(1982)
M.T.Swinhoe(1984)
E.Goldberg(1985)
M.T.Swinhoe(1985)
S.Chiba(1985)
J.W.Meadows(1987)
S.M.Qaim(1987)
7Li (n,nt) α

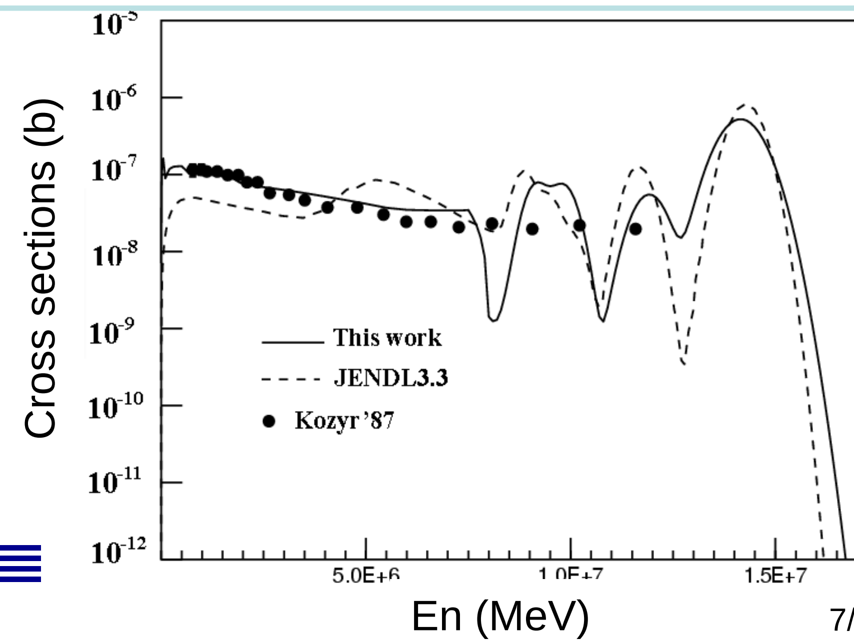
Structure Nuclei



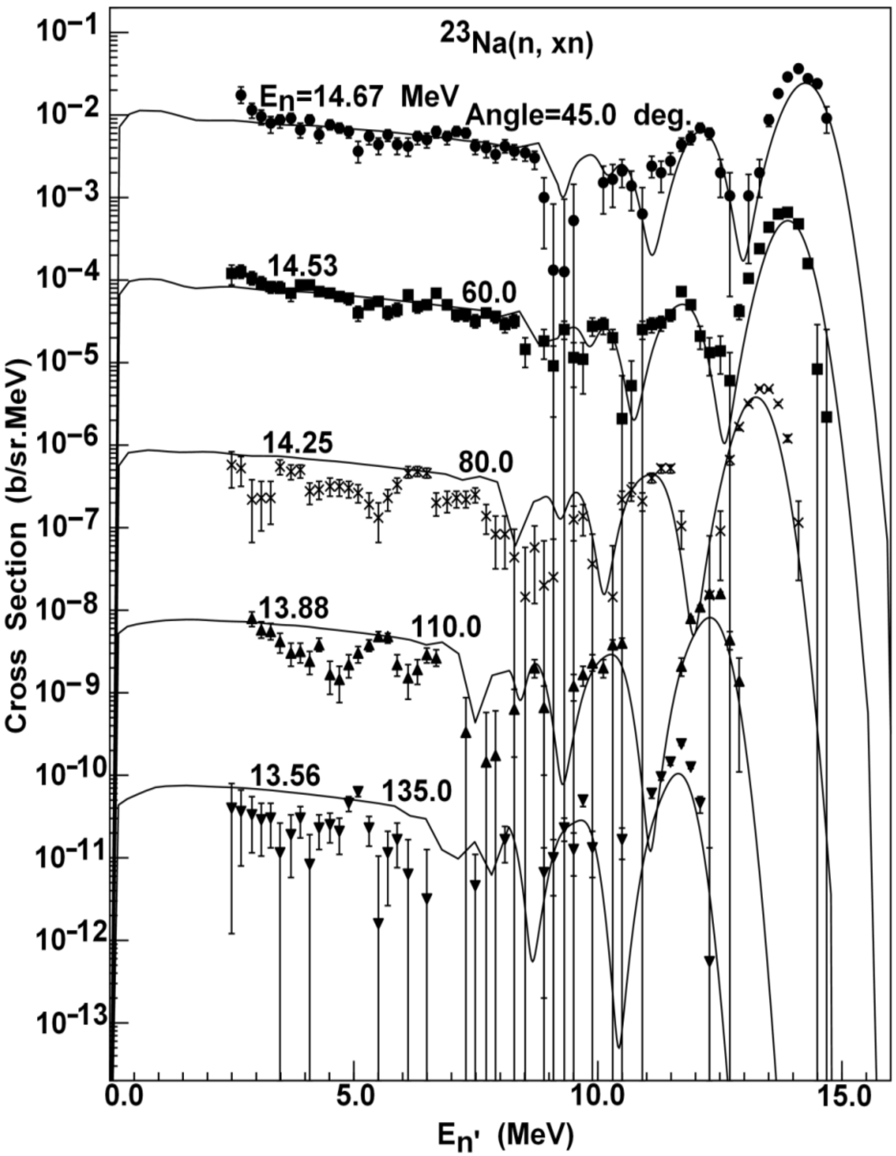


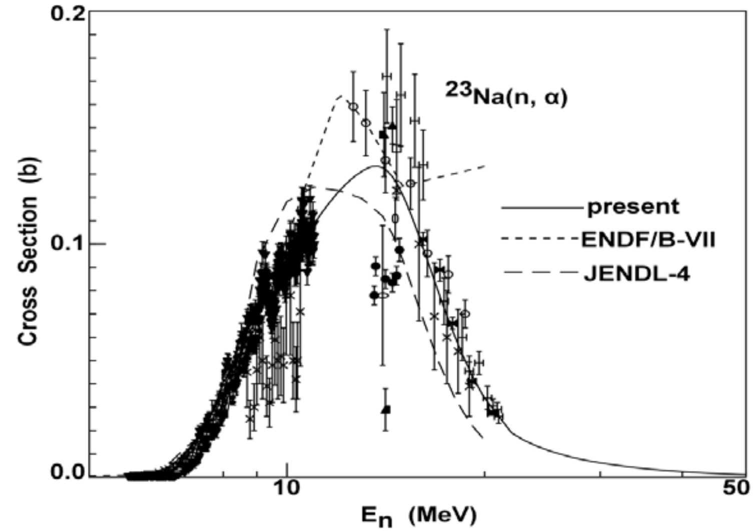
New evaluation and calculation for the isotopes of Sulfur

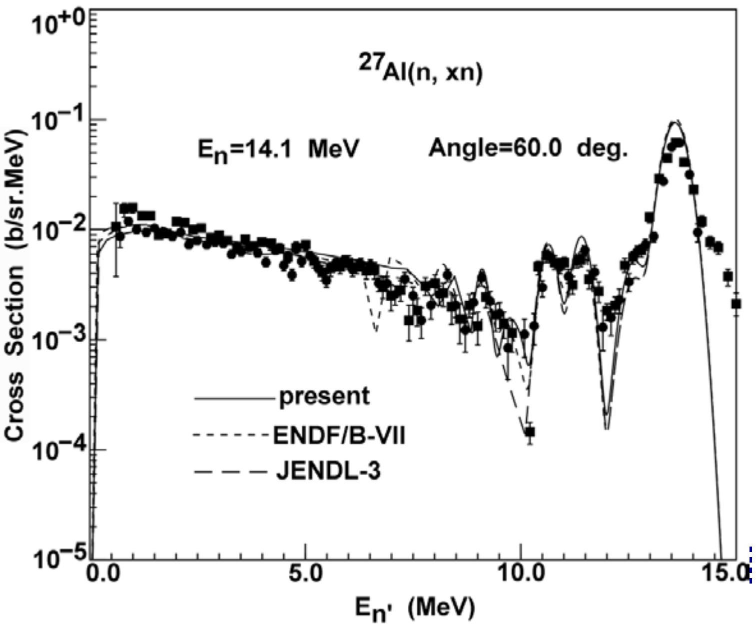




The nuclear data of ^{23}Na, ^{27}Al are obtained through theoretical calculation by UNF and the analysis to experimental data available.

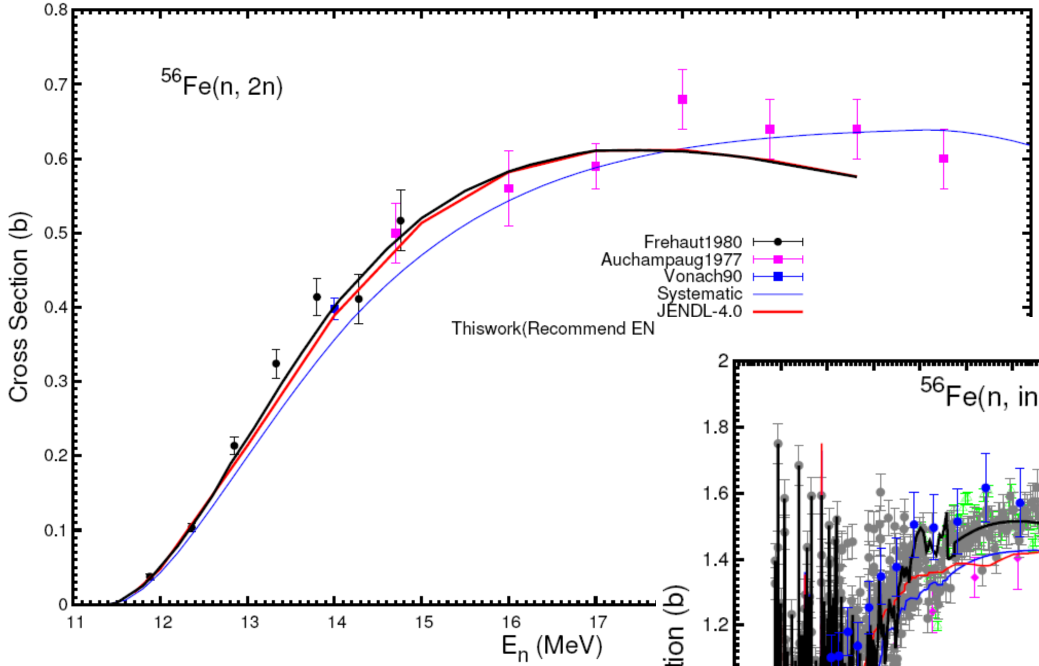


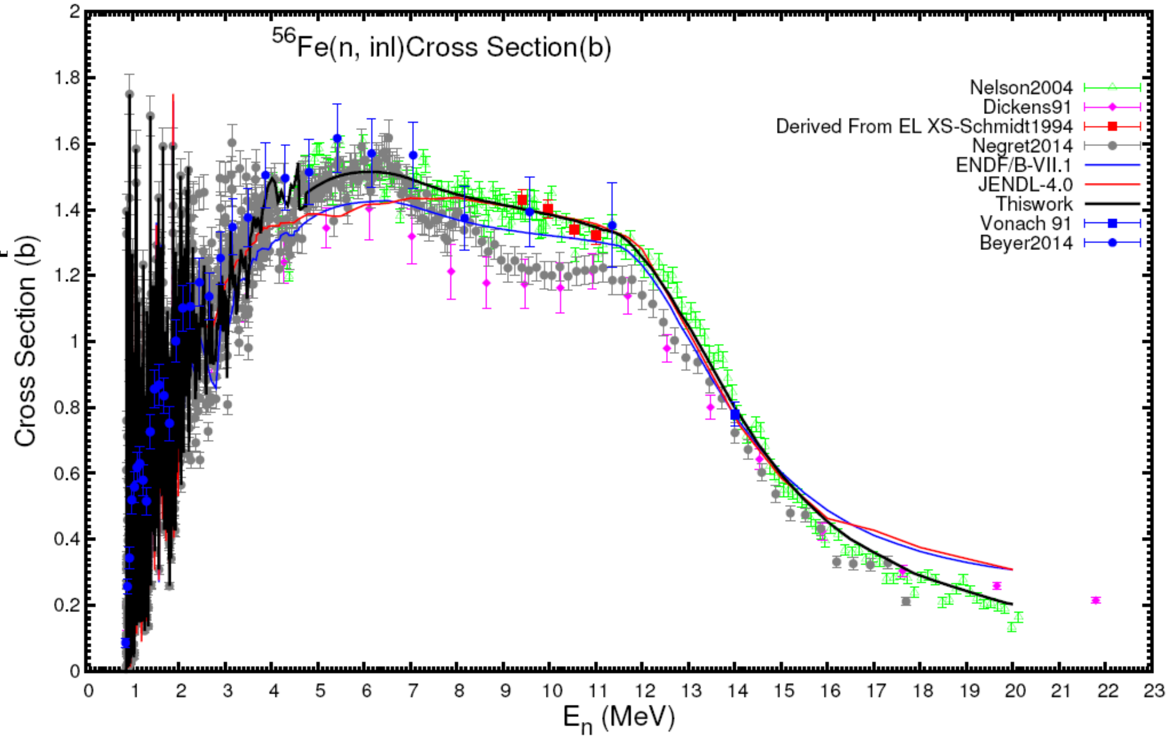




Neutron emission reactions of ^{56}Fe

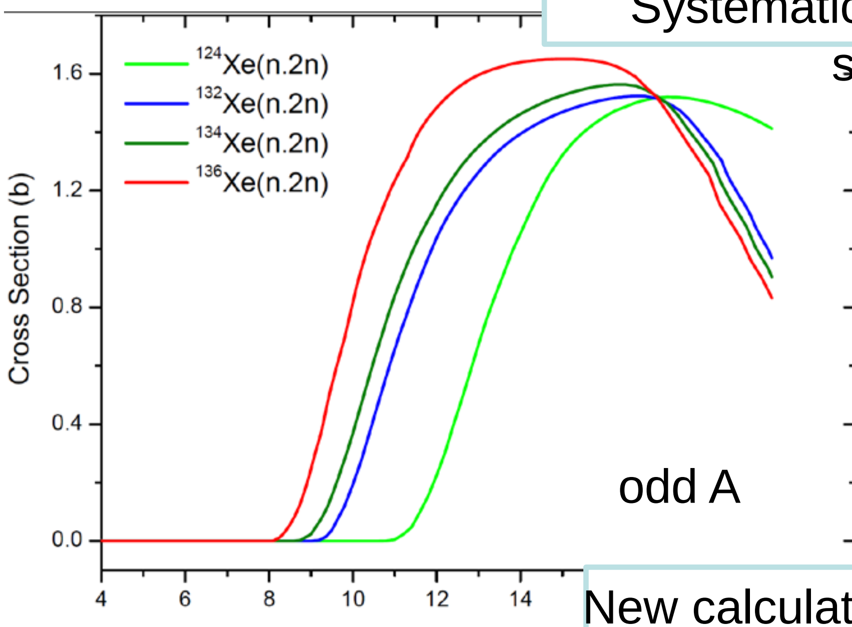
Fe-56

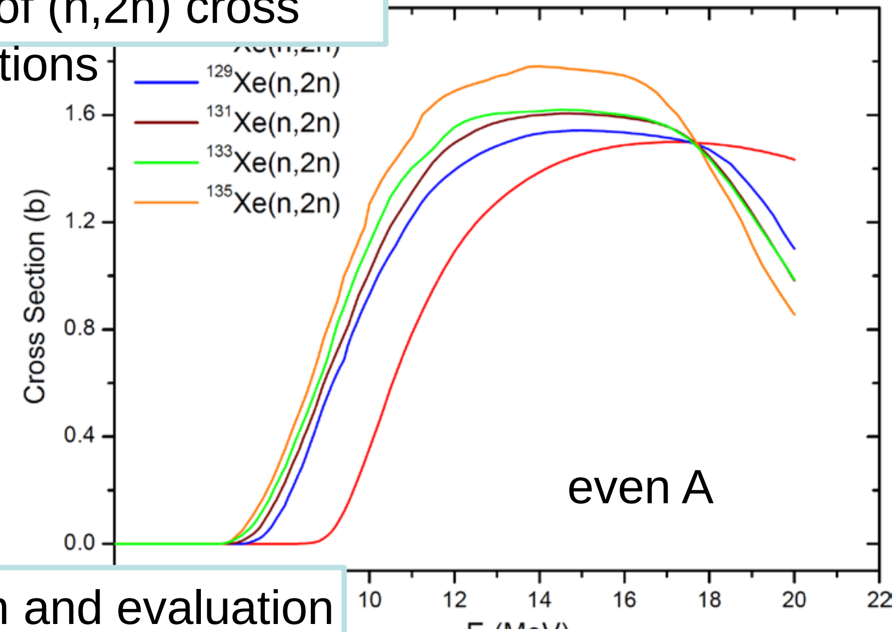




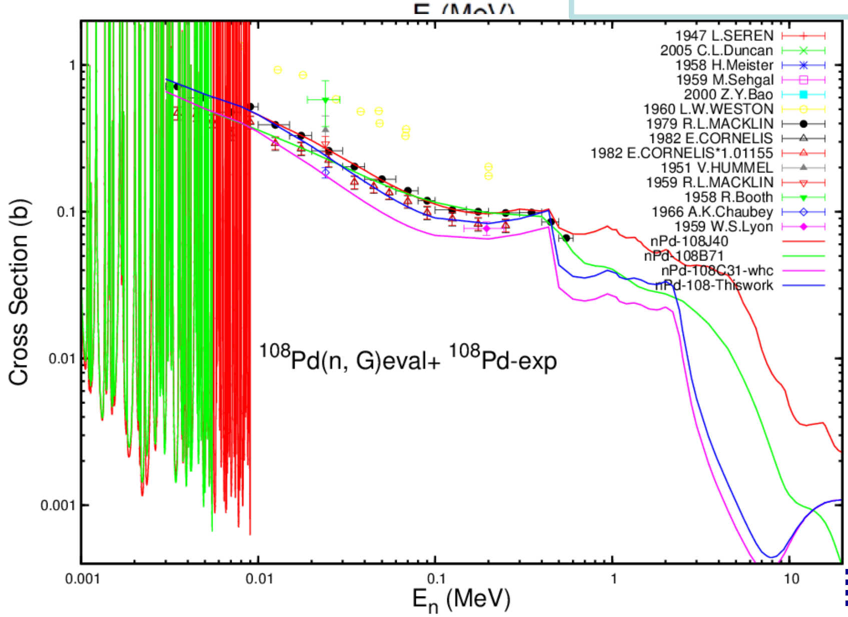
Fission Product Nuclide

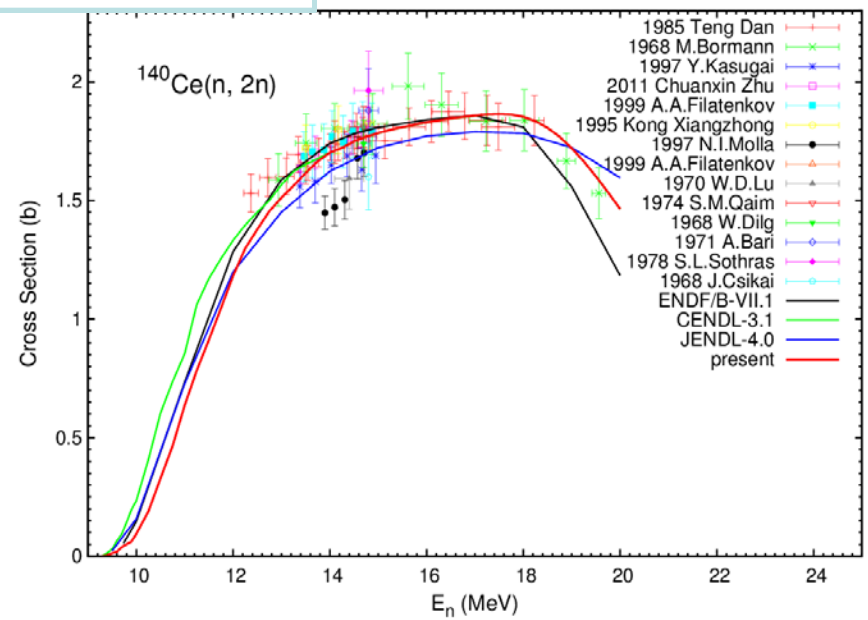
Systematics of (n,2n) cross sections



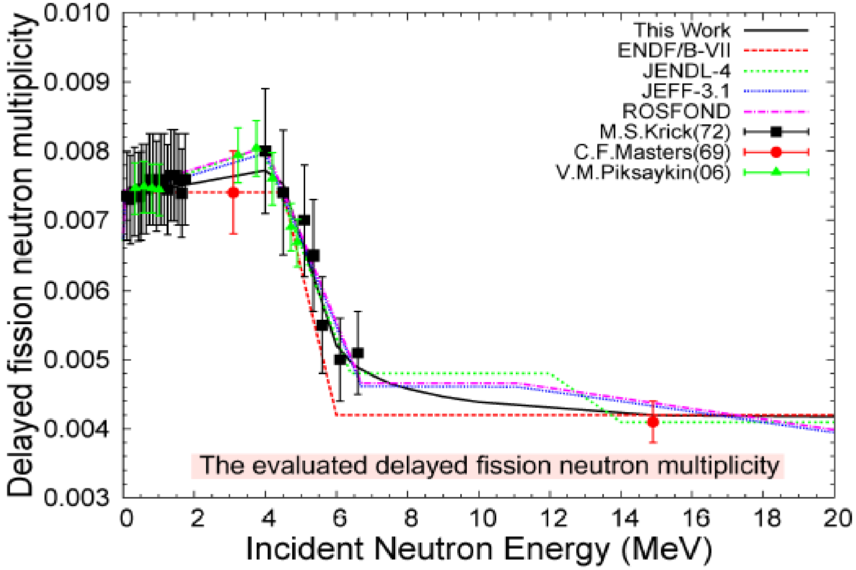


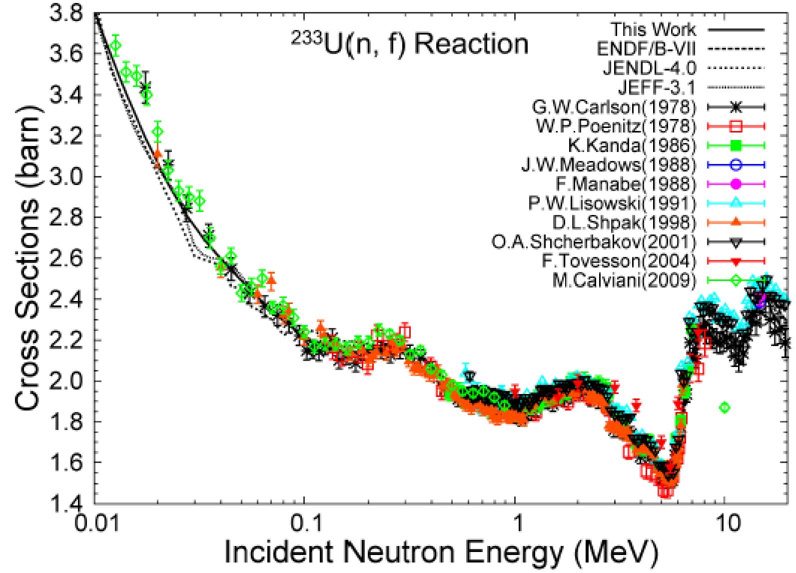
New calculation and evaluation

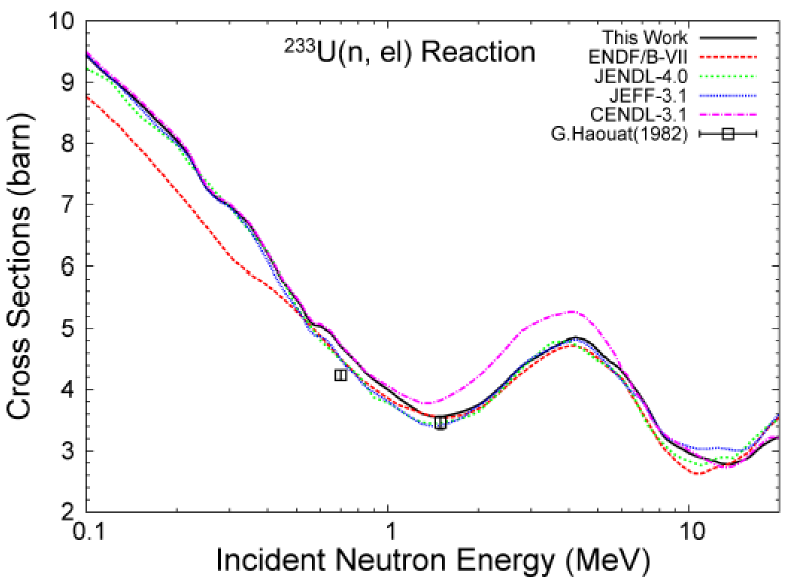


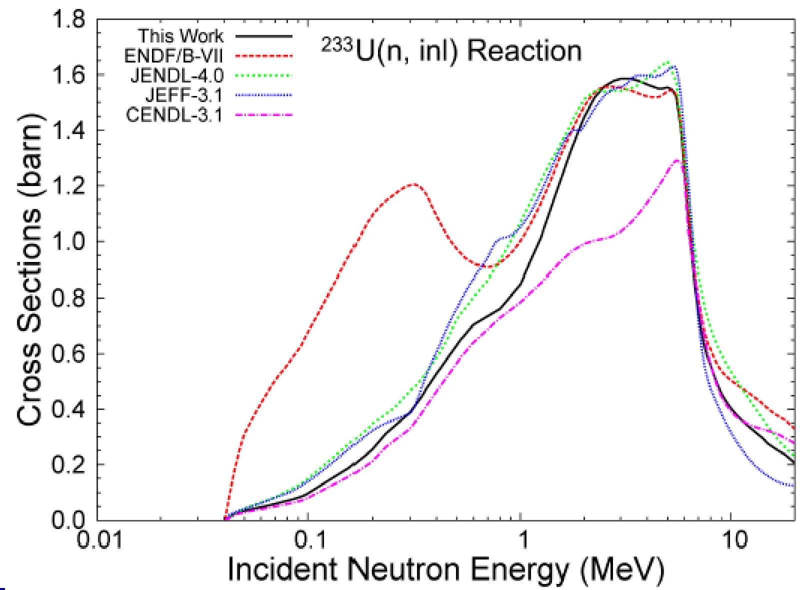


Nuclear data for U-233

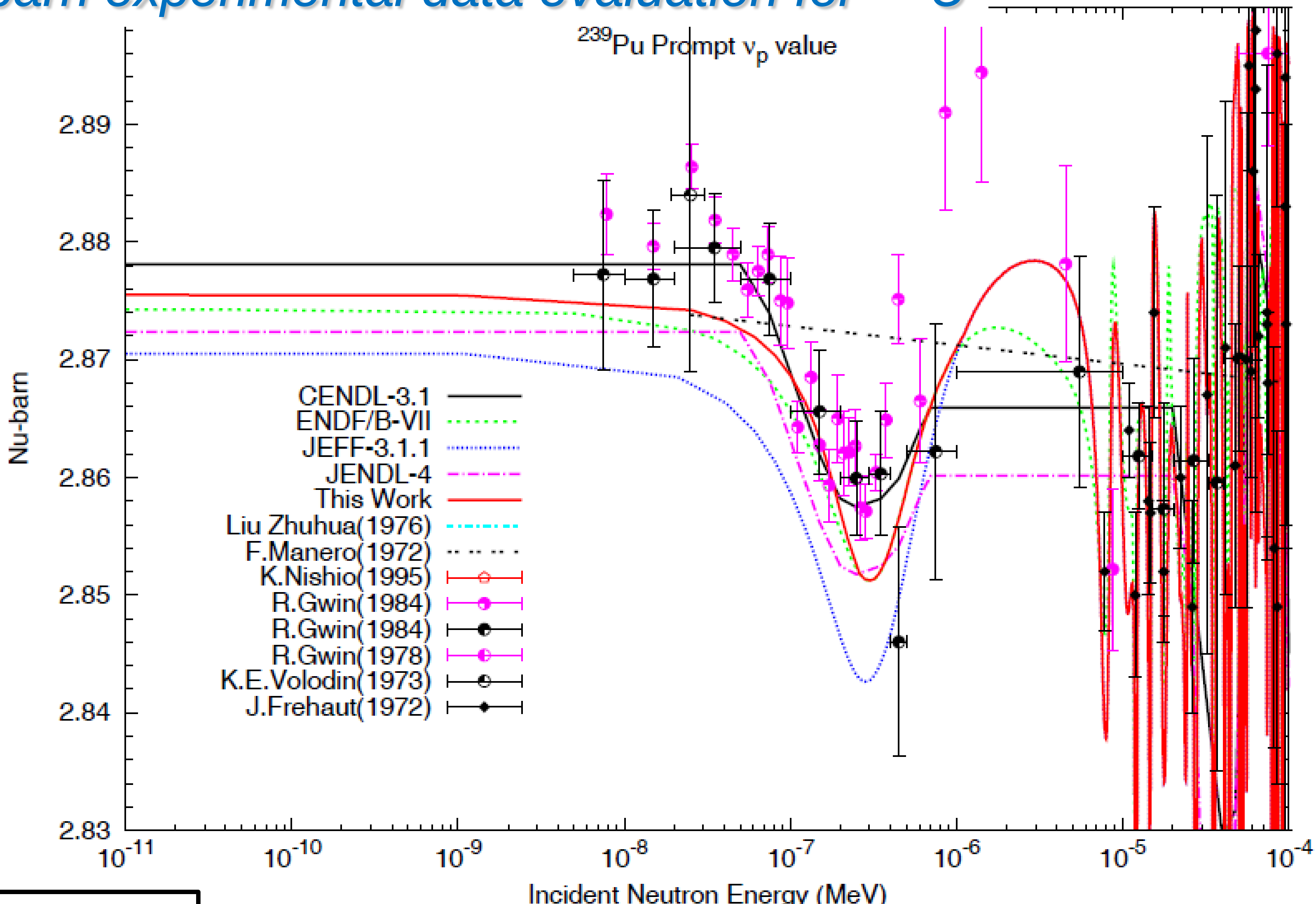






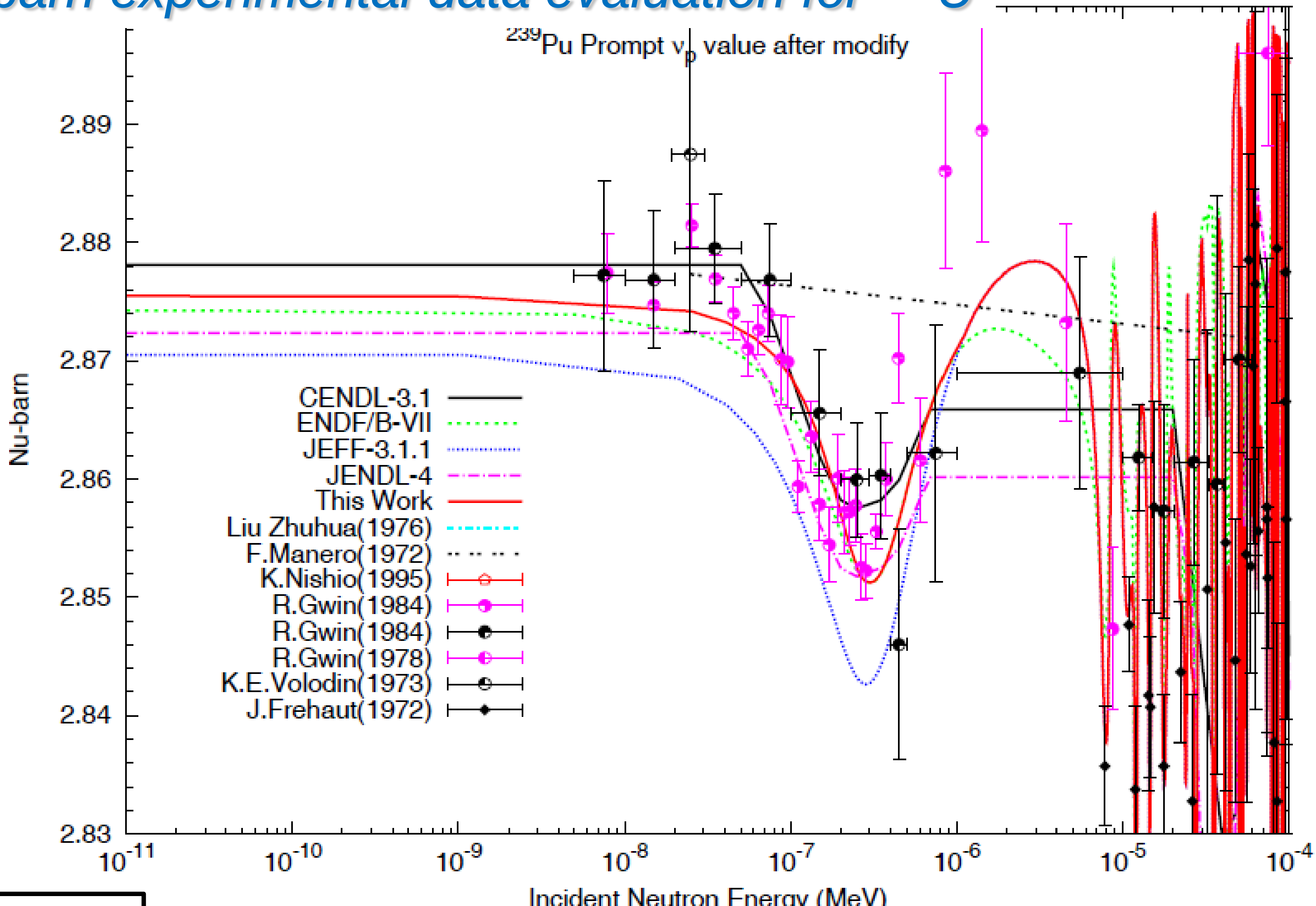


Nu-barn experimental data evaluation for ^{239}U



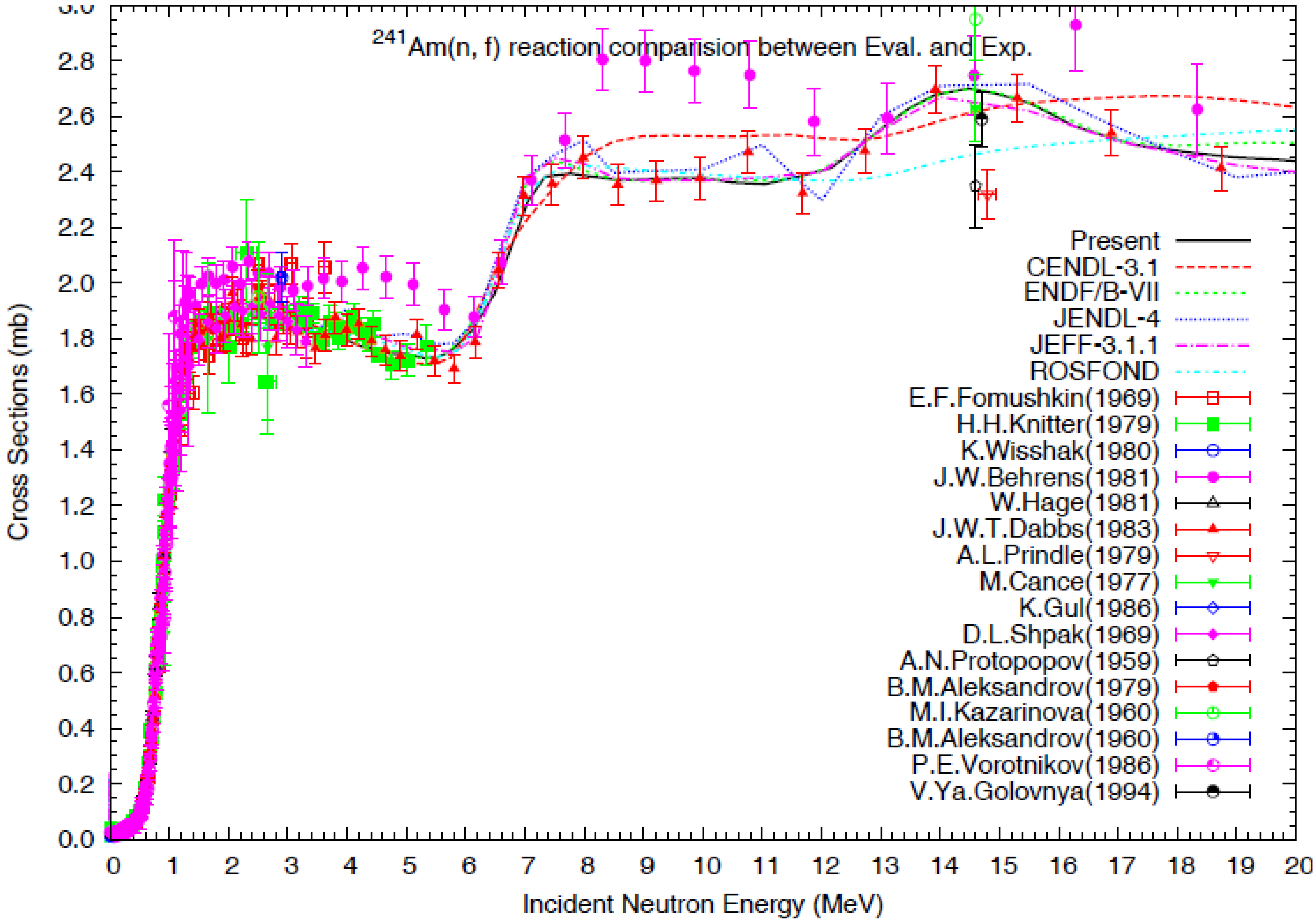
Before

Nu-barn experimental data evaluation for ^{239}U



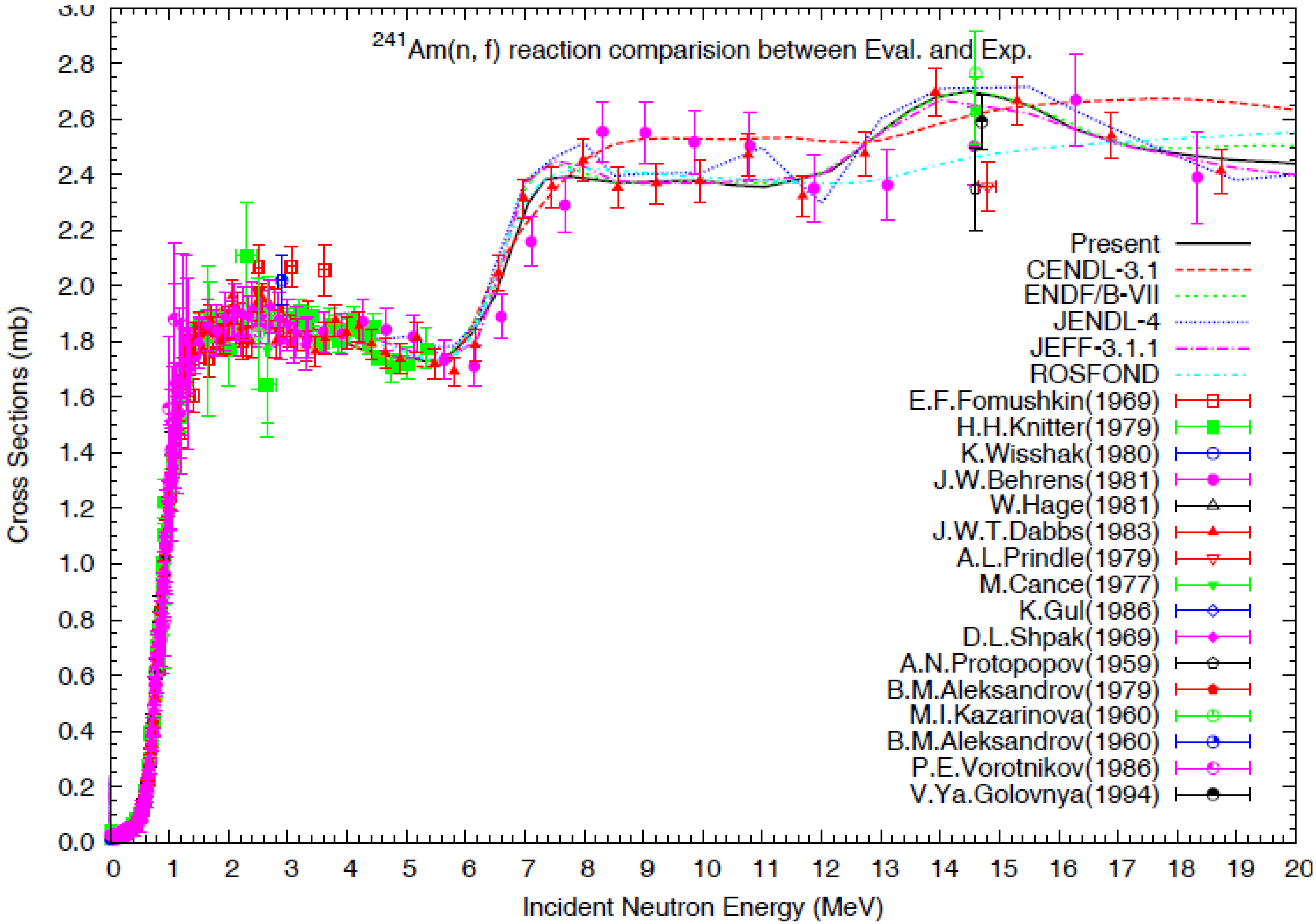
After

(n, fission) experimental data evaluation for ^{241}Am



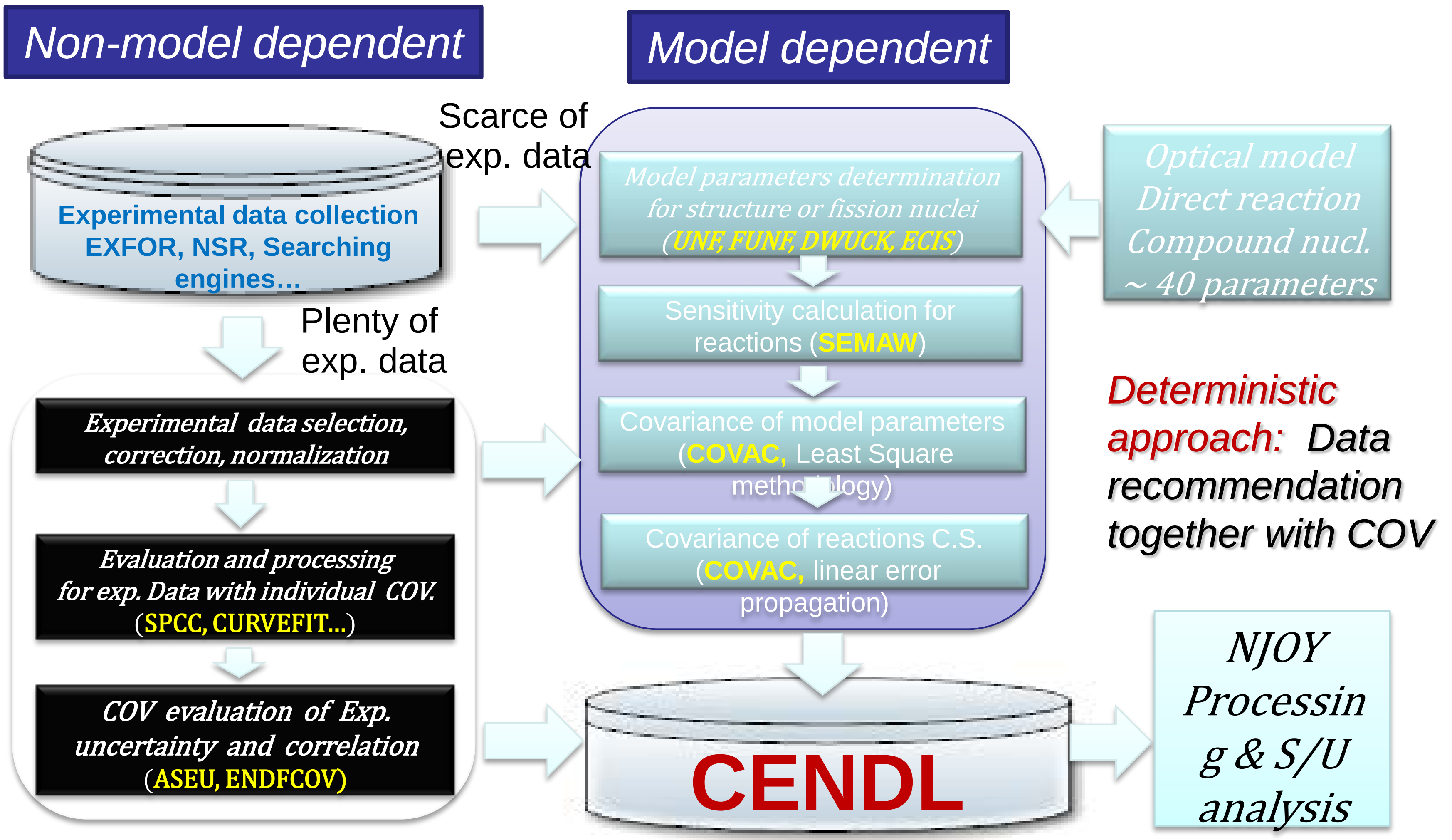
Before

(n, fission) experimental data evaluation for ^{241}Am



After

II. Covariance evaluation of CENDL 3.230



Correlations among single (or multiple) set(s) of experimental data are vital elements to get an 'honest' covariance. But it is almost inaccessible in the real evaluation.

The formulism of the non-model dependent covariance

Analysis of the sources of experimental uncertainties (ASEU)

Physics quantity y is derived based on N sets of experimental observables X following function F:

$$y = f(x_1, x_2, \cdots, x_N)$$

Taylor expansion around <X>, and the high order items are ignored:

$$y = f(\langle x \rangle) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle) + \frac{1}{2!} \sum_{i=1,j=1}^{N} \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) + \cdots,$$

$$y = f(\langle x \rangle) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle)$$

Covariance is derived based on the uncertainties of diversified experimental observables X, which the experimental uncertainty sources.

$$\sigma^2(y) \approx \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2\Big|_{x=\langle x \rangle} \sigma_i^2 + \sum_{i \neq j}^{N} \left(\frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j}\right)\Big|_{x=\langle x \rangle} Cov(x_i, x_j)$$

$$\begin{aligned}
Cov(y_i, y_j) &= < \left(\sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \Delta x_{ki}\right)\left(\sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_j \Delta x_{kj}\right) > \\
&= \sum_{kk'=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_{k'}}\Big|_j < \Delta x_{ki} \Delta x_{k'j} > \\
&= \sum_{kk'=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_{k'}}\Big|_j \rho_{ij}^{kk'} \sigma_{ik} \sigma_{k'j} \\
&= \sum_{kk'=1}^{N} \rho_{ij}^{kk'} \left(\frac{\partial f}{\partial x_k}\Big|_i \sigma_{ik}\right)\left(\frac{\partial f}{\partial x_{k'}}\Big|_j \sigma_{k'j}\right) \\
&= \sum_{kk'=1}^{N} \rho_{ij}^{kk'} \Delta y_{ki} \Delta y_{k'j}
\end{aligned}$$

$^{90}Zr(n, 2n)^{89}Zr$

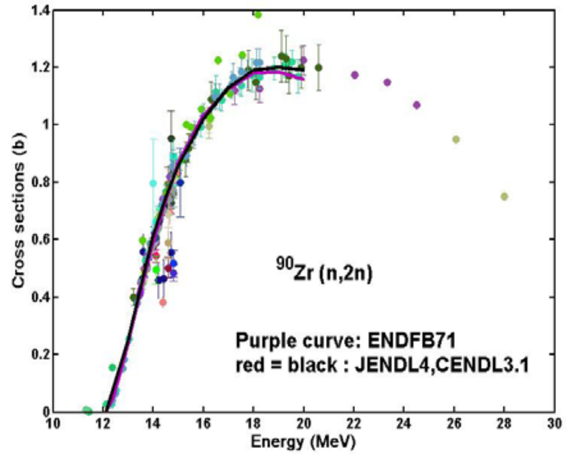
To an extend, ASEU is trying to express the current skill level of experiment.

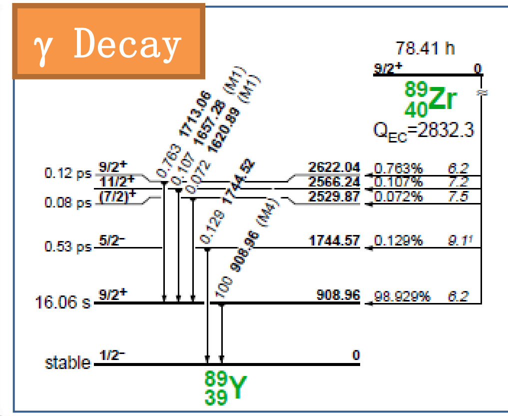
Observables in measurement		Uncertainties of $^{90}Zr(n,2n)^{89}Zr$		Correlations
	Error source	12-20MeV	13.5-15MeV	
Statistics	Count	4.0-0.6%	0.3-0.6%	0.0
Neutron flux	● Differential C.S. $T(d,n)^4He$ ● Background correction from D-D and other nuclei ● correction for neutron scattering	3-1% 1% 1.5-0.6%	1% 0.5% 0.5%	0.3 1.0 0.0
Sample	● Sample weighting ● Isotopic abundance ● γ self-absorption	0.5% 0.2% 0.5%	Same Same Same	1.0 1.0 1.0
Monitor err. $^{27}Al(n,\alpha)^{24}Na$	Cross section error of Monitor	4-2%	1.3-0. 5%	0.6
Detector err.	Efficiency of dectetor	2%	Same	1.0
Activation	Decay data	1%	Same	1.0
others	Time of irradiation	0.1%	Same	1.0

$^{90}Zr(n, 2n)^{89}Zr$

ASEU for $^{90}Zr(n,2n)^{89}Zr$:

Experiment conditions in ASEU interests	
1	Time
2	Energy region
3	Num. of reported Energies
4	Institute
5	Accelerator
6	Neutron source
7	Method
8	Detector
9	Monitor cross sections



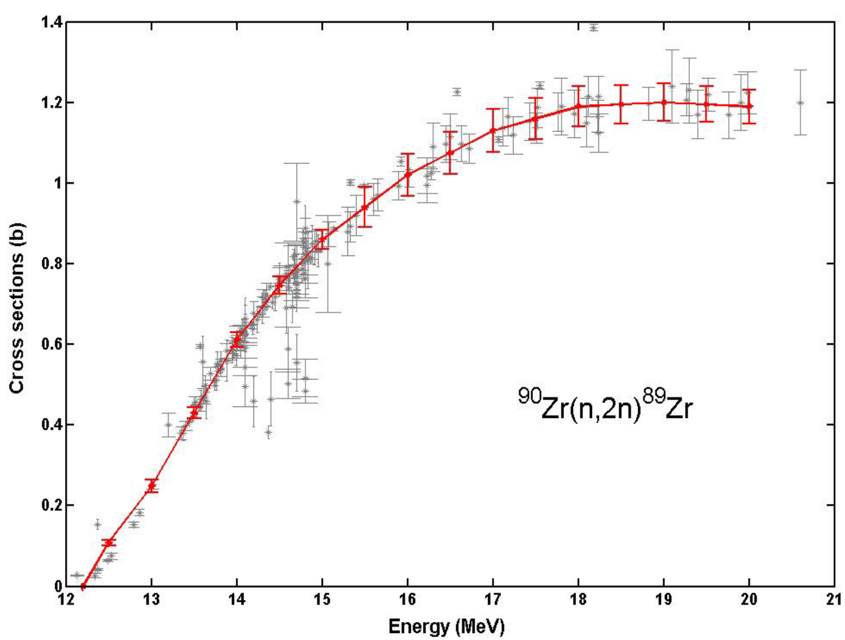


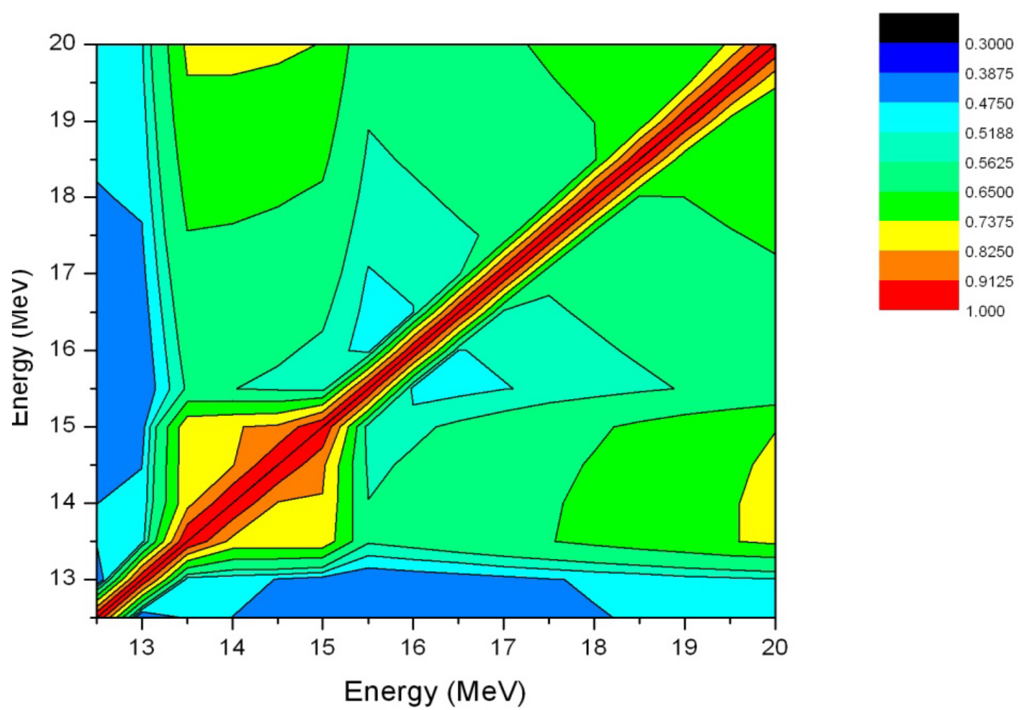
- E_{th} = 12.1MeV, relative higher, easy avoid the influence from neutrons at low energies;
- $T_{1/2}$ of ^{89}Zr = 78hour, sample is easy to be irradiated, cooled and detected;
- Few cascading in ^{89}Y decay, better to be detected.
- 39 measurements are available in EXFOR

Activation measurement is adopted for all experiments. Most of γ energies are selected as 909keV from ^{89}Y

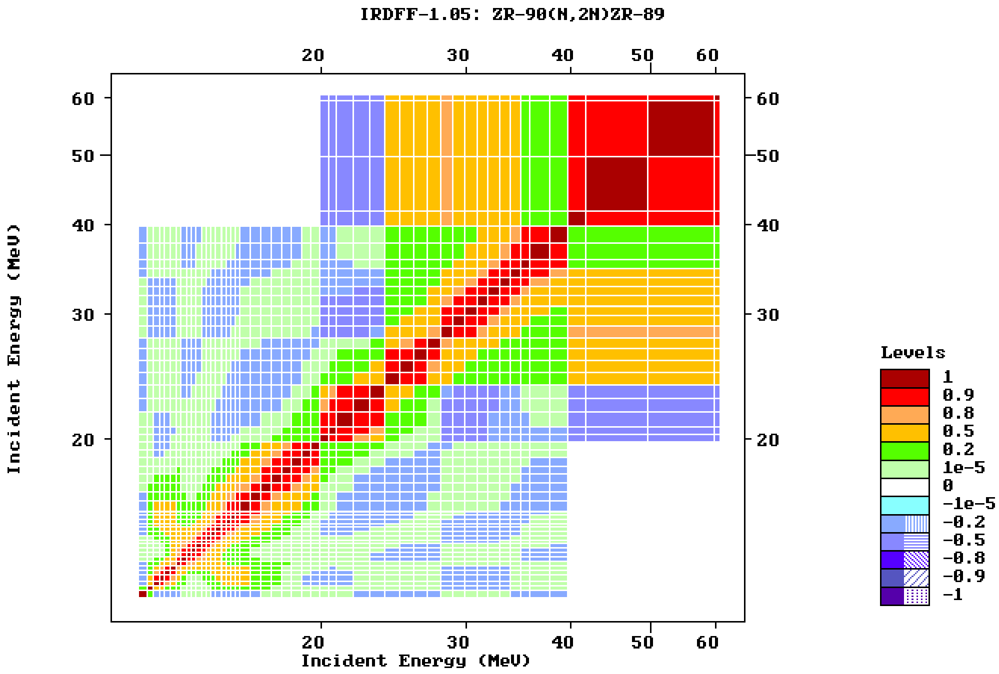
$^{90}Zr(n, 2n)^{89}Zr$

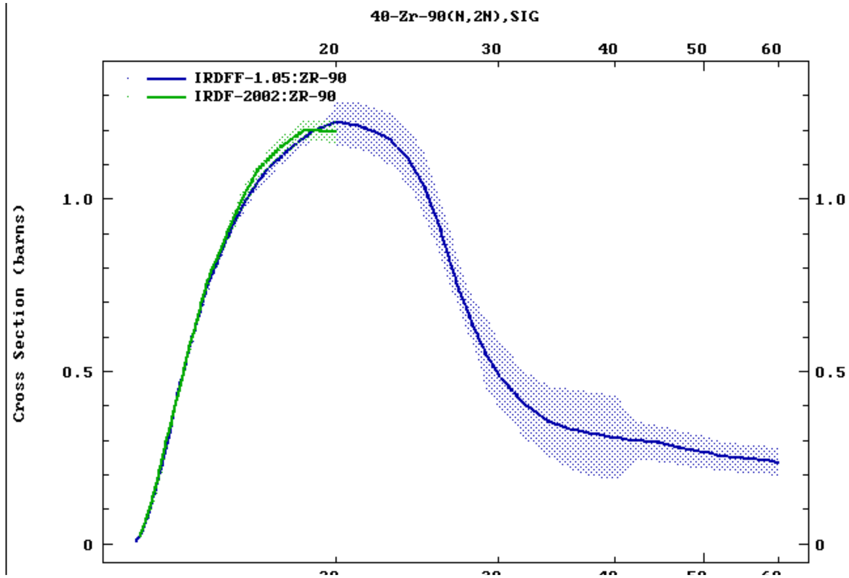
- This covariance is directly produced from experimental observable uncertainties in Table above but not SLS.
- 39 sets of experimental data, which are used in cross section fitting by SLS, are adopted in the separated covariance evaluation.
- The linear energy dependence is taken both for uncertainty and correlation.
- Correlated uncertainty will be decreased in future regarding multi-sets of data are available at same energy region.





$^{90}Zr(n, 2n)^{89}Zr$



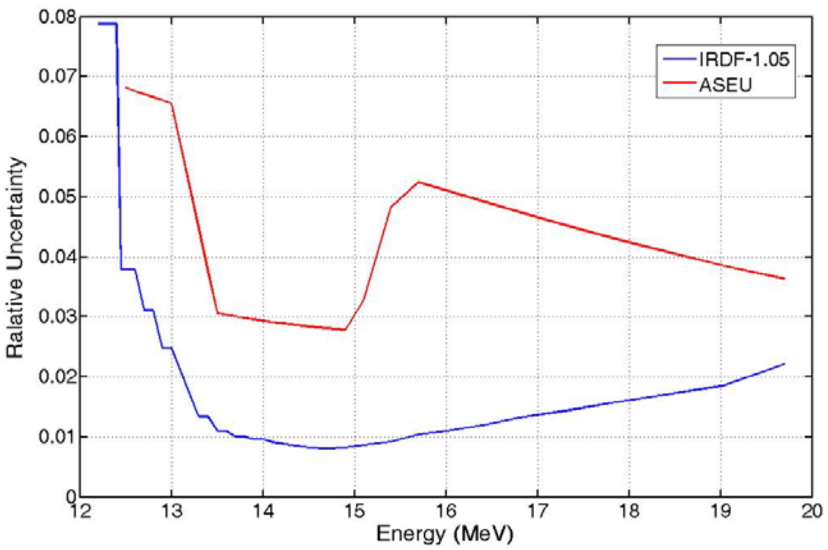


IRDF-1.05:

0-20MeV: K. I. Zolotarev

20-60MeV: Trkov

Produced by LS method



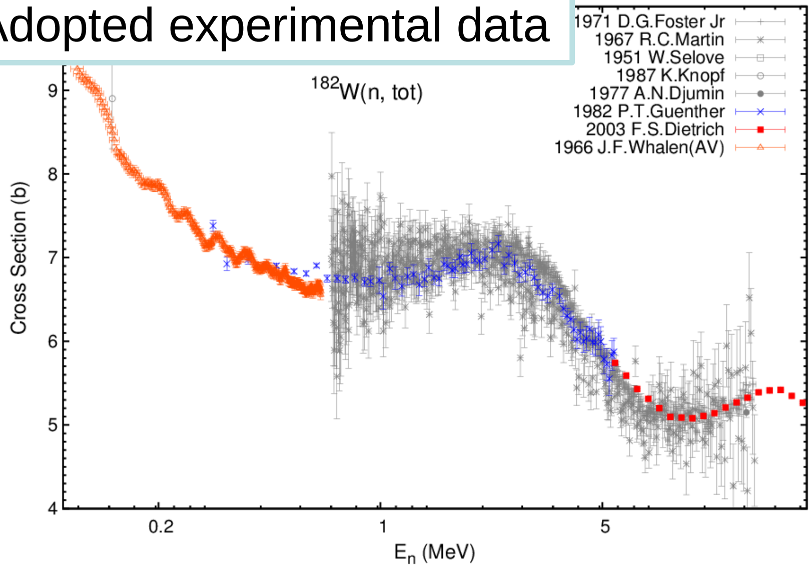
ASEU is performed to the covariance evaluation for ^{182}W(n, tot) cross section

* Three energy regions are separated based on the status of experimental data:
I[0.1, 0.5], II[0.5, 5.45], III[5.45, 20]

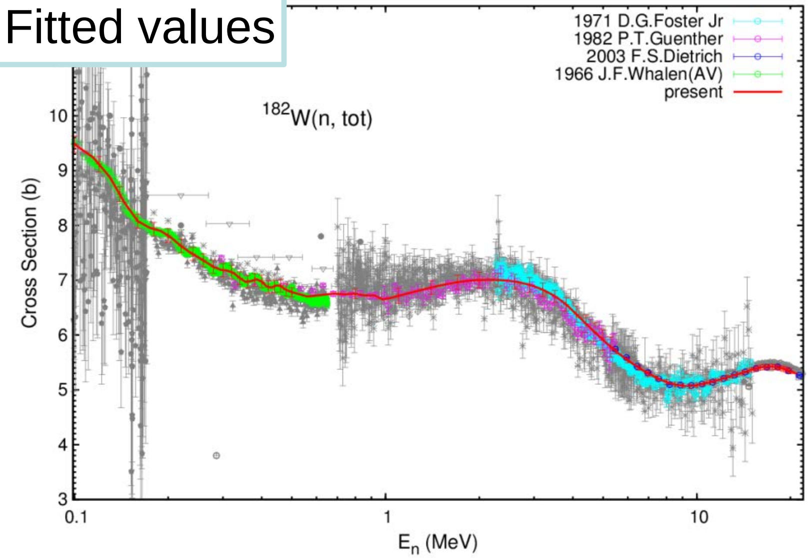
* The uncertainties and correlations are evaluated according to different energy regions

Uncertainty items			Statistics	B.G.	Inner scat.	Dead time correction	Energy Shift	Geometry	Sample
Corr.			Uncorr.	MRC	MRC	MRC	MRC	LRC	LRC
I	Values		Linear interplation	0.006	0.006	0.005	0.005	0.003	0.008
	C.C	linear	0	0.2	0.3	0.3	0.1	1.0	1.0
		Gaus./ full half width	0	0.02	0.01	0.01	0.01	1.0	1.0
II	Values			0.005	0.005	0.0045	0.005	0.002	0.006
	C.C	linear	0	0.2	0.3	0.3	0.1	1.0	1.0
		Gaus./ full half width	0	0.6	0.5	0.5	0.5	1.0	1.0
III	Values			0.003	0.004	0.003	0	0.002	0.005
	C.C	linear	0	0.2	0.3	0.3	0.1	1.0	1.0
		Gaus./ full half width	0	1.2	1.0	1.0	/	1.0	1.0

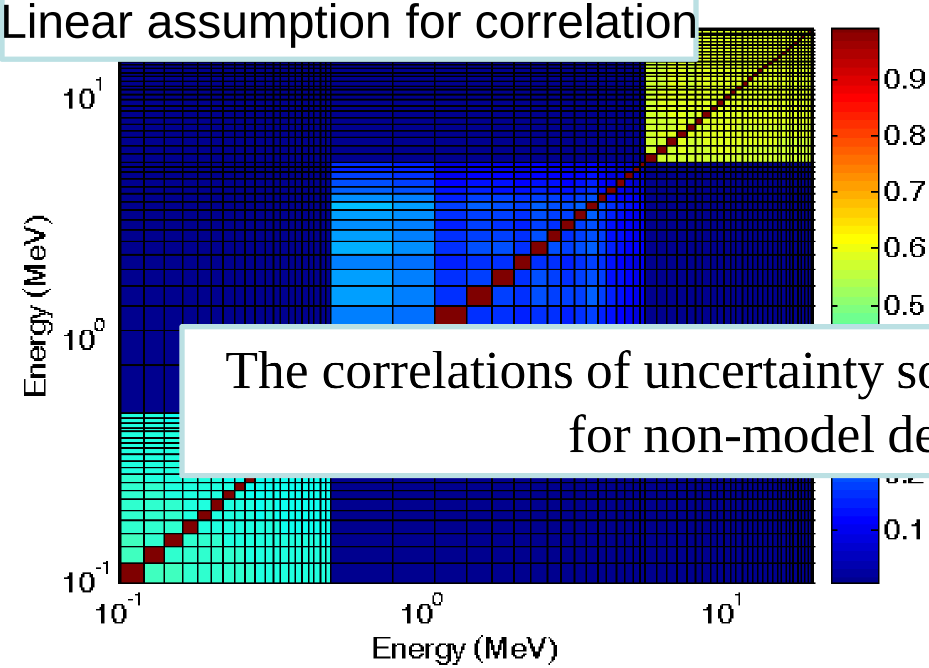
Adopted experimental data



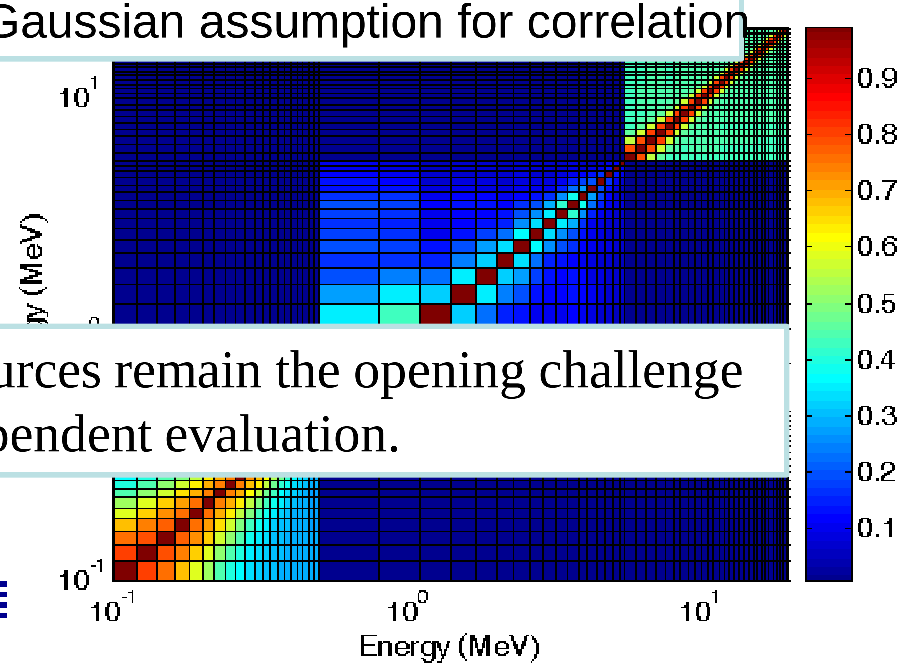
Fitted values



Linear assumption for correlation



Gaussian assumption for correlation



The correlations of uncertainty sources remain the opening challenge for non-model dependent evaluation.

The formulism of the model dependent covariance calculation

The parameters estimation by Bayes

$$p(\mathbf{p}|D) = L(D|\mathbf{p})p_a(\mathbf{p})/[\int L(D|\mathbf{p}')p_a(\mathbf{p}')d\mathbf{p}']$$

COV of Parameter

$$(\mathbf{V}_p)_{kq} = \langle(p_k-\langle p_k\rangle)(p_q-\langle p_q\rangle)\rangle = \int(p_k-\langle p_k\rangle)(p_q-\langle p_q\rangle)p(\mathbf{p}'|D)d\mathbf{p}'$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})]\}$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})]\}p_a(\mathbf{p})$$

$p_a(\mathbf{p}) = 1$ (equal probability assumption)

$$[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] = \text{minimum}$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] + (-1/2)(\mathbf{p}-\mathbf{p}_a)^+\mathbf{V}_a^{-1}(\mathbf{p}-\mathbf{p}_a)\}.$$

$$[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] + (\mathbf{p}-\mathbf{p}_a)^+\mathbf{V}_a^{-1}(\mathbf{p}-\mathbf{p}_a) = \text{minimum}$$

LS for model-dependent case:

$$\Delta\hat{C} = (F^TV^{-1}F)^{-1}F^TV^{-1}(Y-Y_0)$$

$$\hat{V}_C = (F^TV^{-1}F)^{-1}$$

$$\hat{Y} = F\Delta\hat{C} + Y_0$$

$$\hat{V}_{\hat{Y}} = FV_cF^T$$

Important inputs:

Sensitivities(F)

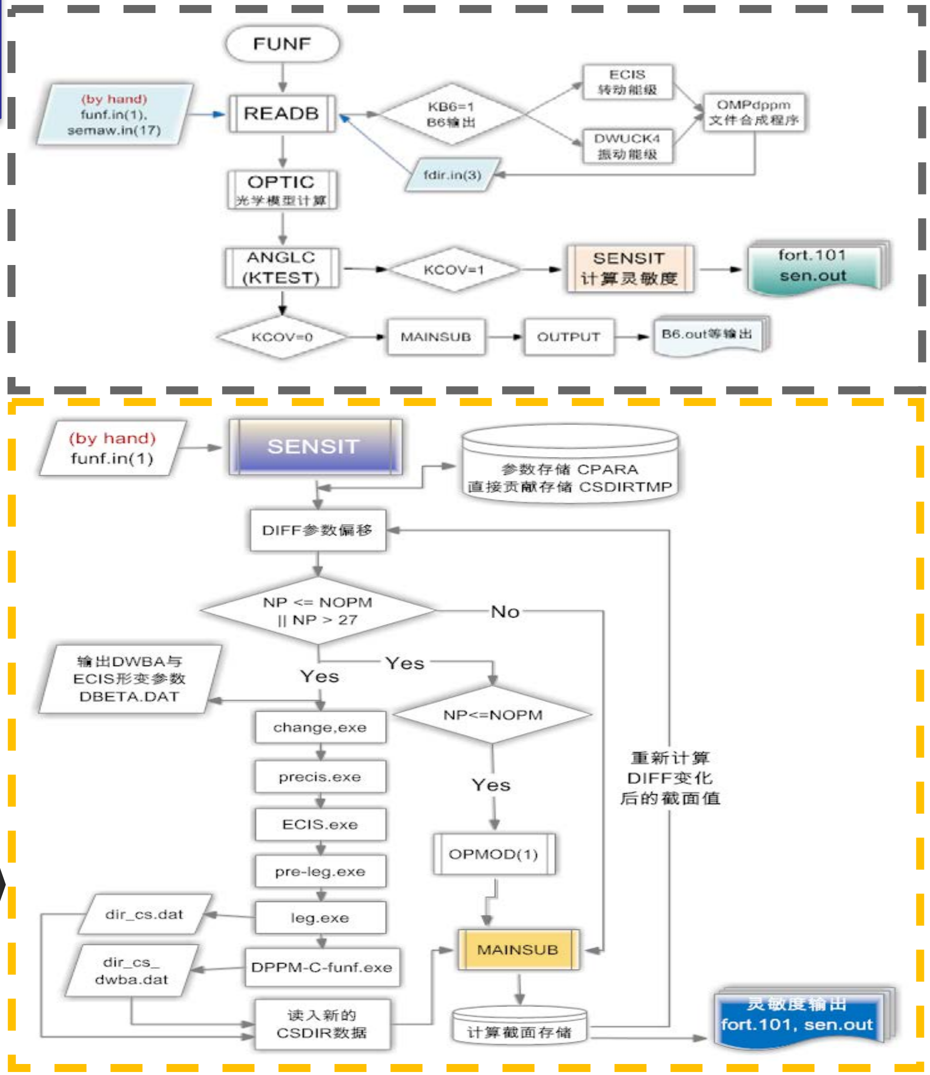
COV of exp. Data (V_Y)

Sensitivity Matrix Workstation (SEMAW)

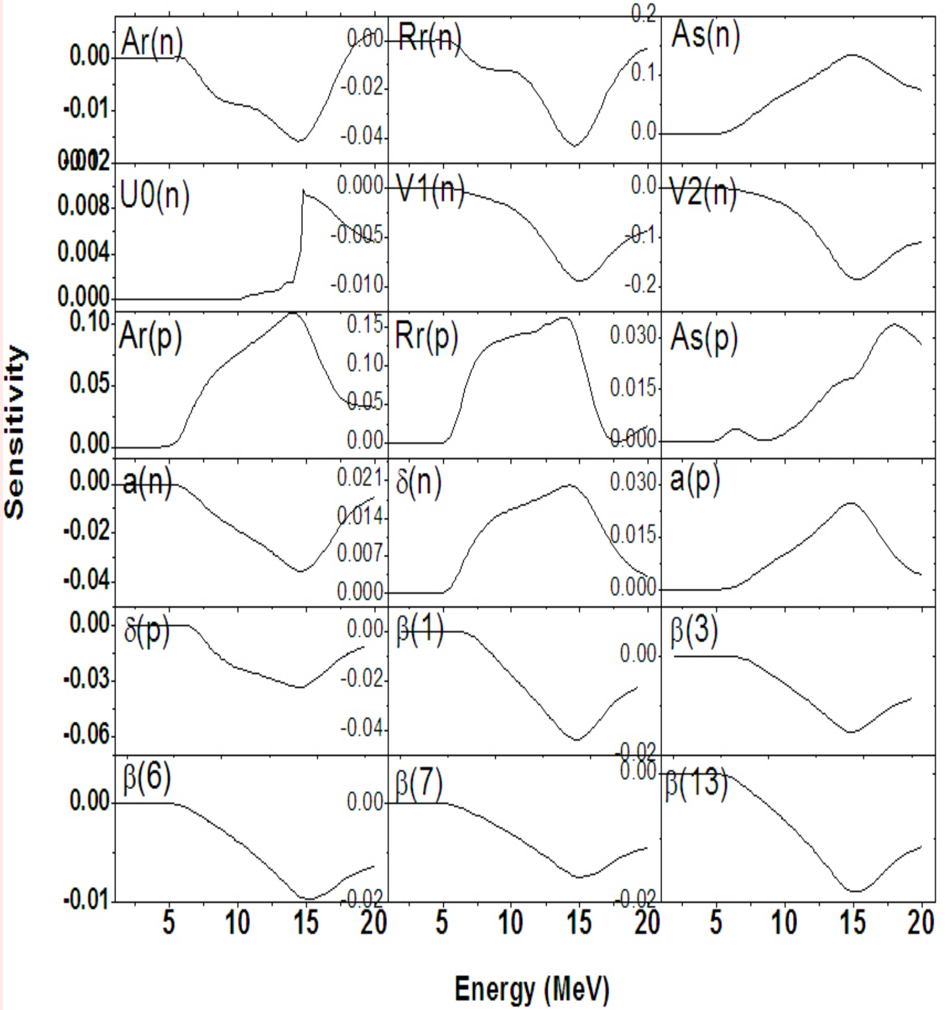
- Nuclear reaction codes UNF, ECIS, DWUCK4
- 40 model parameters are involved
- Applied in fission nuclei, middle-heavy nuclei evaluation

Numerical solution：

$$f'(x_0) = \frac{(y_3 - y_{-3}) + 9(y_{-2} - y_2) + 45(y_1 - y_{-1})}{60h}$$



Sensitivity to ^{48}Ti(n, p)^{48}Sc

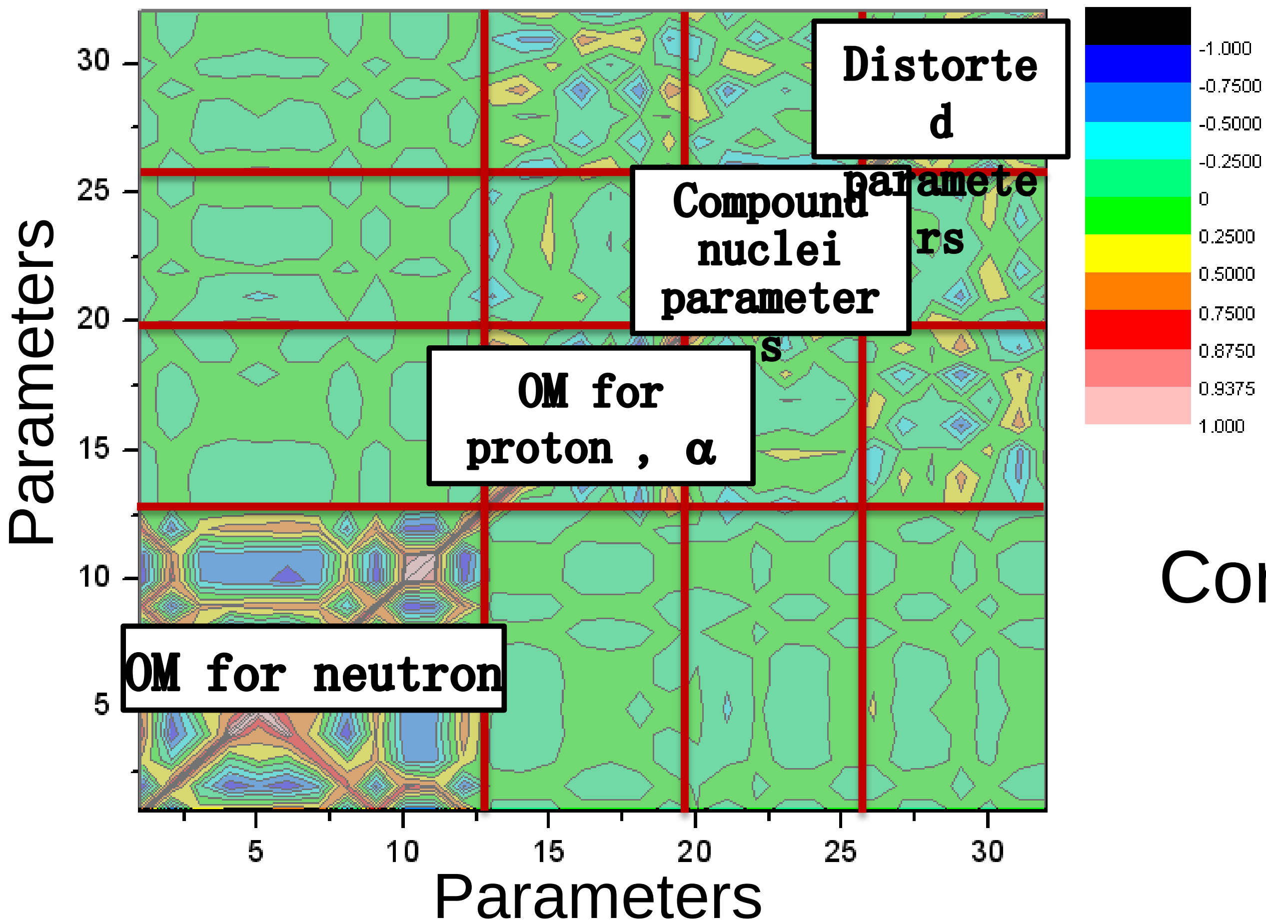


34 theoretical parameters

- OM for neutron：U0, V0, V1, V2, VSO, W0, Rr, Ar, As, Aso
- OM for proton：V0, W0, Rr, Ar, As
- OM for ^{4}He：U0, Rr, Ar
- Level density and pair:
  (n,inl), (n,p), (n,^{4}He), (n,2n)
- E1 giant dipole resonance for
  (n,inl), (n, γ)
- Kalbach parameter：K
- Distorted parameters of 5 discrete levels

➡ Sensitivities > 10^{-3}

Covariance of theoretical model parameter



Corr. Coef. of model para. in n+^{48}Ti calculation

* Covariance for parameters exhibit the correlations among various models para.;

• It is derived based on experimental data and sensitivities;

• The model-dependent covariance is always larger than the non-model dependent ones.

III. Benchmark Testing of CENDL 3.2b0

CENDL-3.2b0(C32b0) has been tested with all the criticality benchmarks in ENDITS-1.0.

^{233,235}U, ^{232}Th have been improved significantly. For ^{235}U, by loading the fission cross sections from IAEA 2006 standard, reevaluating the α values and revising the resolved resonance parameters according to the nuclear data adjustment based on the selected HMT benchmarks, the predictions of the k_{eff} values for the uranium fuelded system have been significantly improved.

The normalized χ^2 values for most of the systems calculated with the C32b0 have been generally improved compared to C3.1.

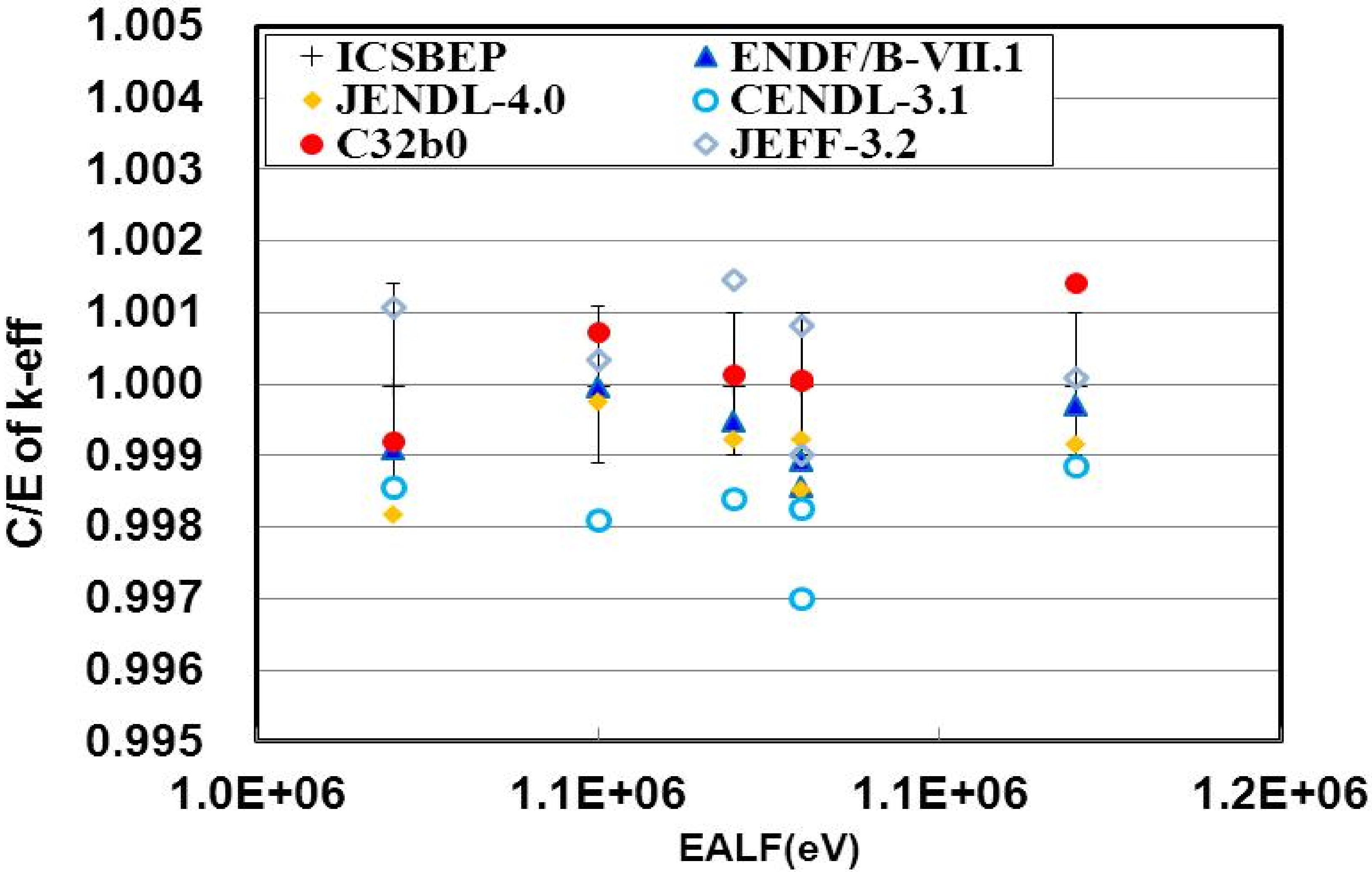
For all the uranium fueled benchmarks in the ENDITS-1.0, C32b0 gives the best prediction of k_{eff} values compared with the other libraries.

For the bare and uranium reflected ^{233}U spheres, the C/E values closed to unit due to the revised ^{233}U(n,inl) cross sections.

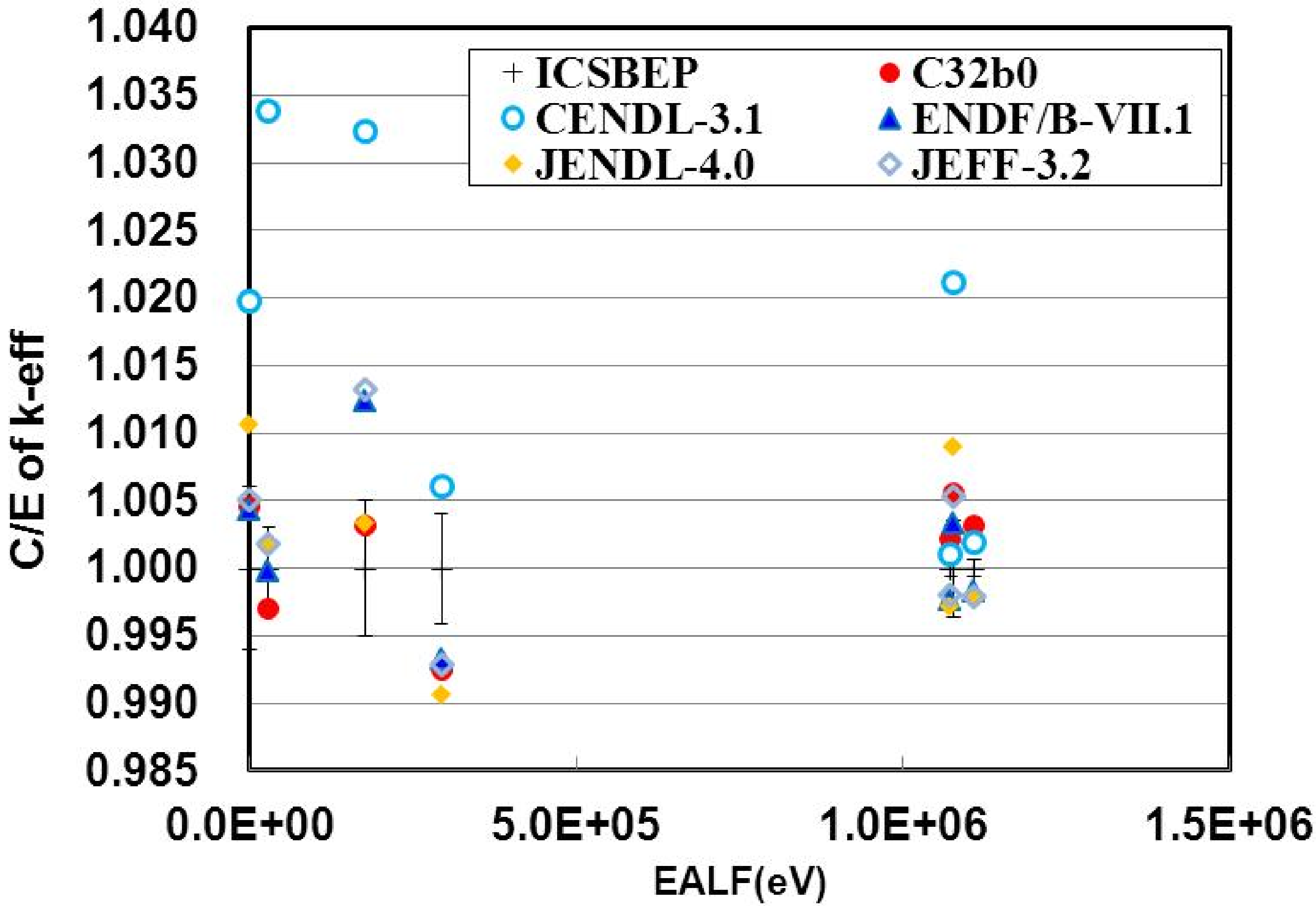
For the fast and intermediate spectra benchmark KBR and Thor, the k_{eff} values are sensitive to the data of ^{232}Th, the C/E values of the k_{eff} have been improved significantly by revised ^{232}Th(n,γ) cross sections.

Type	Cores	C32b0	C31	B71	J40	F32
HCF	5	1.2	0.8	2.6	2.0	1.8
HCI	8	825	843	915	642	741
HCM	18	1.1	47.4	136	25.2	86.9
HCT	43	2.9	4.3	2.5	8.1	2.5
HMF	151	460	539	500	526	560
HMI	6	48.6	40.3	24.9	20.4	95.4
HMT	89	29.4	130	47.0	48.8	23.3
HST	118	2.1	1.9	1.7	1.6	1.9
ICF	2	-1.0	39.6	4.9	128	10.3
ICI	2	-1.0	132	-0.5	2.6	0.2
ICT	33	-0.2	1.9	0.6	4.6	0.7
IMF	17	1.6	10.4	2.6	61.3	9.2
LCT	122	6.3	4.2	3.5	3.4	3.1
LMT	26	-0.4	0.0	-0.3	-0.1	0.4
LST	58	2.0	6.2	3.7	2.6	2.4
U235	698	114	145	128	130	135

Comparison of (χ^2-1) of k_{eff} values for uranium fueled criticality benchmarks



The comparison of the C/E values of the k_{eff} for the bare and uranium reflected ^{233}U spheres.



The C/E results of fast and intermediate spectra benchmarks sensitive to ^{232}Th (KBR and Thor).

Ⅳ. Other Information Related to CENDL Project

- ✓ Regular update and maintenance of IAEA/NDS mirror-site in China with the support of NDS.
- ✓ Nuclear data services is providing to all the nuclear data users in China and other regions by CNDC.
- ✓ The photonuclear data of light and middle-heavy nuclei are being evaluated, the new evaluation and theoretical source codes are being carried out so as to fulfill the requirement of CRP(IAEA)
- ✓ Compiled 30 new entries for 35 articles, and updated 1 entry for EXFOR database
- ✓ A budget (~8.5 millions USA$) about the "13th Five Year Plan" (2016-2020) for CENDL project has been approved, which contains nuclear data evaluations and measurements.
- ✓ A proposal (~2.8 millions USA$, 2018-2023) of the fundamental study for fission nuclear data has been submitted to the National Natural Science Foundation of China (NSFC) which was approved two days ago.

Thank you for your attention !
Comments and suggestion welcome !