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Validation of EXFOR, the world nuclear data libraries, and TALYS

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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 NEA/DB/DOC(2014)3: 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 NEA/DB/DOC(2017)1: 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.

Main contributors

- Emmeric Dupont, NEA (-2014), for help to initiate this project and feedback on the first results
- Oscar Cabellos, NEA (2014-2017), for continuing this project
- Viktor Zerkin, IAEA: for releasing XC4 databases and extensions of the format
- Naohiko Otsuka: for feedback on erroneous compilations

Approach

For purposes like:

- TENDL
- Machine learning
- Automated plotting
- Automated optimization, etc.

ALL data in EXFOR need to directly available (i.e. not via a clickable web interface).

Thus:

- Produce a directory structured database out of EXFOR
- Perform statistical checks in the process

Newbase code and database

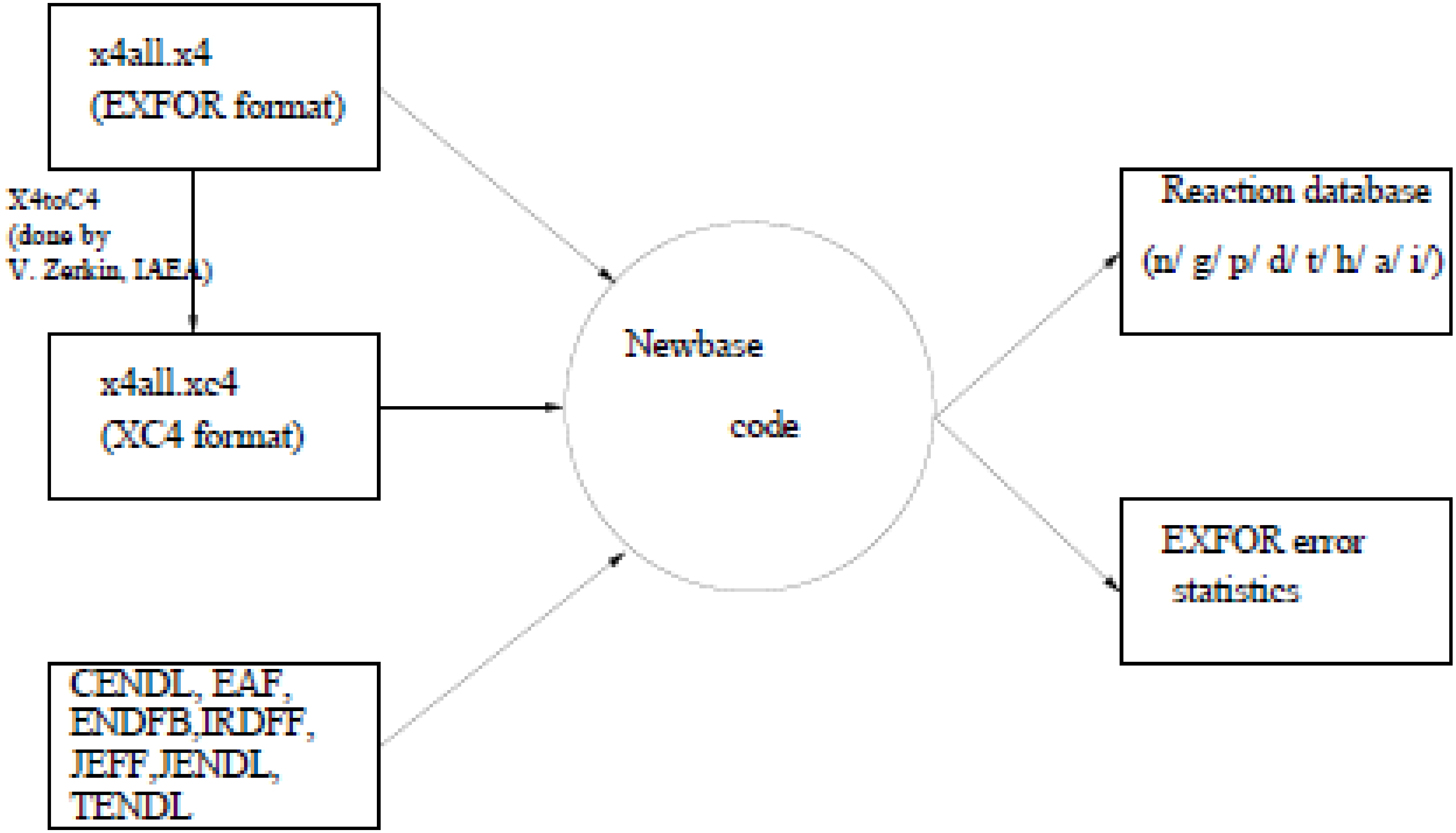


Figure 2.1: Databases produced out of EXFOR.

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.)
- See NEA/DB/DOC(2017)1

Reaction	All	Compared	F < 3	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	
[illegible]	53	53	36	22	9	0	4	2	0	[illegible]	6	0	0	0	0	y

Goodness-of-fit estimators

χ^2 per point:

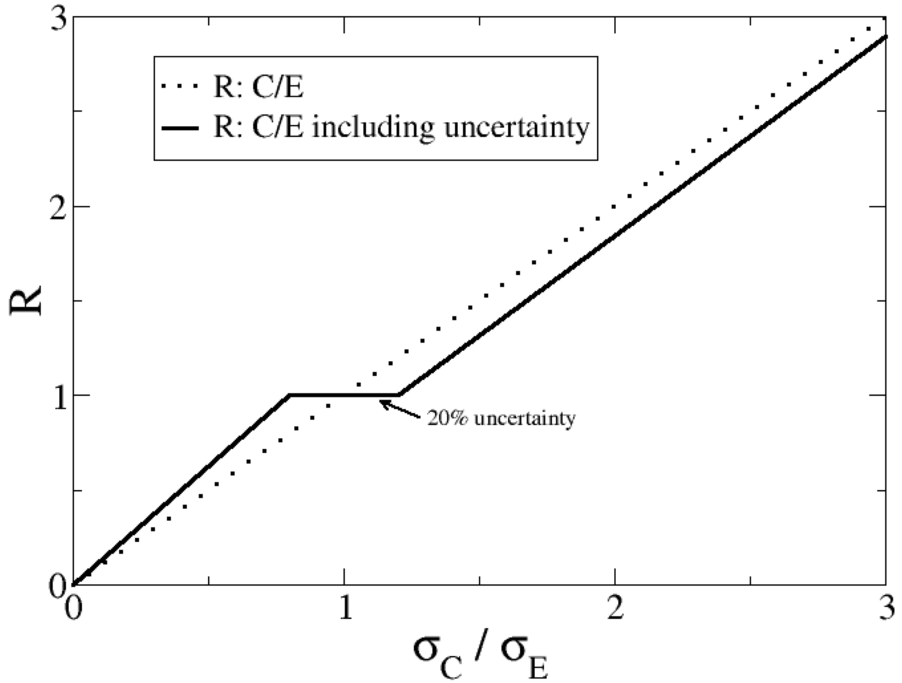
$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sigma_T^i - \sigma_E^i}{\Delta\sigma_E^i}\right)^2 .$$

Root-mean-square asymmetry per point:

$$A = \exp\left[\frac{1}{N}\sum_{i=1}^{N}\ln R_i\right]$$

Root-mean-square deviation per point:

$$F = \exp\left[\frac{1}{N}\sum_{i=1}^{N}\ln^2 R_i\right]^{1/2}$$

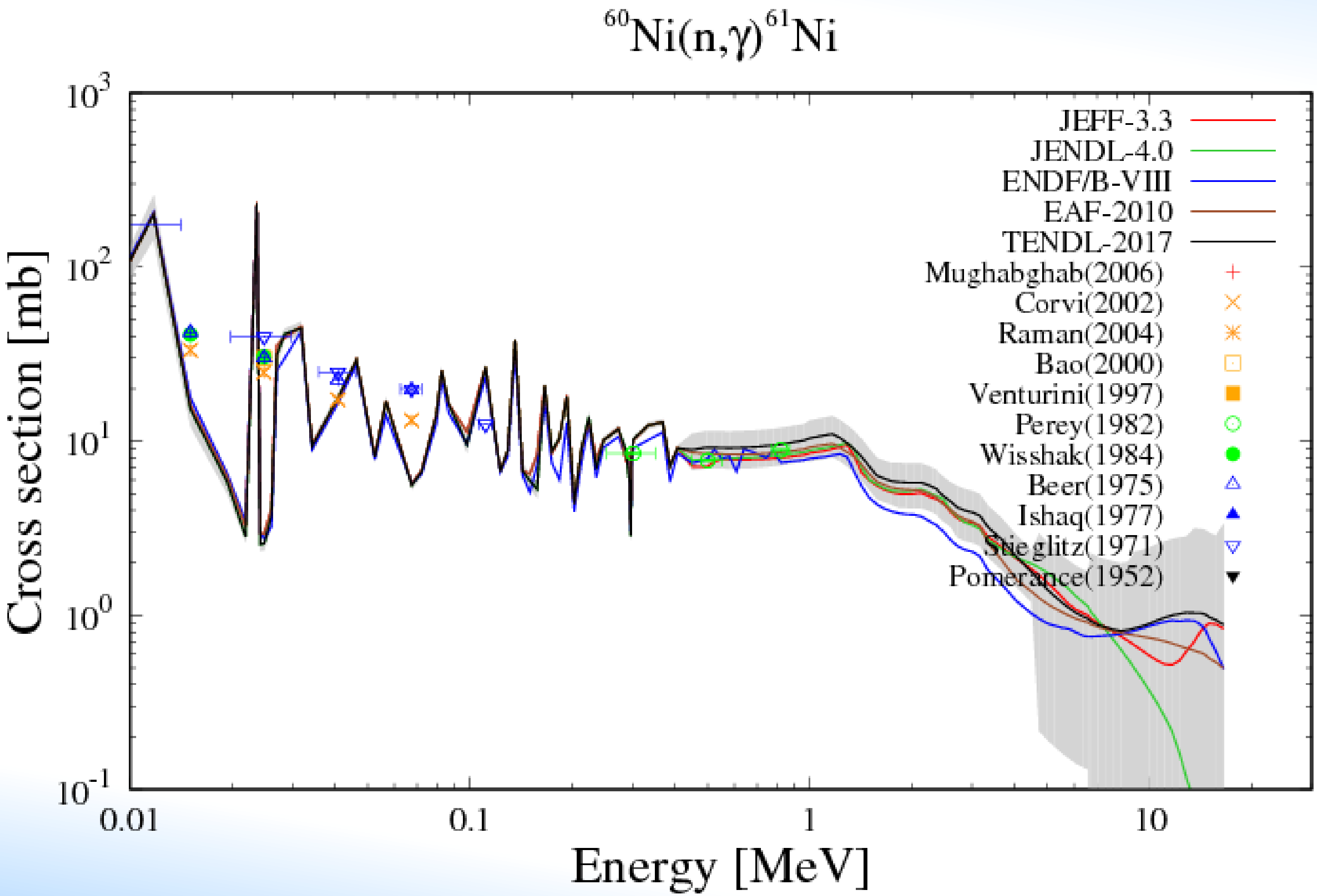


where R_i is the ratio of theory and experiment taking into account the experimental uncertainty:

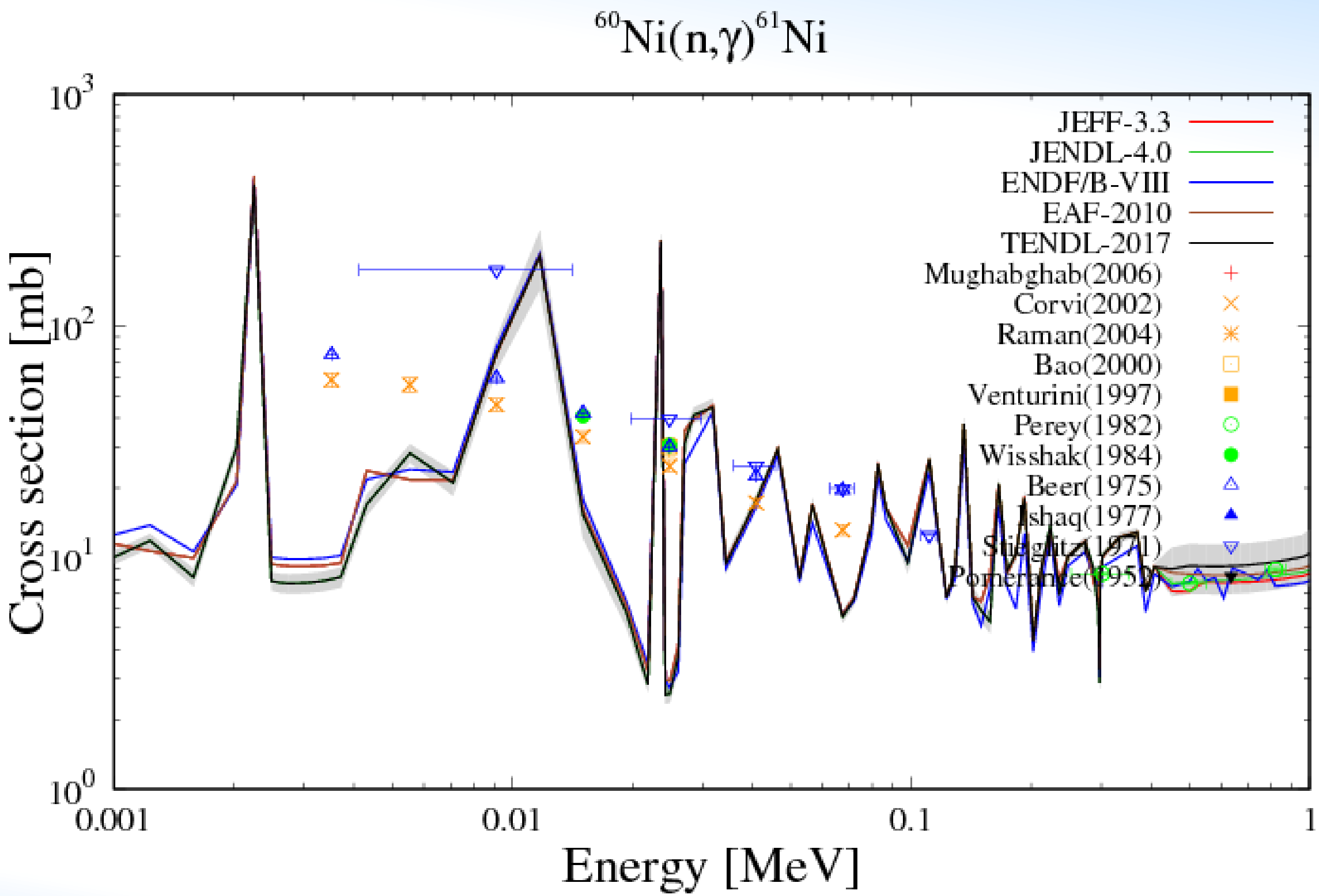
$$\begin{aligned} R_i &= \frac{\sigma_T^i}{\sigma_E^i - \Delta\sigma_E^i}, \text{ if } \sigma_T^i < \sigma_E^i - \Delta\sigma_E^i \\ &= \frac{\sigma_T^i}{\sigma_E^i + \Delta\sigma_E^i}, \text{ if } \sigma_T^i > \sigma_E^i + \Delta\sigma_E^i \\ &= 1, \text{ otherwise} \end{aligned} \quad (66.4)$$

Utsunomiya et al, to be published PRC (2018)

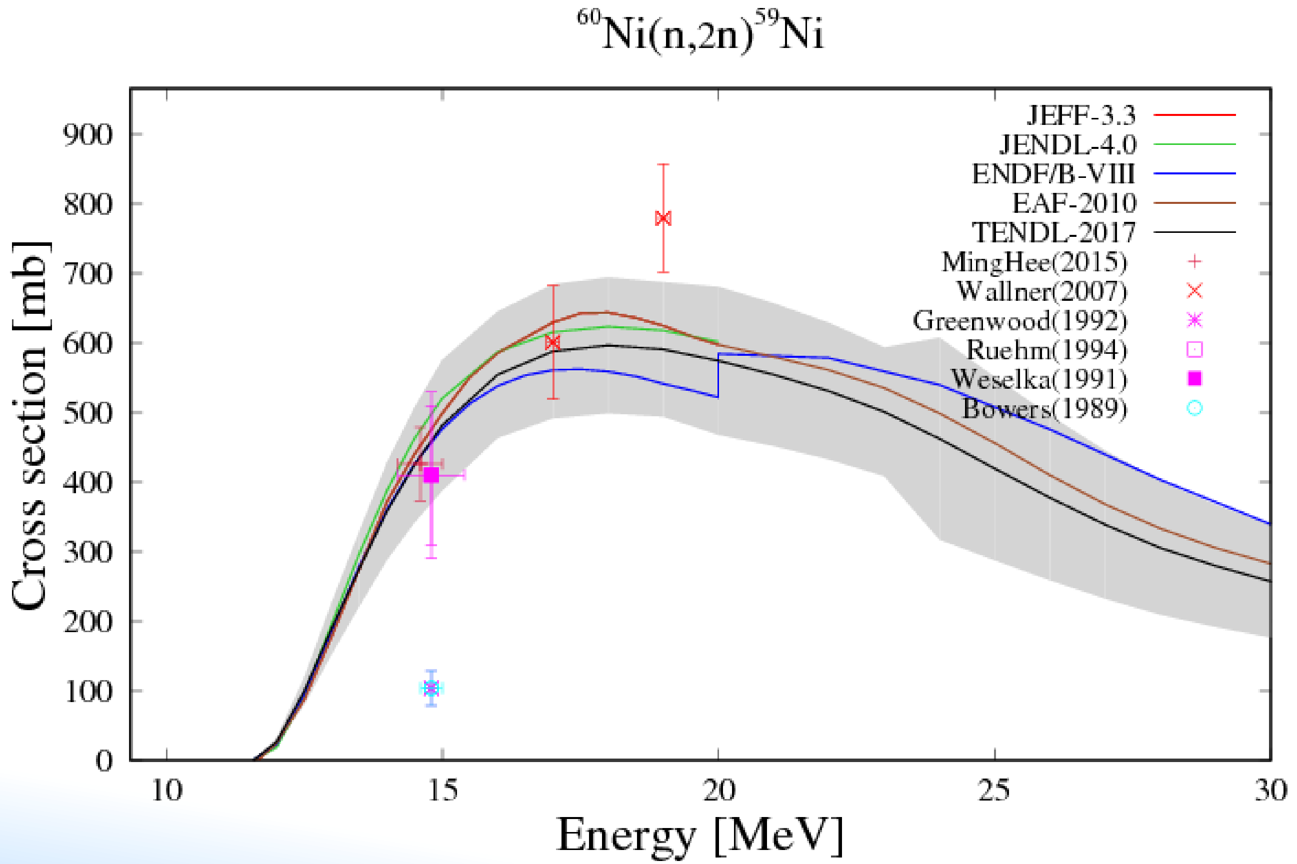
Example: capture (groupwise)



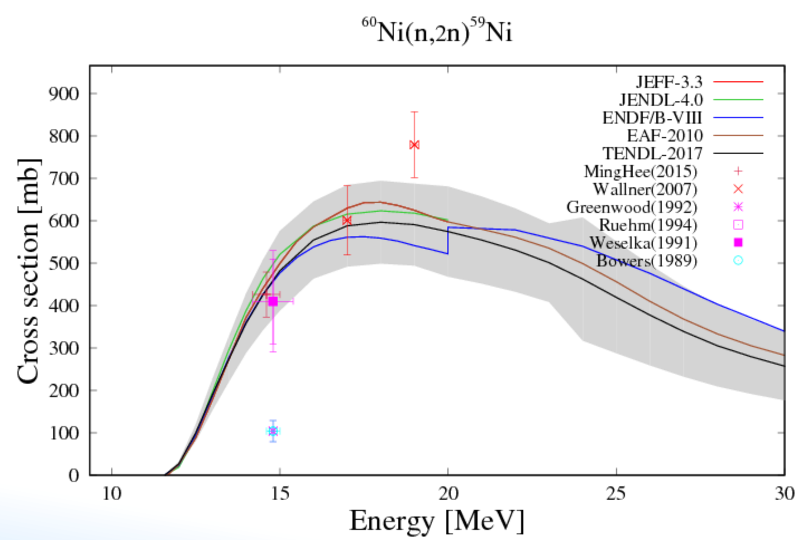
Example: capture (groupwise)



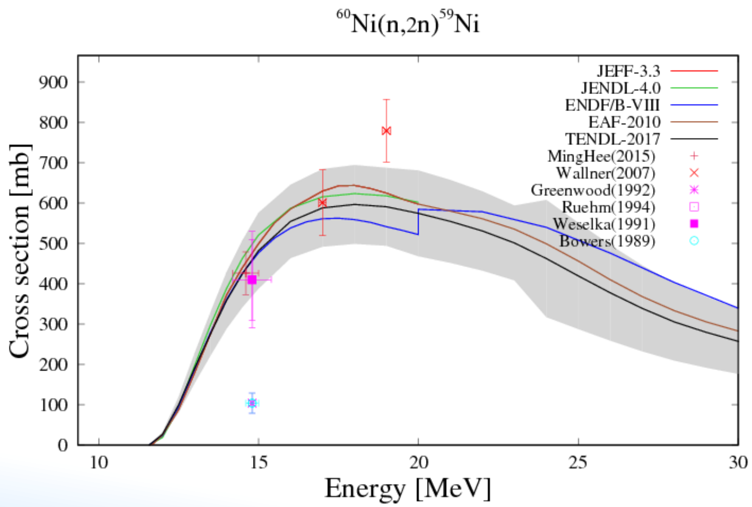
Automated plots for all nuclides, projectiles, reactions available at ftp://ftp.nrg.eu/pub/www/talys/plots/



Quality 22583002 : T1
Date 22583002 : 20-06-2014
Reaction 22583002 : NP: 1 E-range: 14.8 - 14.8 MeV 28-NI-60(N,2N)28-NI-59,,SIG pdf: y
Paper 22583002 : W.Ruehm+ Jour. Planetary and Space Science Vol.42, Issue.3, p. 227, 1994 A new half-life determination of 59Ni
Action 22583002 :
Comment 22583002 : Evaluation N= 1 F= 1.16 A= 1.16 chi-2= 0.444
Comment 22583002 : TALYS N= 0 F= 0.00 A= 0.00 chi-2= 0.00
Comment 22583002 : cendl3.1 N= 1 F= 1.19 A= 1.19 chi-2= 0.591
Comment 22583002 : eaf.2010 N= 1 F= 1.16 A= 1.16 chi-2= 0.427
Comment 22583002 : endfb8.0 N= 1 F= 1.11 A= 1.11 chi-2= 0.215
Comment 22583002 : irdff1.0 N= 0 F= 0.00 A= 0.00 chi-2= 0.00
Comment 22583002 : jeff3.3 N= 1 F= 1.16 A= 1.16 chi-2= 0.427
Comment 22583002 : jendl4.0 N= 1 F= 1.21 A= 1.21 chi-2= 0.765
Comment 22583002 : tendl.2017 N= 1 F= 1.12 A= 1.12 chi-2= 0.240



```
# Quality  13132005 : R2
# Date     13132005 : 10-08-2012
# Reaction 13132005 : NP:    1 E-range:   14.8     -   14.8      MeV 28-NI-60(N,2N)28-
NI-59,,SIG          pdf: y
# Paper    13132005 : D.L.Bowers+ Rept. American Soc. of Testing and Materials Repor
ts No.1001, p.508, 1989 Analysis of long-lived isotopes by liquid scintillatio
# Action   13132005 : pdf not available, correct in IAEA database
# Comment  13132005 : Evaluation         N=     1    F=   4.57     A=   4.57      chi-
2=   221.
# Comment  13132005 : TALYS              N=     0    F=   0.00     A=   0.00      chi-
2=   0.00
# Comment  13132005 : cendl3.1           N=     1    F=   4.68     A=   4.68      chi-
2=   235.
# Comment  13132005 : eaf.2010           N=     1    F=   4.57     A=   4.57      chi-
2=   221.
# Comment  13132005 : endfb8.0           N=     1    F=   4.39     A=   4.39      chi-
2=   199.
# Comment  13132005 : irdff1.0           N=     0    F=   0.00     A=   0.00      chi-
2=   0.00
# Comment  13132005 : jeff3.3            N=     1    F=   4.57     A=   4.57      chi-
2=   221.
# Comment  13132005 : jendl4.0           N=     1    F=   4.78     A=   4.78      chi-
2=   248.
# Comment  13132005 : tendl.2017         N=     1    F=   4.41     A=   4.41      chi-
2=   202.
```



Distribution of F-values

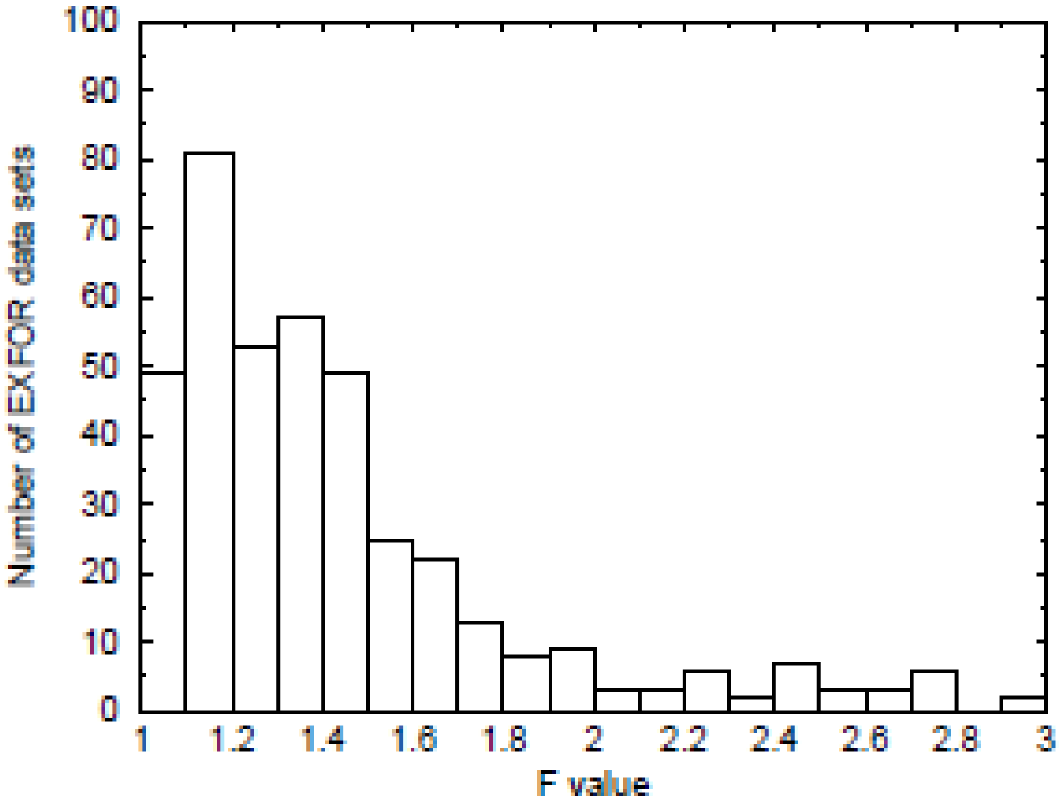


Figure 4.3: Distribution of F-values for the (n,p) reaction.

Energy dependent predictive power

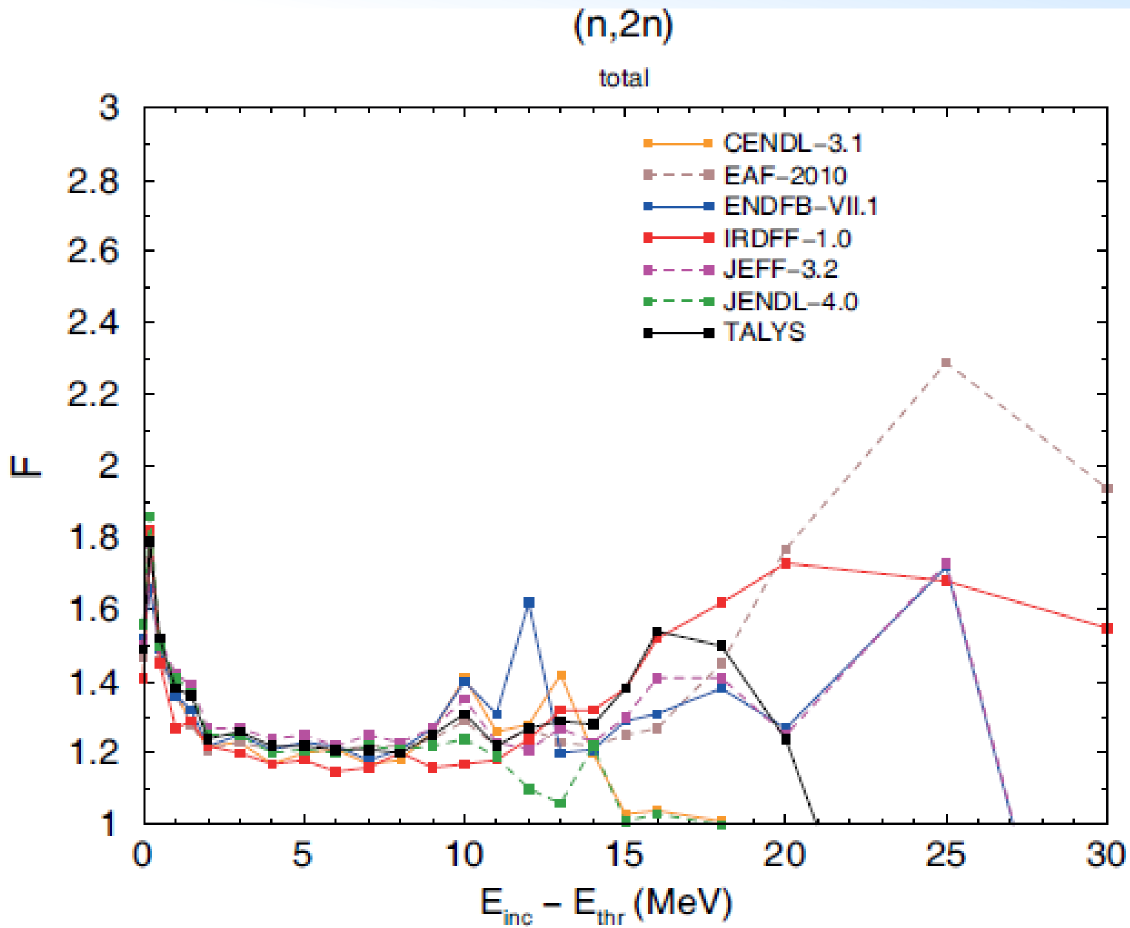


Fig. 3. Energy dependent deviation of all calculated (n, 2n) cross sections compared to the values in EXFOR. For reference, also the values for other world libraries are given.

Sorted uncertainties for neutron capture

No uncertainties

```
  5958 reactions for neutron d MT=102 isomer=  -1
 SUBENT      AUTHOR      YEAR  N              Reaction              Av. Exp   Rel. Err.

V1002716 S.F.Mughabghab  2006  0 100-FM-256(N,G)100-FM-257,,SIG 4.500E+04  0.00
V10027131S.F.Mughabghab  2006  0 100-FM-254(N,G)100-FM-255,,SIG 7.600E+04  0.00
V10026891S.F.Mughabghab  2006  0 97-BK-250(N,G)97-BK-251,,SIG,, 3.500E+05  0.00
V1002543 S.F.Mughabghab  2006  0 86-RN-220(N,G)86-RN-221,,SIG,,  200.      0.00
```

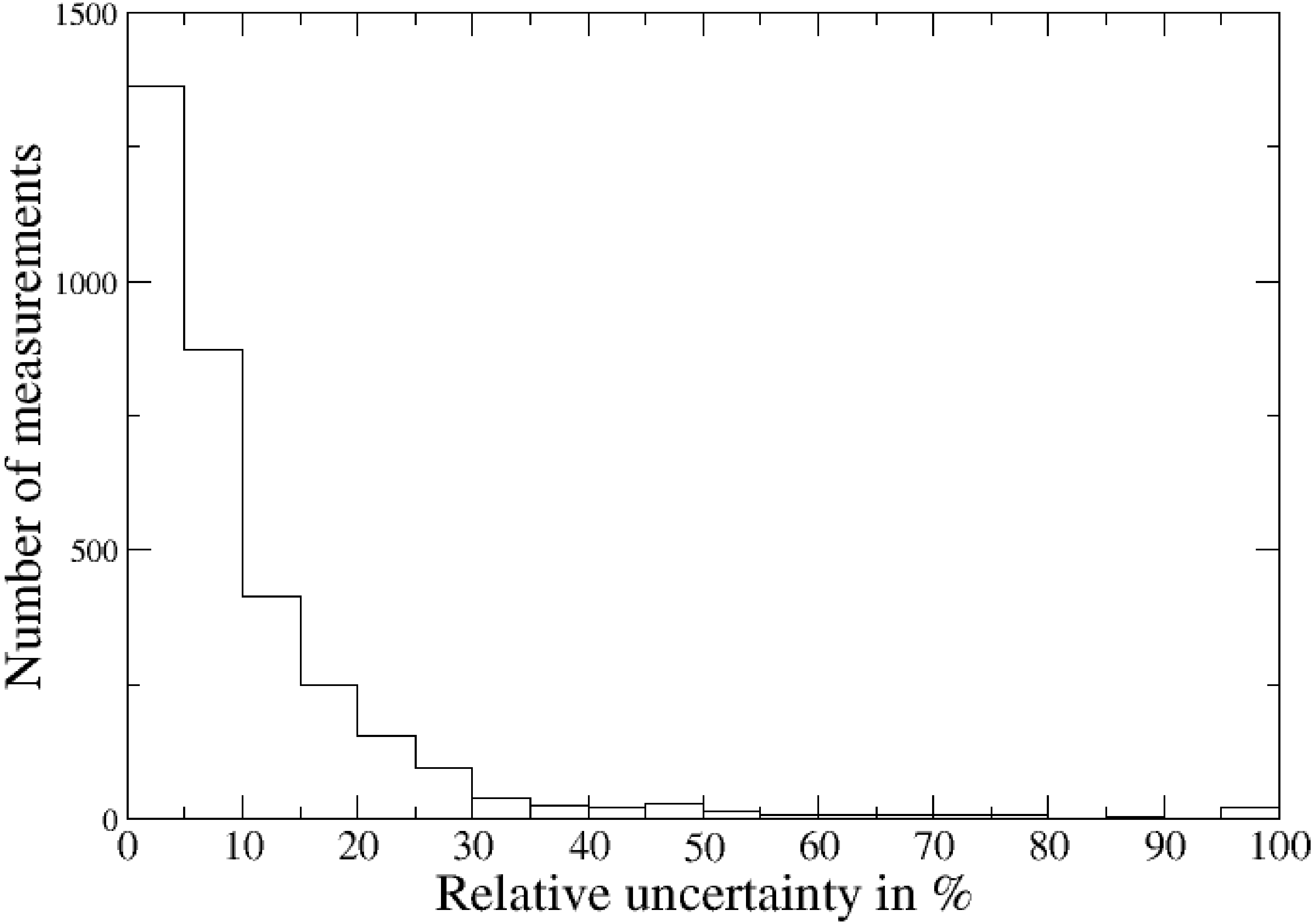
Small uncertainties

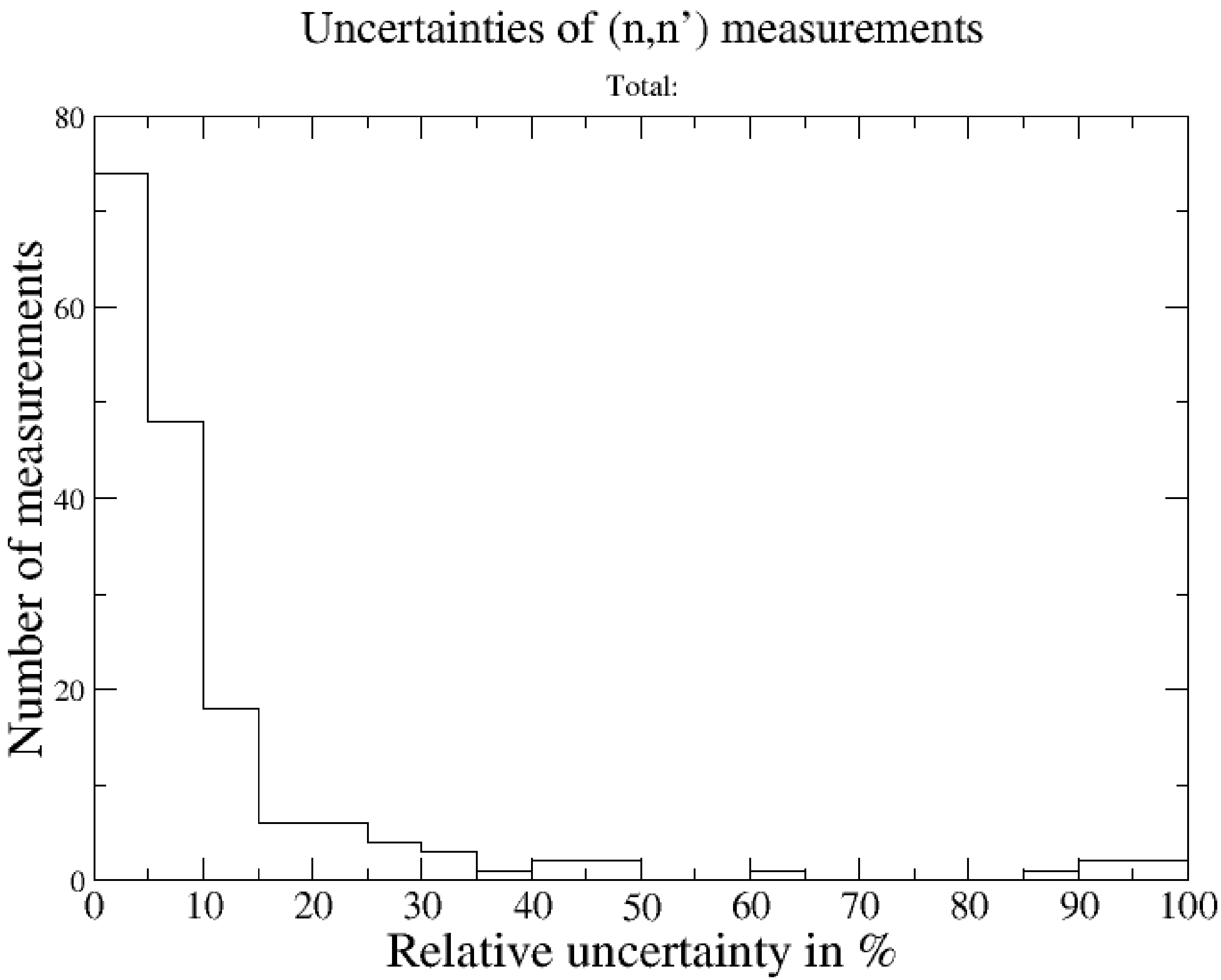
```
22450036 K.Knopf+          1997  1 68-ER-CMP(N,G),,SIG,,,DERIV     9.410E+05 0.213
11028021 J.W.Meadows+      1961  1 64-GD-0(N,G),,SIG               4.662E+07 0.215
22968004 E.Uberseder+      2007  6 9-F-19(N,G)9-F-20,,SIG,,MXW,DE   2.66     0.246
23266122 F.Farina Arboc    2013  1 56-BA-138(N,G)56-BA-139,,SIG     403.     0.248
23260117 F.Farina Arboc    2014  1 64-GD-152(N,G)64-GD-153,,SIG    7.720E+05 0.259
12964002 H.Beer+           1988 12 64-GD-152(N,G)64-GD-153,,SIG,,  1.113E+03 0.282
```

Huge uncertainties

```
23141004 A.Kimura+         2012 11 96-CM-246(N,G)96-CM-247,,SIG   3.630E+04  817.
14155003 K.H.Guber+        2007 17 (19-K-CMP(N,G),,SIG,,RAW)=(17-  25.3      858.
14244004 O.Roig+           2016 56 71-LU-176(N,G)71-LU-177,,SIG   1.422E+06 1.389E+03
22360029 1M.C.Moxon+       1974 23 72-HF-0(N,G),,SIG              1.271E+05 2.090E+03
11329106 J.H.Gibbons+      1961  3 49-IN-0(N,G),,SIG               490.     1.033E+04
22541003 M.C.Moxon         2006 20 92-U-238(N,G)92-U-239,,SIG     1.483E+04 4.952E+04
 SUBENT      AUTHOR        YEAR  N             Reaction           Av. Exp   Rel. Err.
```

Uncertainties of (n,γ) measurements





If a measurement has no uncertainty, but we still want to use it, should we assign uncertainties on the basis of all other measurements? (of course, OUTSIDE EXFOR)

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.

F value per EXFOR entry

- Suggests a ‘quality’ per paper
- These F values can be sorted over the entire EXFOR, from ‘best’ paper to ‘worst’ paper
- Can lead to a ‘quality’ per author
- …but we should use that with care!!!!

#ENTRY	AUTHOR	YEAR	Evaluation	Quality
22820	V.Semkova+	2004	F= 1.19	T1: 3 T2: 0 T3: 0 N1: 0 N2: 0 N3: 0 R1: 7 R2: 0 R3: 0

#SUBENT	N	Reaction	F	Quality	endfb8.0	tendl.2017
22820002	12	28-NI-58(N,P)27-CO-58,,SIG	1.22	R1	1.20	1.16
22820004	12	28-NI-58(N,X)27-CO-57,,SIG	1.05	T1	1.04	1.04
22820006	7	28-NI-58(N,P)27-CO-58-M,,SIG	1.35	R1	0.00	1.31
22820007	9	28-NI-58(N,2N)28-NI-57,,SIG	1.07	R1	1.06	1.06
22820008	4	28-NI-60(N,P)27-CO-60-M,,SIG	1.11	R1	0.00	1.12
22820009	1	28-NI-61(N,X)27-CO-60-M,,SIG	1.18	T1	0.00	1.12
22820010	5	28-NI-61(N,P)27-CO-61,,SIG	1.15	R1	1.06	1.11
22820011	4	28-NI-62(N,X)27-CO-61,,SIG	1.54	T1	1.29	1.75
22820012	13	27-CO-59(N,2N)27-CO-58,,SIG	1.06	R1	1.07	1.04
22820013	5	27-CO-59(N,2N)27-CO-58-M,,SIG	1.10	R1	0.00	1.14
#SUBENT	N	Reaction	F	Quality	endfb8.0	tendl.2017
		Average:	1.19		1.13	1.19

Experimental nuclear data evaluation

- Essential: numerical operations on every existing data set in EXFOR, e.g.
  - Reject: 0
  - Accept: 1
  - Fuzzy Accept: e.g. 0.7
  - Suggested normalization (standards)
  - Other corrections
- This is subjective per evaluator, but at least his/her opinion is quantified and this is better than reinventing the wheel every time.
- THIS should be called an evaluation, or perhaps more explicit: quantified knowledge.
- Create a new database between EXFOR and ENDF in the nuclear data chain
- The person who creates the ENDF or GND data library decides to use a model code, or least-square fit, using this information (i.e. this evaluation)
- Most importantly: information is no longer lost
- ….. This has not yet been agreed and organized.

Plan

- Clean up the **newbase** code and its output
- Use the latest XC4, or perhaps XC5 (including systematic vs. statistical uncertainties) database
- Extend analysis to angular distributions and spectra
- Reduce false negatives (mostly due to unrecognized EXFOR formats)
- Give NRDC a ‘cleaner’ list of (almost) sure errors to be corrected.
- Define format for EXFOR evaluation (including quality scores)

Conclusions

- **WPEC SG30 on the quality of the EXFOR database has resulted in more NEA activities in the 2010-2017 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 (and perhaps forever) 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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Thank you!