Global validation of the EXFOR database with the world nuclear data libraries

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Outline

- Introduction
- EXFOR Quality classes
- Some statistics
- Visual inspection
- Summary

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Introduction

- **Usual route: Use EXFOR data to build data libraries.**
- **Here, inverse route: Use nuclear data libraries, and TALYS, to check quality of EXFOR data**
- **Started in 2007 with WPEC SG30 on Quality assessment of EXFOR**
- **NEA report xx (2014) : Statistical verification and validation of the EXFOR database: (n,n'), (n,2n), (n,p), (n,alpha) and other neutron-induced reaction cross sections**
- **NEA report xx (2016) : Statistical verification and validation of the EXFOR database: (n,gamma), (n,n'), (n,2n), (n,p), (n,alpha) and other neutron-induced reaction cross sections. Almost in print**

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Main contributors

- Emmeric Dupont, NEA (-2014), for help to initiate this project and feedback on the first results
- Oscar Cabellos, NEA (2014-), for continuing this project
- Viktor Zerkin, IAEA: for releasing XC4 databases and extensions of the format
- Naohiko Otsuka: for feedback on erroneous compilations

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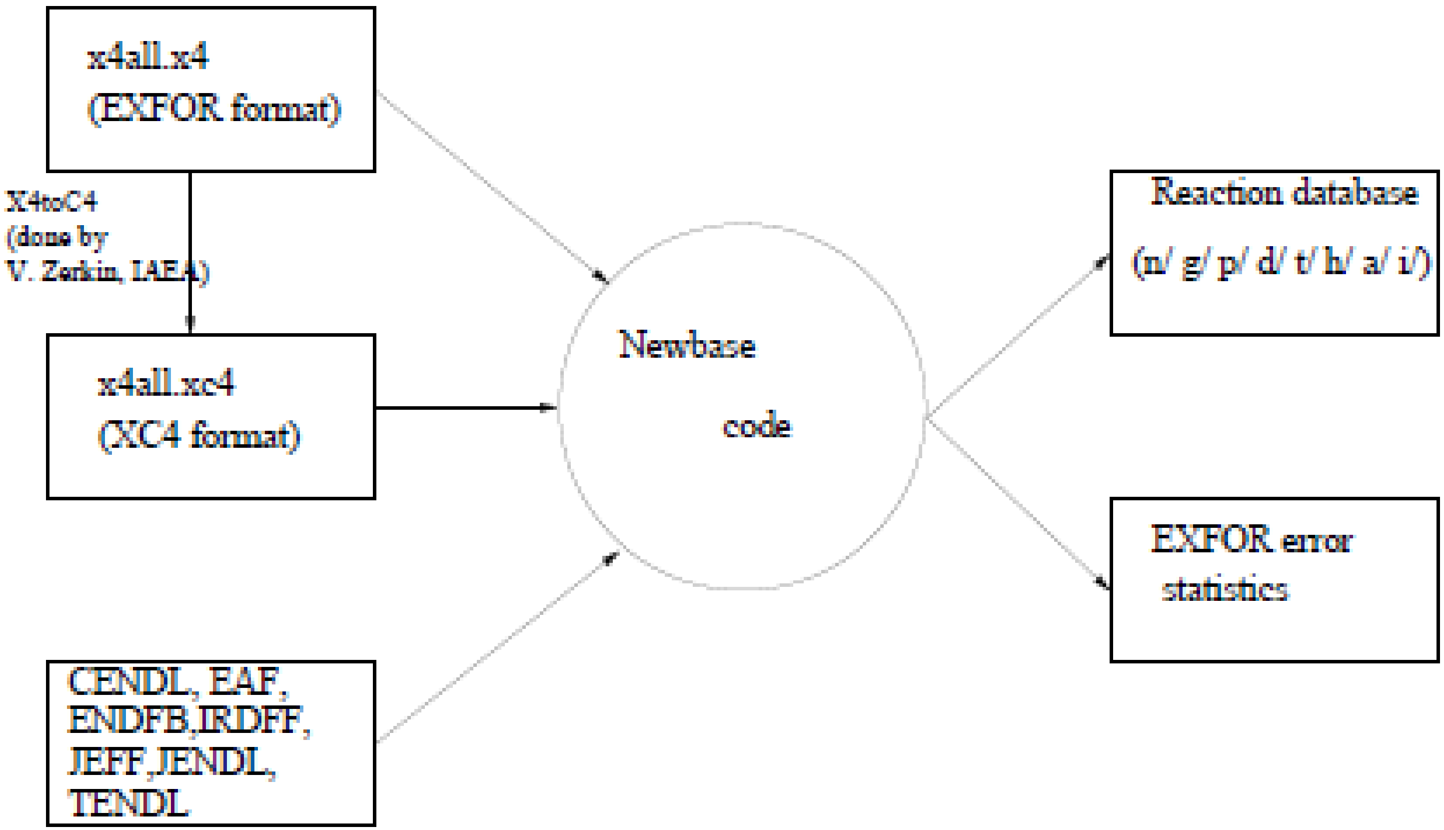

Figure 2.1: Databases produced out of EXFOR.

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Libraries for comparison

- CENDL-3.1: Chinese Evaluated Nuclear Data Library (China), a general purpose library for neutrons.
- EAF-2010: European Activation File (UKAEA Culham/NRG Petten), a special purpose library for activation reactions.
- ENDF/B-VII.1: Evaluated Nuclear Data File (USA), a general purpose library for neutrons.
- IRDFF-1.0: International Reactor Dosimetry and Fusion File (IAEA), a special purpose library for a limited number of reaction channels.
- JEFF-3.2 : Joint Evaluated Fission and Fusion file (NEA Data Bank), a general purpose library for neutrons.
- JENDL-4.0: Japanese Evaluated Nuclear Data Library (Japan), a general purpose library for neutrons.
- TENDL-2015: TALYS Evaluated Nuclear Data Library (NRG Petten), a general purpose library for neutrons and all other incident particles.
- If necessary, alternative nuclear model codes, or the same (TALYS) but run in an entirely different mode, e.g. with only microscopic (non-phenomenological) inputs.

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Quality classes

3.1.2 Subentries which are automatically compared with data libraries (T)

T1 Automatically compared with libraries: small deviations.
The subentry contains (very) probably the reaction and data measured by the author, and although the associated publication has not been checked by the reviewer, the quantities have central values and uncertainties which are close to other measurements, libraries and/or calculations.

T2 Automatically compared with libraries: questionable deviations
The subentry contains maybe the reaction and data measured by the author, and the associated publication has not (yet) been checked by the reviewer. The quantities have central values and uncertainties which are deviating to some extent from other measurements, libraries and/or calculations.

T3 Automatically compared with libraries: strong deviations
The subentry contains probably not the reaction and data measured by the author, and the associated publication has not (yet) been checked by the reviewer. The quantities have central values and uncertainties which are strongly deviating from other measurements, libraries and/or calculations.

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Quality classes

3.1.3 Subentries which are reviewed by checking the publication (R or N)

R1 **Paper reviewed: small deviations.**
The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties, which are close to other measurements, libraries and/or calculations.

R2 **Paper reviewed: questionable deviations**
The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties which are deviating to some extent from other measurements, libraries and/or calculations.

R3 **Paper reviewed: strong deviations**
The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties which are strongly deviating from other measurements, libraries and/or calculations.

N1 **Automatic score T1, but pdf of paper not available for checking**

N2 **Automatic score T2, but pdf of paper not available for checking**

N3 **Automatic score T3, but pdf of paper not available for checking**

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Quality classes

- **T: compared with theory/libraries**
- **N: no pdf file available**
- **R: Reviewed**
- **E: Error in compilation (according to me)**
- **Quality classes 1, 2 and 3 (R1, R2…etc.)**

Reaction	All	Compared	F < 5	T1	T2	T3	N1	N2	N3	R1	R2	R3	E1	E2	E3	Reviewed
(n,tot)	4528	4421	4390	2187	963	0	816	430	0	0	0	0	0	0	0	
(n,el)	871	852	846	446	225	0	112	67	0	0	0	0	0	0	0	
(n,non)	375	365	364	213	100	0	32	20	0	0	0	0	0	0	0	
(n,n')	229	151	149	52	12	4	49	5	12	6	3	8	0	0	0	y
(n,n')m	255	248	242	57	30	1	92	18	9	16	6	19	0	0	0	y
(n,n')n	3	3	2	0	1	0	0	0	0	0	2	0	0	0	0	y
(n,2n)	1643	1600	1593	378	126	30	331	48	20	408	202	53	2	2	0	y
(n,2n)g	384	377	376	70	20	8	80	24	4	105	35	27	2	0	3	y
(n,2n)m	712	701	691	109	26	6	154	55	5	214	83	47	1	0	2	y
(n,2n)n	42	41	33	7	3	3	5	5	0	3	5	10	0	0	0	y
(n,3n)	94	83	78	17	9	0	34	11	0	6	4	2	0	0	0	y
(n,3n)g	8	6	4	3	0	0	0	3	0	0	0	0	0	0	0	y
(n,3n)m	19	16	16	6	4	0	1	4	0	1	0	0	0	0	0	y
(n,f)	1229	1153	1127	515	131	112	267	68	56	0	0	0	0	0	0	

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Goodness-of-fit estimators

$$F = 10^{\sqrt{\frac{1}{N}\sum_i^N f_i}} \qquad (4.1)$$

where the term for each individual data point is

$$f_i = \left(\log \frac{\sigma_T^i}{\sigma_E^i}\right)^2, \qquad (4.2)$$

$$\chi^2 = \frac{1}{N}\sum_i^N \chi_i^2,$$

where the term for each individual data point is

$$\chi_i^2 = \left(\frac{\sigma_T^i - \sigma_E^i}{\Delta\sigma_E^i}\right)^2,$$

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Reaction	$F_{1\sigma}$	$F_{2\sigma}$	#Sets
(n,n')	1.40	5.8	213
(n,n')m	1.52	3.5	251
(n,2n)	1.25	2.50	1675
(n,2n)g	1.41	2.45	397
(n,2n)m	1.28	3.6	719
(n,3n)	2.27	23.6	84
(n,n$_1$)	2.6	20.	491
(n,n$_{2-40}$)	3.3	80.	312
(n,γ)	1.47	6.55	5188
(n,γ)g	2.11	10.5	143
(n,γ)m	2.10	11.3	211
(n,p)	1.31	3.55	1846
(n,p)g	1.82	8.0	188
(n,p)m	1.70	7.0	426
(n,d)	3.0	15.0	45
(n,t)	2.1	27.0	137
(n,a)	2.0	12.0	1068
(n,a)g	2.4	13.0	78
(n,a)m	2.75	13.0	196
(n,np)	7.5	121.7	148
(n,na)	7.2	6.75	54
(n,xp)	1.43	2.99	87
(n,xt)	2.00	159.	23
(n,xa)	2.07	9.07	164

Table 4.1: $F_{1\sigma}$ and $F_{2\sigma}$ values per reaction channel. A fraction of 68.27 and 95.45 %, respectively, of all F values fall inside the given boundaries. To indicate the statistical significance,

Class 1 : (T1, N1, R1 and E1): $1 \leq F \leq F_{1\sigma}$

Class 2 : (T2, N2, R2 and E2): $F_{1\sigma} < F \leq F_{2\sigma}, \chi^2 < 30, Q_t < 0.10$
$F > F_{1\sigma}, \chi^2 < 30, Q_t < 0.05$

Class 3 : (T3, N3, R3 and E3): $F_{1\sigma} < F \leq F_{2\sigma}, \chi^2 > 30, Q_t > 0.10$
$F > F_{2\sigma}, \chi^2 > 30, Q_t > 0.05$

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Distribution of F-values

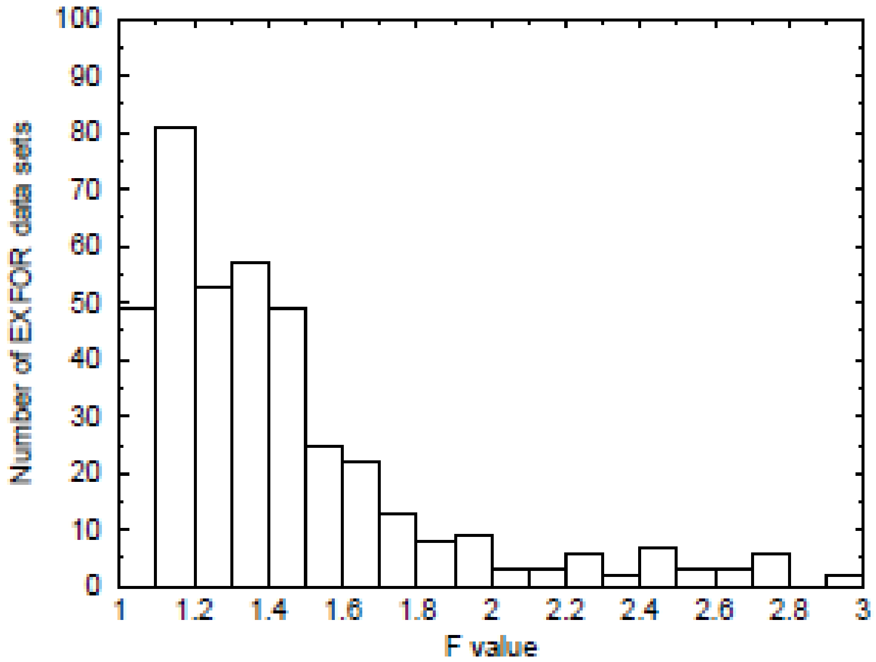

Figure 4.3: Distribution of F-values for the (n,p) reaction.

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Energy dependent predictive power

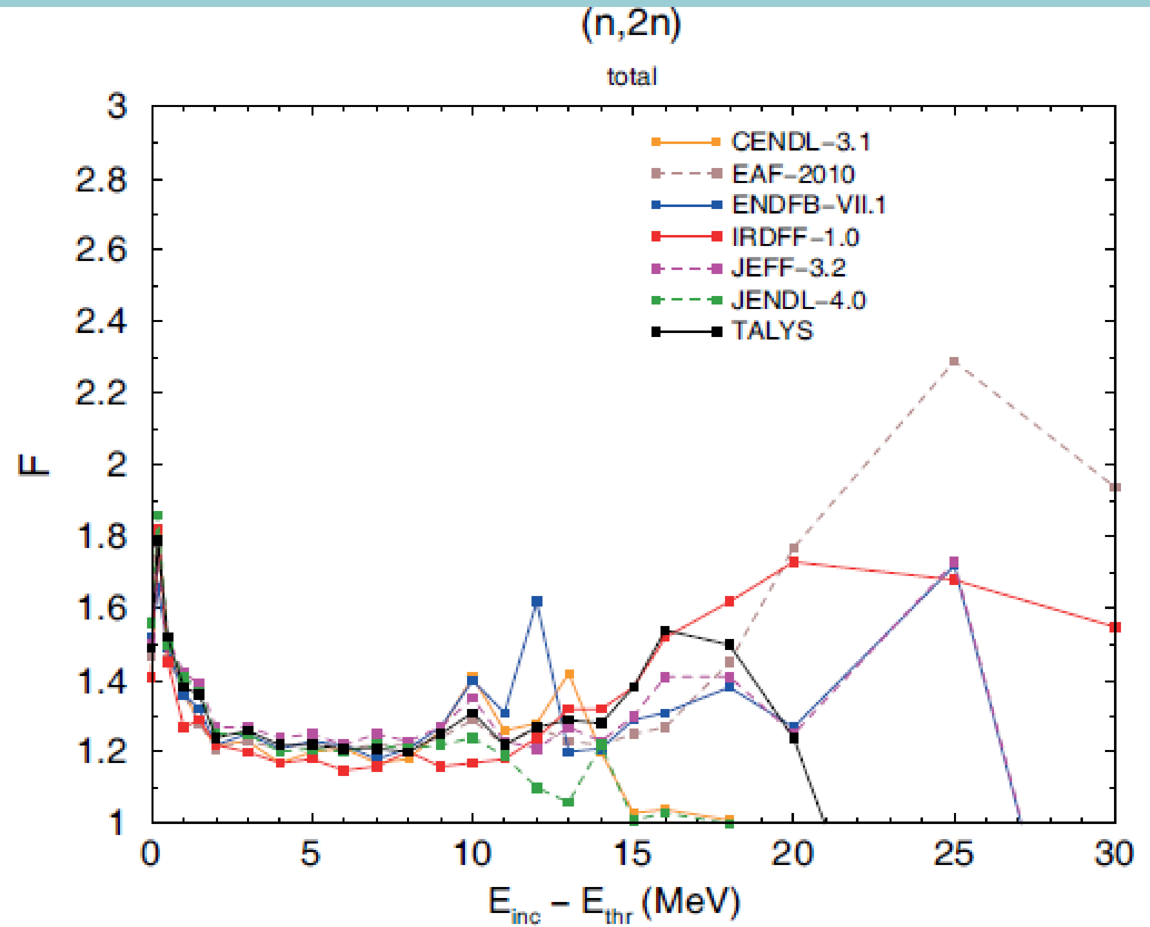

Fig. 3. Energy dependent deviation of all calculated (n, 2n) cross sections compared to the values in EXFOR. For reference, also the values for other world libraries are given.

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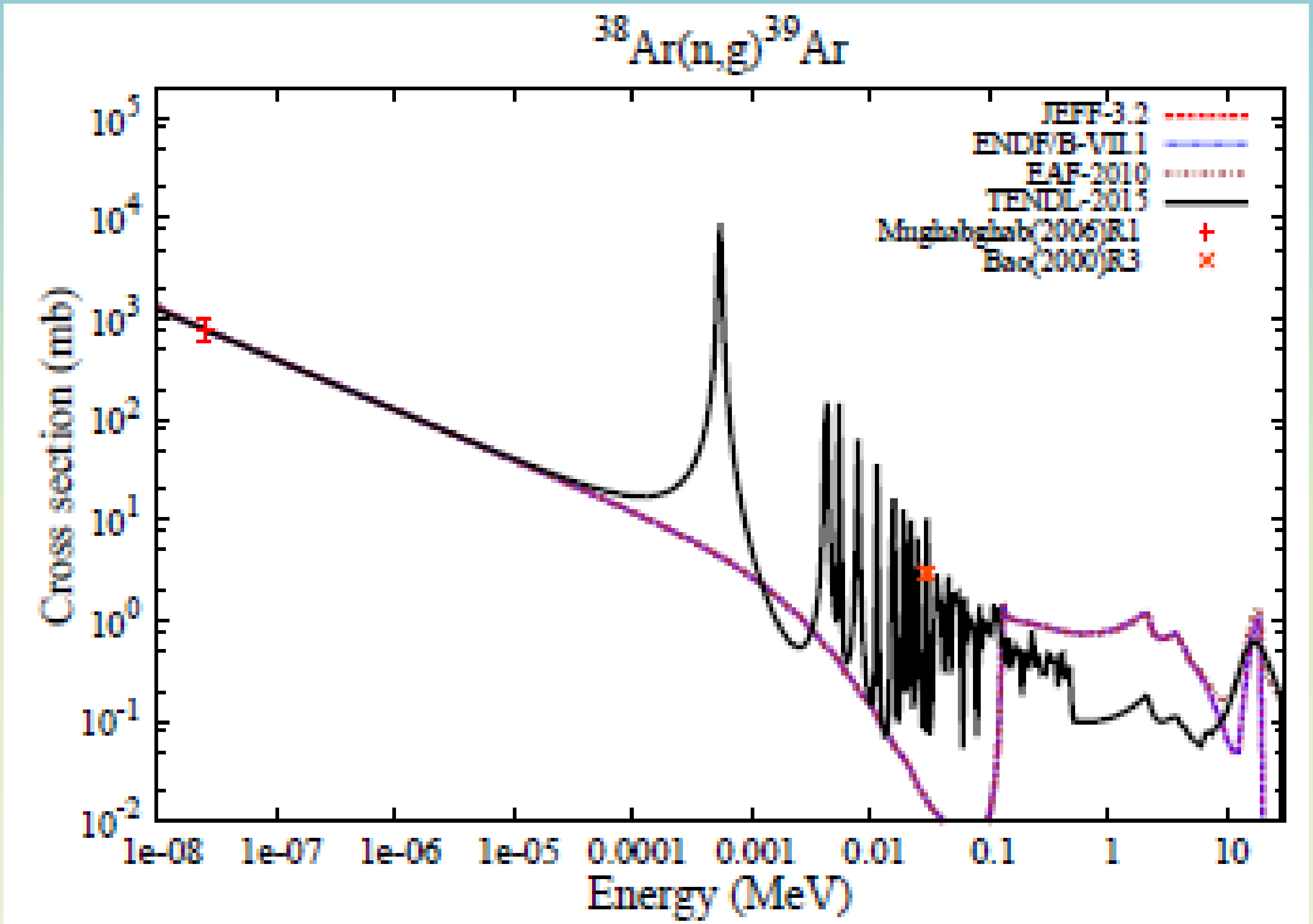

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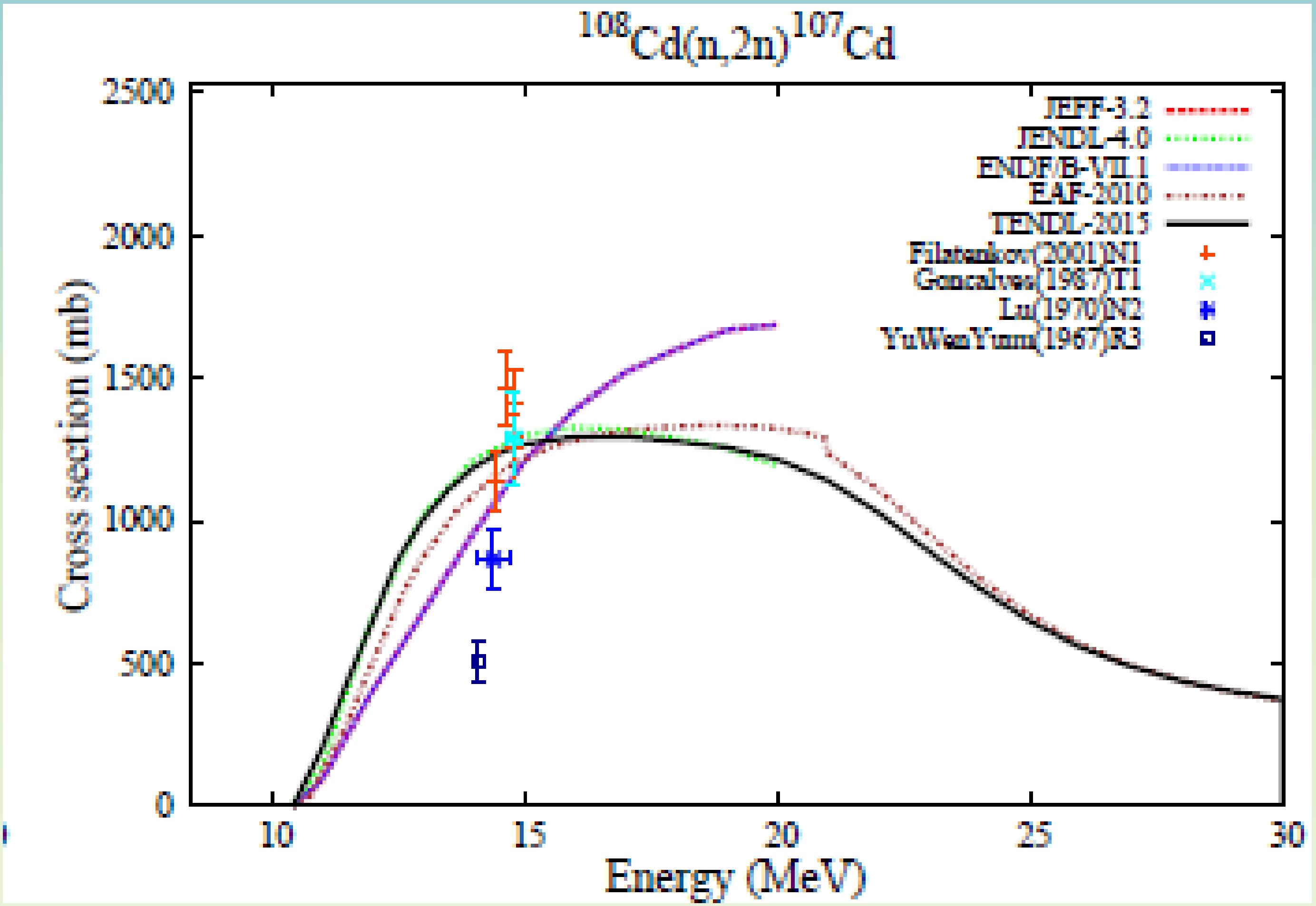

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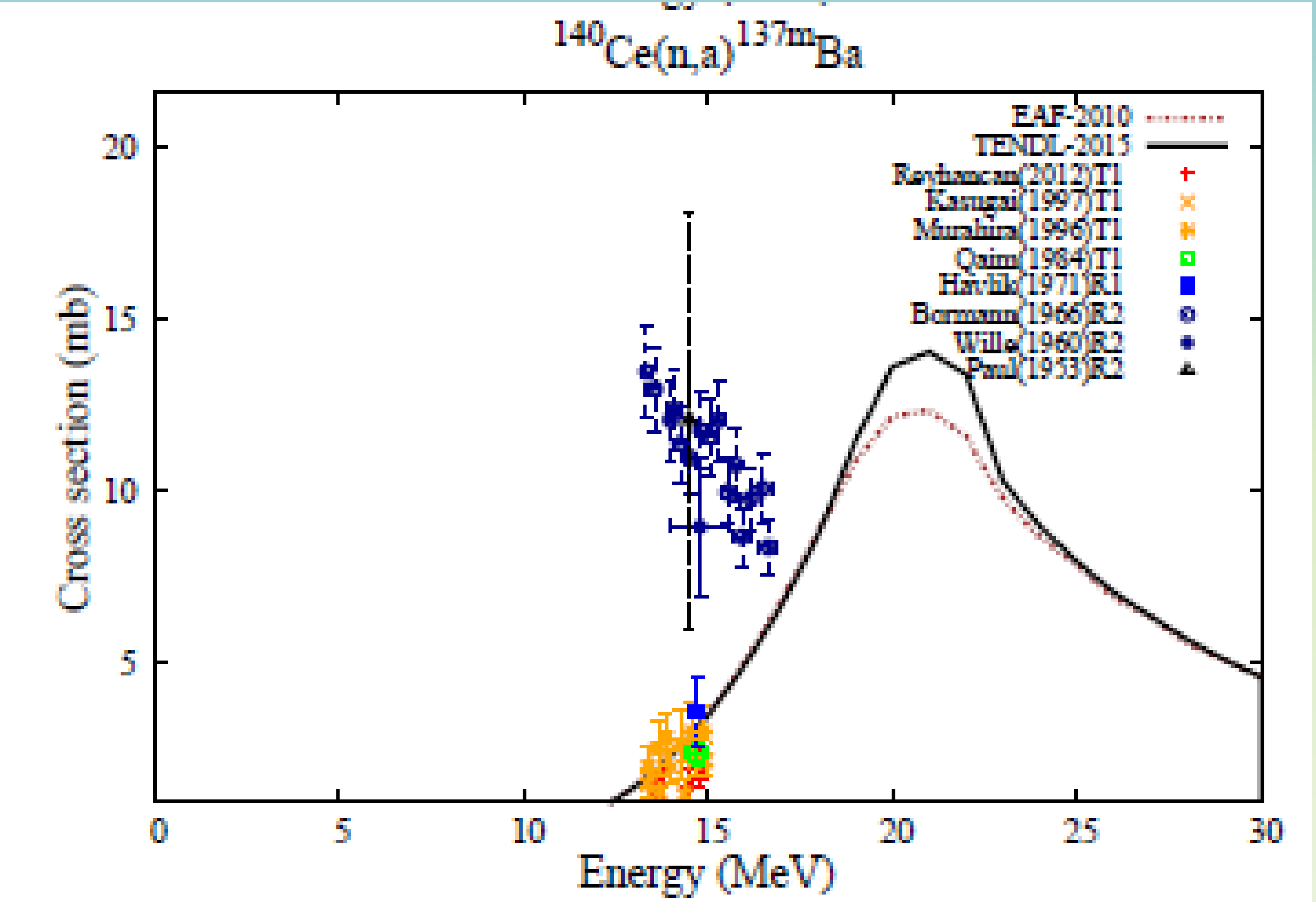

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Other information available

- F factors averaged over subentry
- F factors averaged over entry (“Quality of the entire experiment, or experimentalist”)
- Statistical distribution of uncertainties
- F factors averaged per reaction channel
- F factors per projectile, target
- Etc. etc.

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Starting point: "Expert" (Gaussian) parameter uncertainties

(A.J. Koning and D. Rochman, ``Modern nuclear data evaluation with the TALYS code system", Nucl. Data Sheets 113, 2841 (2012).) Origin: *Fingerspitzengefühl*

Parameter	uncertainty (%)	Parameter	uncertainty (%)
Optical model			
r_V^n	2	d_1^n	10
a_V^n	2	d_2^n	10
v_1^n	2	d_3^n	10
v_2^n	3	r_{SO}^n	10
v_3^n	3	a_{SO}^n	10
v_4^n	5	v_{so1}^n	5
w_1^n	10	v_{so2}^n	10
w_2^n	10	w_{so1}^n	20
r_D^n	3	w_{so2}^n	20
a_D^n	4		
r_V^p	4	d_1^p	20
a_V^p	4	d_2^p	20
v_1^p	4	d_3^p	20
v_2^p	6	r_{SO}^p	20
v_3^p	6	a_{SO}^p	20
v_4^p	10	v_{so1}^p	10
w_1^p	20	v_{so2}^p	20
w_2^p	20	w_{so1}^p	40
r_D^p	6	w_{so2}^p	40
a_D^p	8	r_C^p	10
λ_V	5	λ_{V1}	5
λ_W	5	λ_{W1}	5
λ_{Vso}	5	λ_{Wso}	5

Level density			
a	11.25-0.03125.A	σ^2	30
γ	30	δW	± 1 MeV
α	30	β	30
R_σ	30	γ	30
E_0	20	E_M	20
T	10	δ	± 2 MeV
K_{rot}	80		
C_{HFM}	30	δ_{HFM}	30
Gamma-ray strength			
Γ_γ	20	$\sigma_{E\ell}$	20
$\Gamma_{E\ell}$	20	$E_{E\ell}$	10
$E_{\rm nor}$	20	$E_{\rm shift}$	± 0.8 MeV
Fission			
B_f	10	$\hbar\omega_f$	10
Pre-equilibrium			
M^2	30	$R_{\pi\pi}$	30
$R_{\nu\pi}$	30	$R_{\pi\nu}$	30
$R_{\nu\nu}$	30	R_γ	50
g_ν	11.25-0.03125.A	$E_{\rm surf}$	20
g_π	11.25-0.03125.A	$C_{\rm break}$	80
$C_{\rm knock}$	80	$C_{\rm strip}$	80

Multiply these uncertainties by 5 and sample ~200 parameters from uniform distribution

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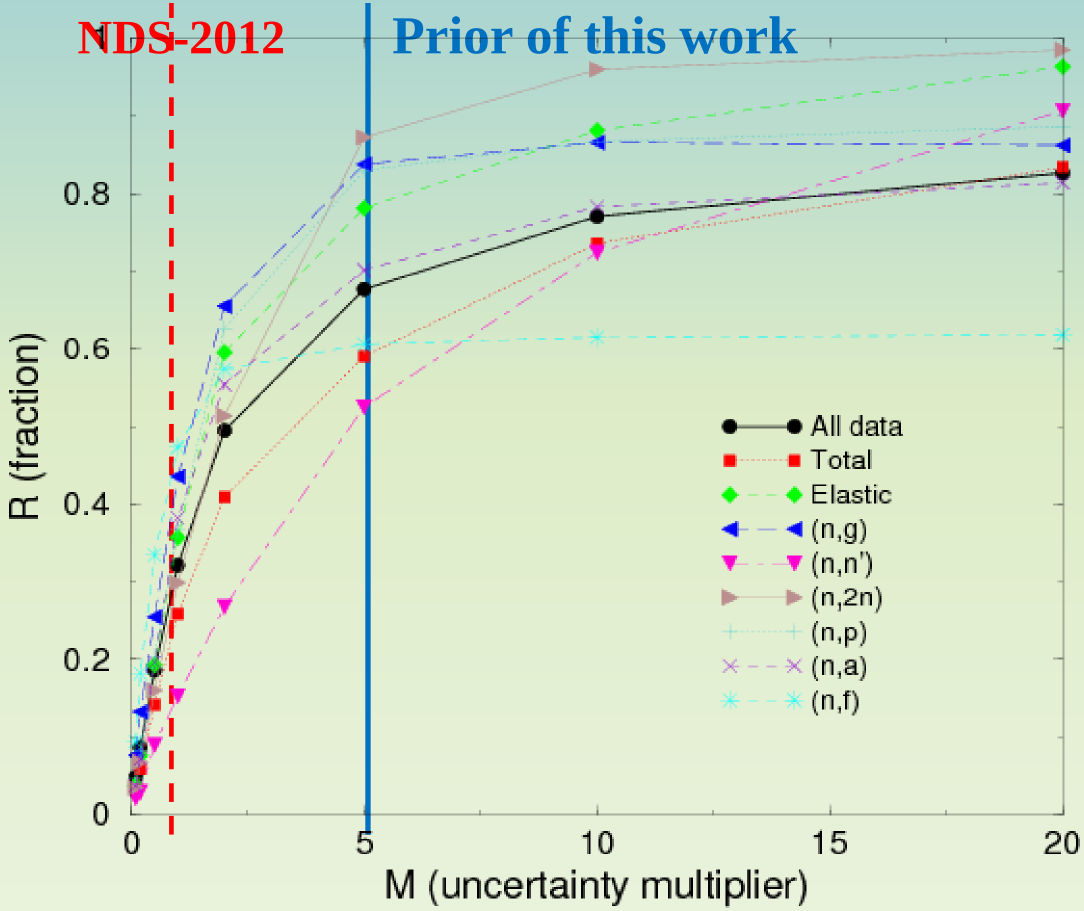
Fraction of EXFOR data inside 1-sigma uncertainty band



Random TALYS calculations for all nuclides compared with 23490 experimental data sets = 2.7 million data points

WPEC-2016, 12-13 May 2016
NEA Data Bank, Paris

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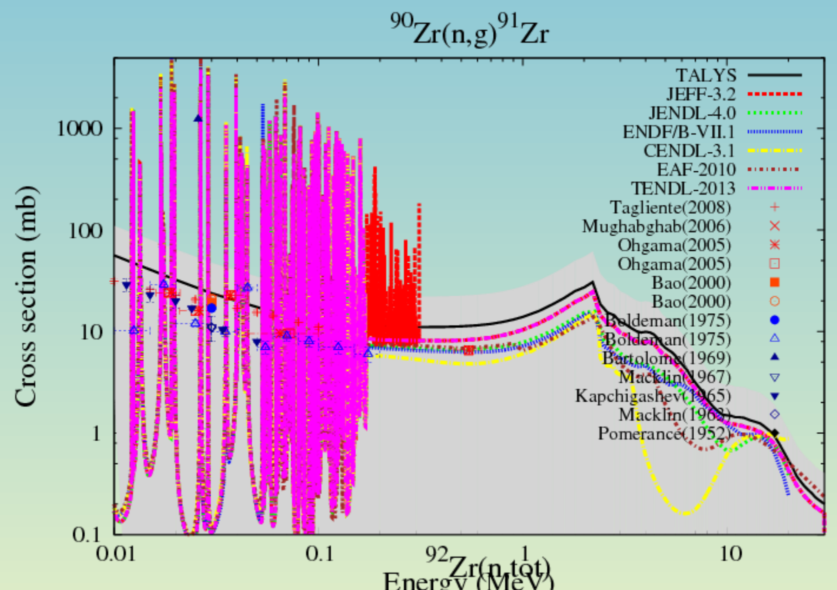
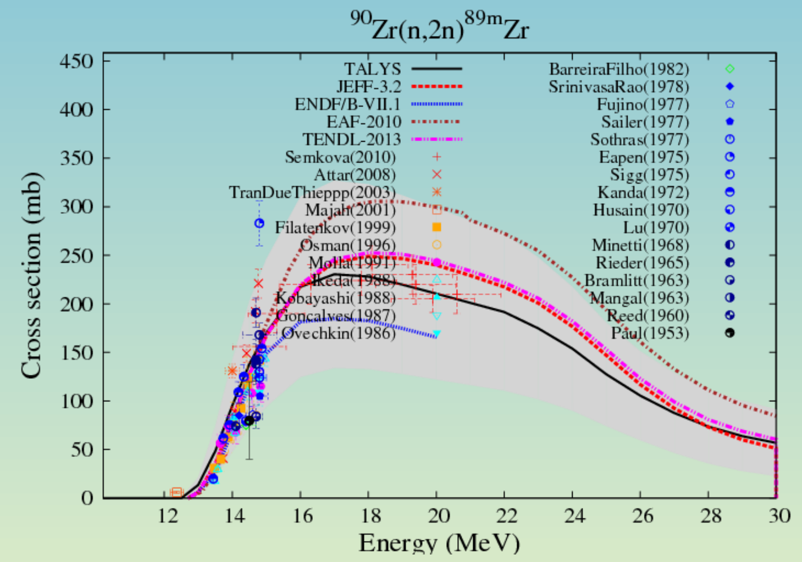
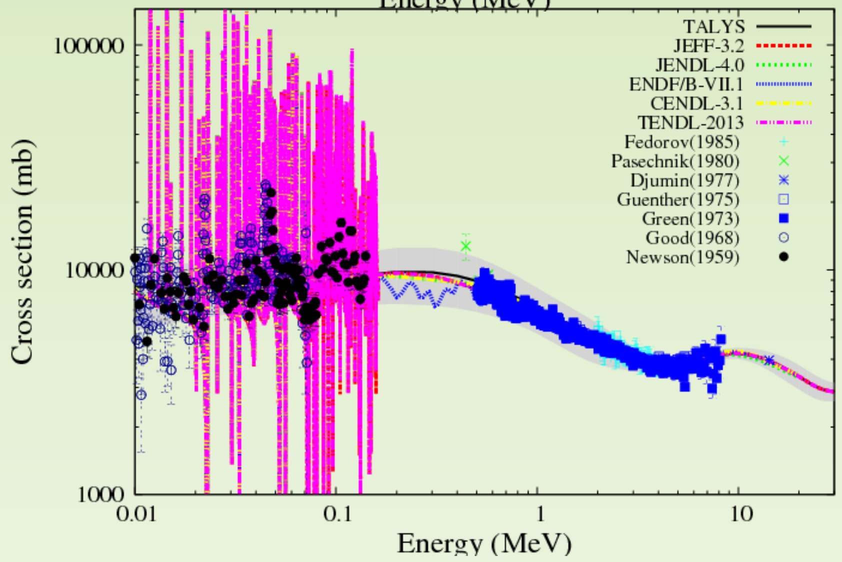
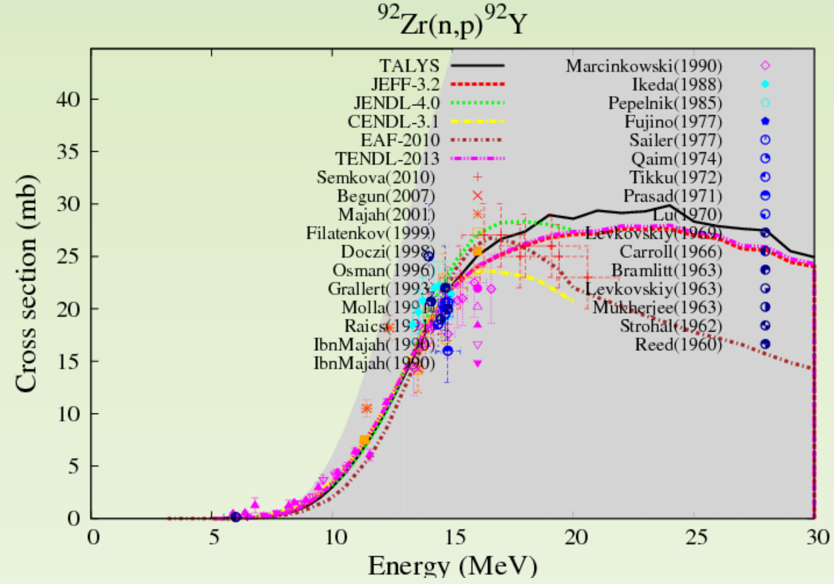
“Knowing nothing”: Random TALYS parameters from initial parameter pdf: uniform distribution with uncertainty multiplier = 5









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Initial probability distribution for cross sections

- Perform 1 global, unadjusted TALYS calculation for the entire periodic table of elements
- Compare the results with all EXFOR data: 23490 experimental data sets = 2.7 million data points
- Determine the average deviation between TALYS and experiment.
- Use the results as knowledge ("pseudo-experimental data") in a Bayesian Monte Carlo updating scheme.

- A.J. Koning, "Bayesian Monte Carlo method for nuclear data evaluation", EPJ A51(12), p1-16 (2015)

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TALYS-based evaluated nuclear data library

Home Reference & us Citations

TENDL-2015

By A.J. Koning[1], D. Rochman[2], J. Kopecky[3], J.Ch. Sublet[4], M. Fleming[4], E. Bauge[7], S. Hilaire[7], P. Romain[7], B. Morillon[7], H. Duarte[7], S.C van der Marck[6], S. Pomp[5], H. Sjostrand[5], R. Forrest[1], H. Henriksson[8], O. Cabellos[9], S. Goriely[10], J. Leppanen[11], H. Leeb[12], A. Plompen[13], and R. Mills[14]

[1] IAEA, [2] PSI,[3] JUKO Research, [4]CCFE, [5]Uppsala Univ., [6]NRG, [7]CEA,[8]Vattenfall, [9]NEA, [10]ULB, [11]VTT, [12]ATI, [13]IRMM, [14]NNL.

We believe that our great goal can be achieved with systematism and reproducibility. We are so outside the box, that the box is a point

Random files

1. Random fission yields

2. Random thermal scattering

Sub-library files

1. neutron

Proton 2.

Deuteron 3.

TENDL-2015: (release date: 18 January 2016)

Last update: 2 May 2016

TENDL is a nuclear data library which provides the output of the **TALYS** nuclear model code system for direct use in both basic physics and applications. The 8th version is **TENDL-2015**, which is based on both default and adjusted **TALYS** calculations and data from other sources (previous releases can be found here: 2008, 2009, 2010, 2011, 2012, 2013, and 2014).

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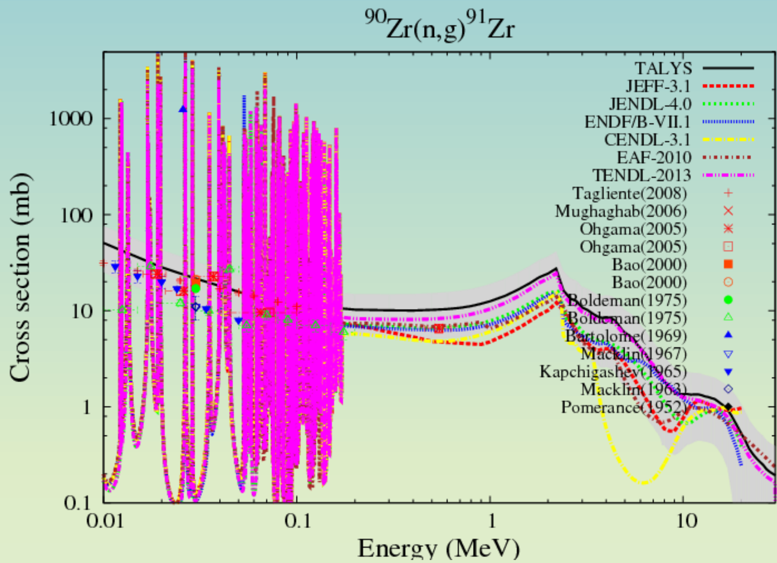
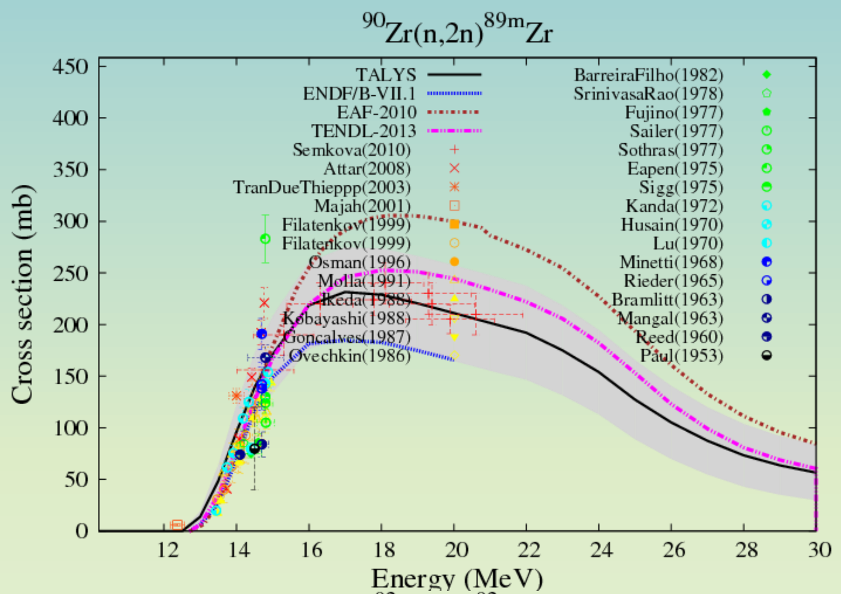
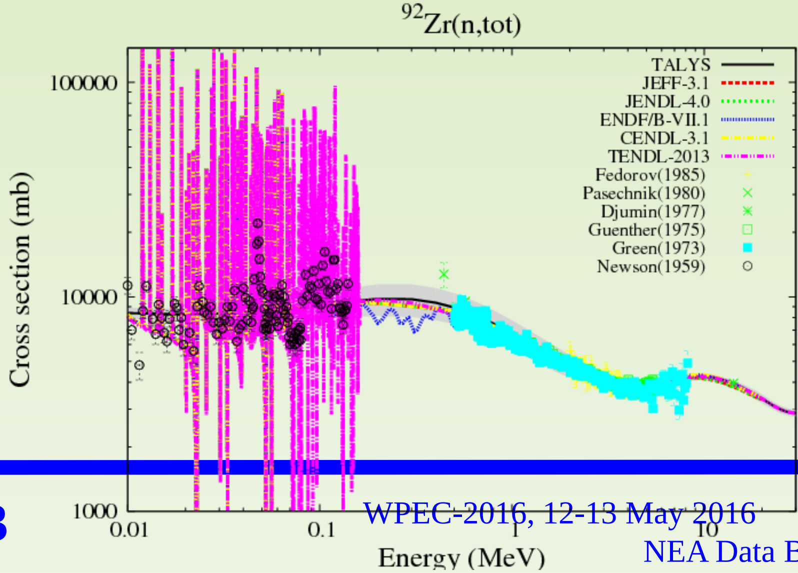
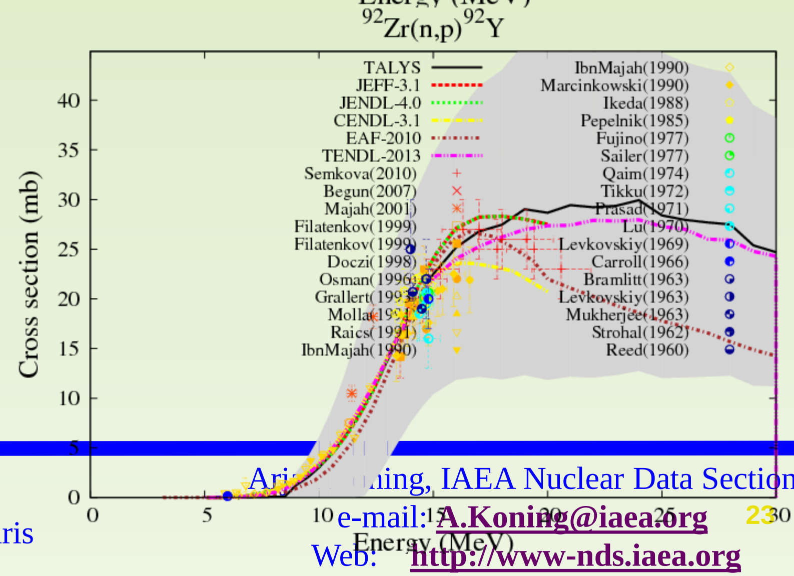
Initial probability distributions for cross sections

Starting point: global TALYS central values and uncertainties based on cross sections for all nuclides









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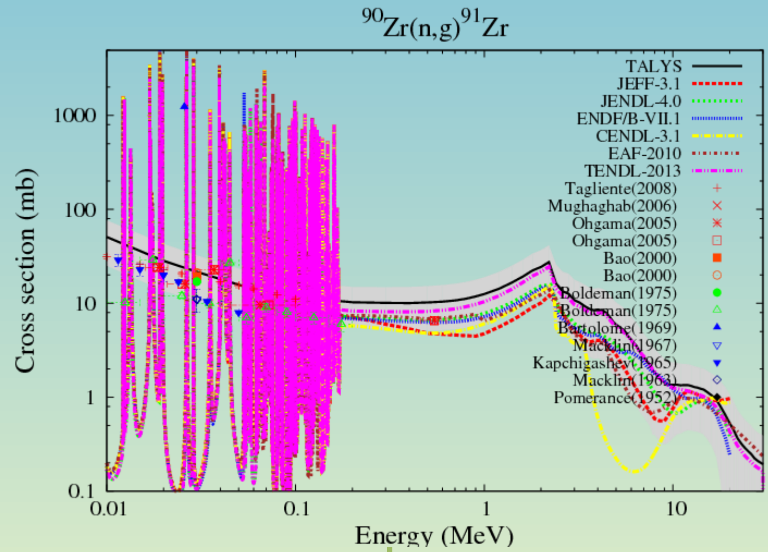
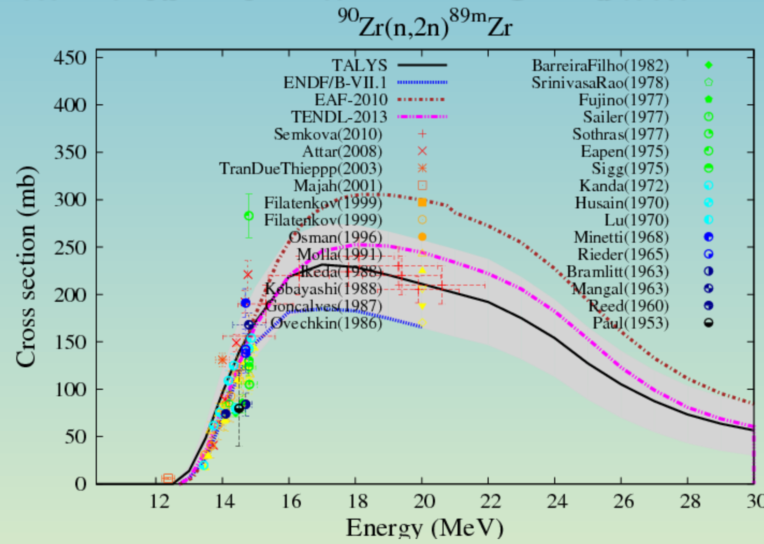
Zooming in

Prior: Global TALYS – uncertainties from all EXFOR data

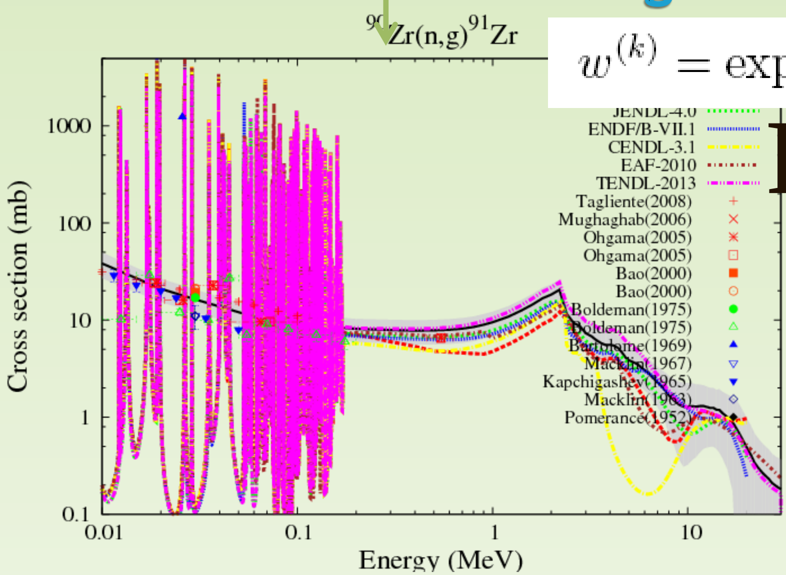


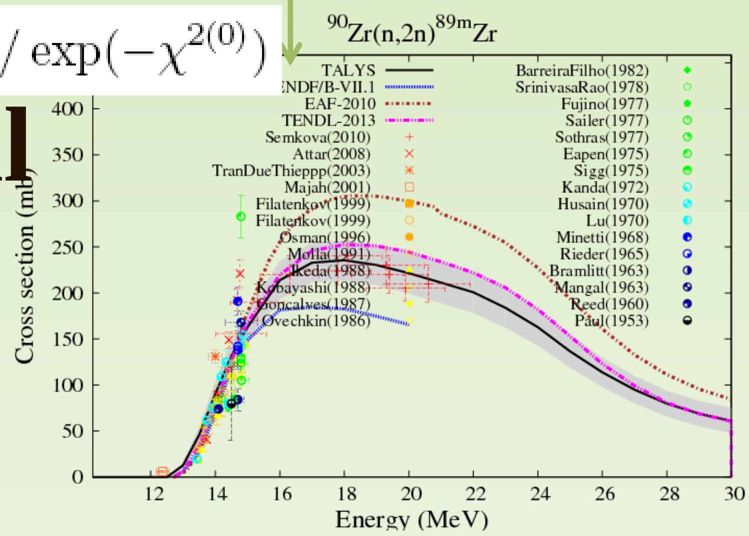


Use weights based on EXFOR for ^{90}Zr

$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$

Final





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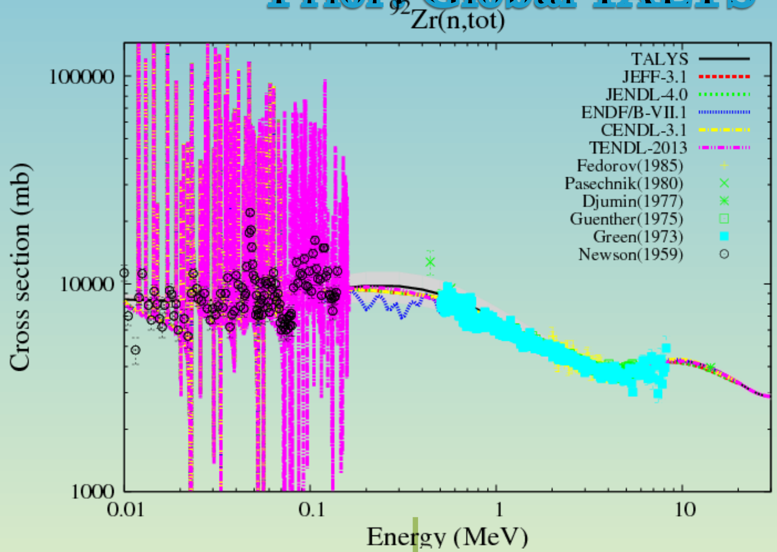
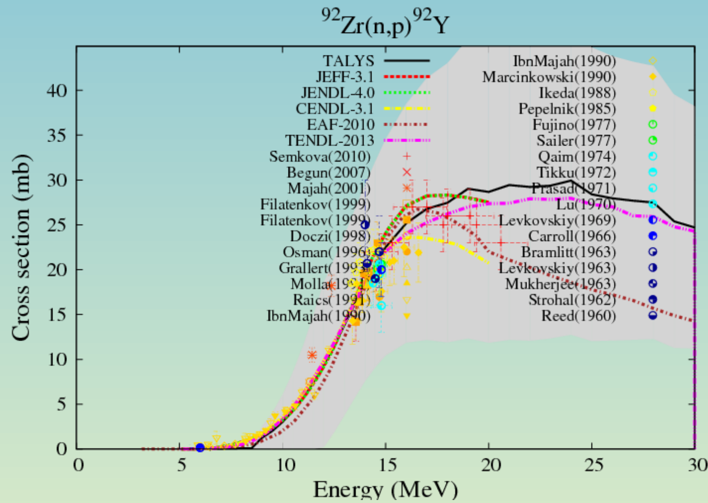
Zooming in

Prior: Global TALYS – uncertainties from all EXFOR data

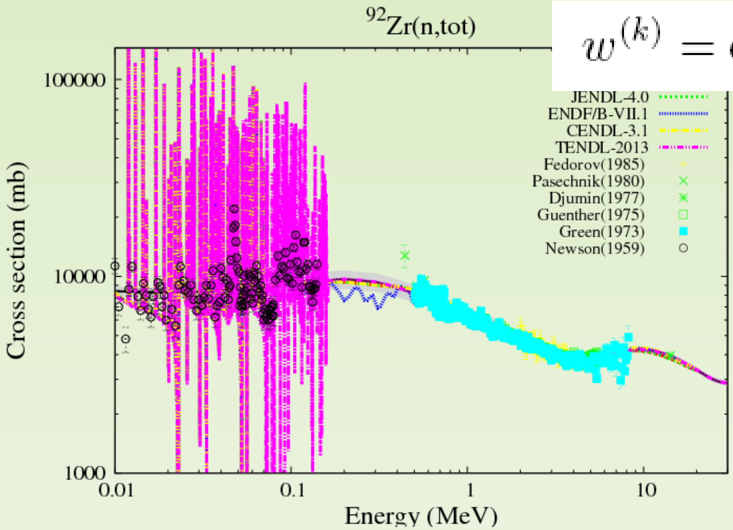


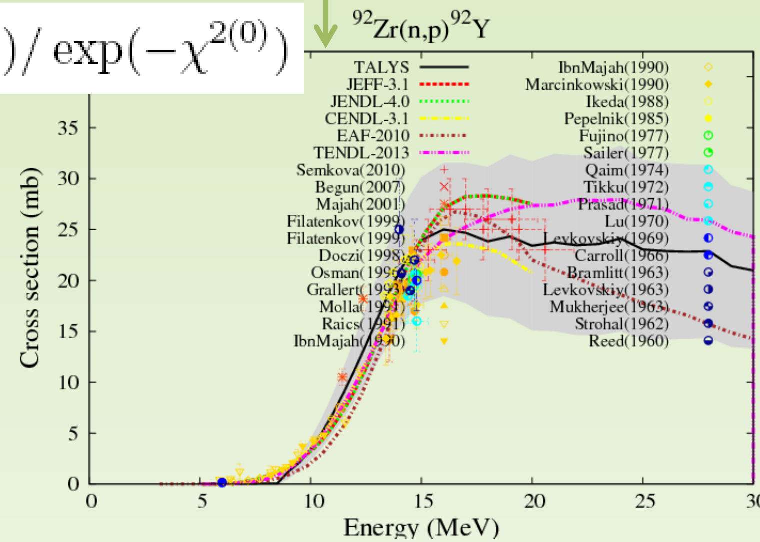


Use weights based on EXFOR for ^{90}Zr

$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$

Final





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Conclusions

- WPEC SG30 on the quality of the EXFOR database has resulted in more NEA activities in the 2010-2016 period.
- EXFOR has been compared, and to a large extent reviewed, for all neutron-induced cross sections – (n,tot), (n,el), (n,non), (n,f) remain to be done.
- A huge subentry scoring table exists, containing quality scores per subentry. The most important score is “R” which means the paper has been “glanced through” to see whether there was no compiler mistake.
- This table should NOT influence the contents of EXFOR, but is important to include or exclude data in nuclear data evaluations. It should be decided how and if this table can be stored and used as an EXFOR tool.
- This is needed for modern nuclear data evaluation.

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