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Thermal capture cross sections for evaluated libraries: selection, validation and recommendation

Technical meeting on thermal capture and capture gammas, IAEA, May 23-27, 2022

Summary

- Introduction/context
- (n_{th},g) sources
- Rule(s)
- Implementation and validation
- Remarks
- Conclusion

Introduction/context

- Evaluated thermal capture cross sections are of prime importance for reactor applications:
  - Fission products, actinides, structural & light element activation
  - Incore, out of core

- Evaluated (n_{th},g) are related to I_g
- Evaluated (n_{th},g) are obtained from resonance parameters

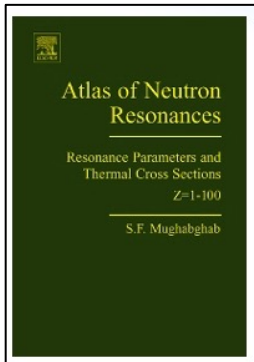
- Evaluation of (n_{th},g) is not based on resonance parameters
  - Using differential measurement (EXFOR)
  - Using integral information (reactor simulations): xs related to other quantities (e.g. FY)

- Some (n_{th},g) are not measured but required for application (spent fuel, or astrophysics). What can be done ?

(n_{th},g) sources (not ordered)

1. EXFOR
2. Holden 1991-1993 (compilation) + RIPL
3. k_0 neutron activation
4. Atlas of Neutron resonances BNL-325, 2006, 2018
5. EAF-2010
6. JUKO Research reports 2000-2017
7. Sukhoruchkin 2009 and 2015
8. Standard
9. Systematics

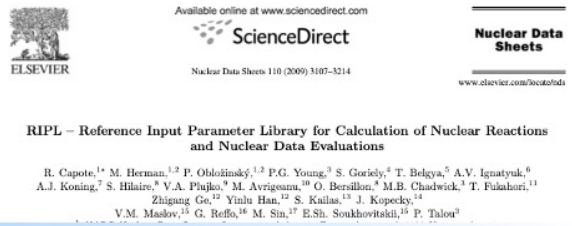
10. ENDF/B
11. JEF(F)
12. JENDL
13. and more



Mughabghab Atlas 2018
Mughabghab Atlas 2006

Sukhoruchkin 2015

Neutron Activation Analysis: http://www.kayzero.com/k0naa

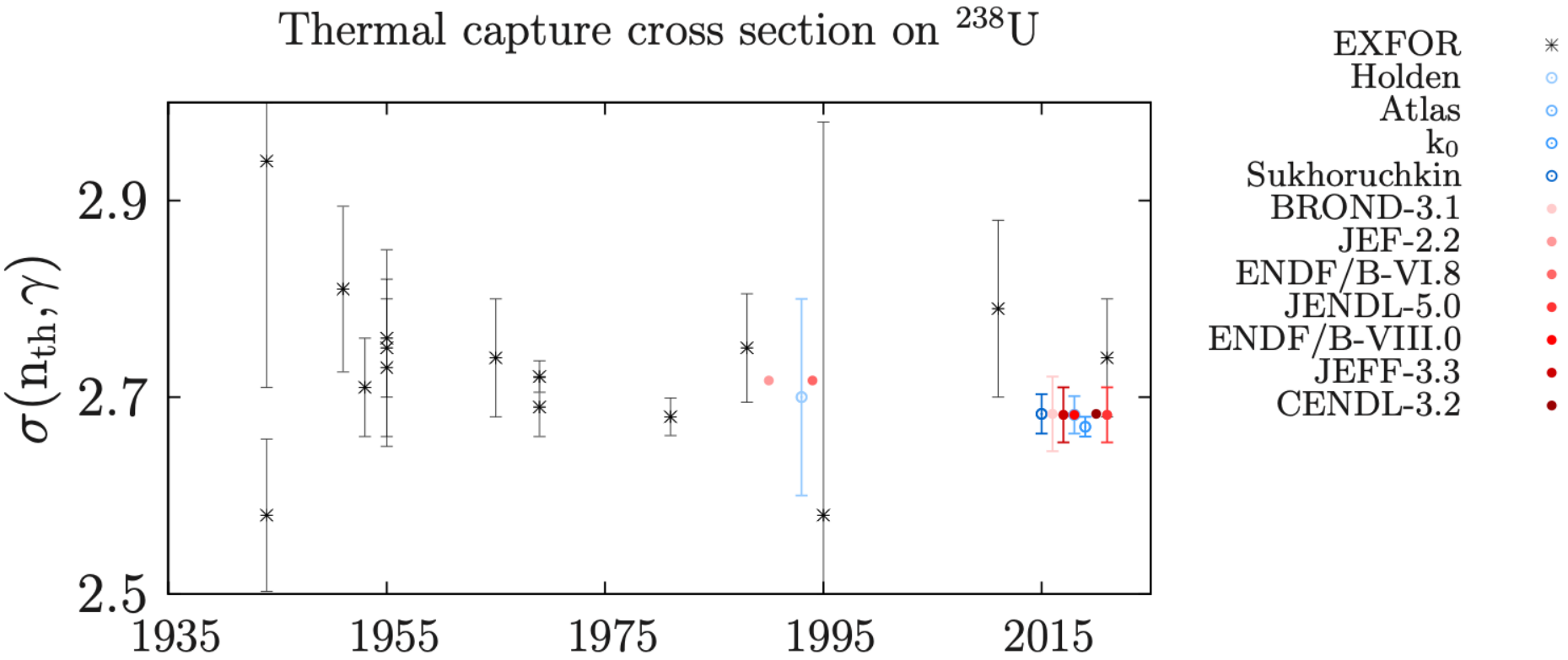


RIPL: Kopecky compilation
(Includes Holden tables)

EXFOR

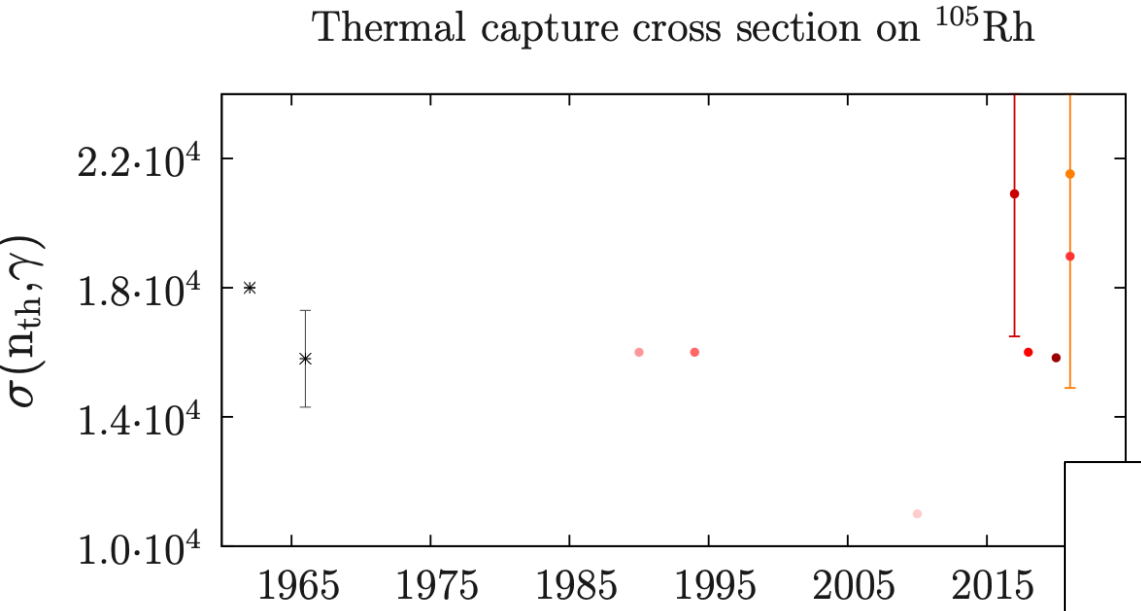
(n_{th},g) sources: Example 1

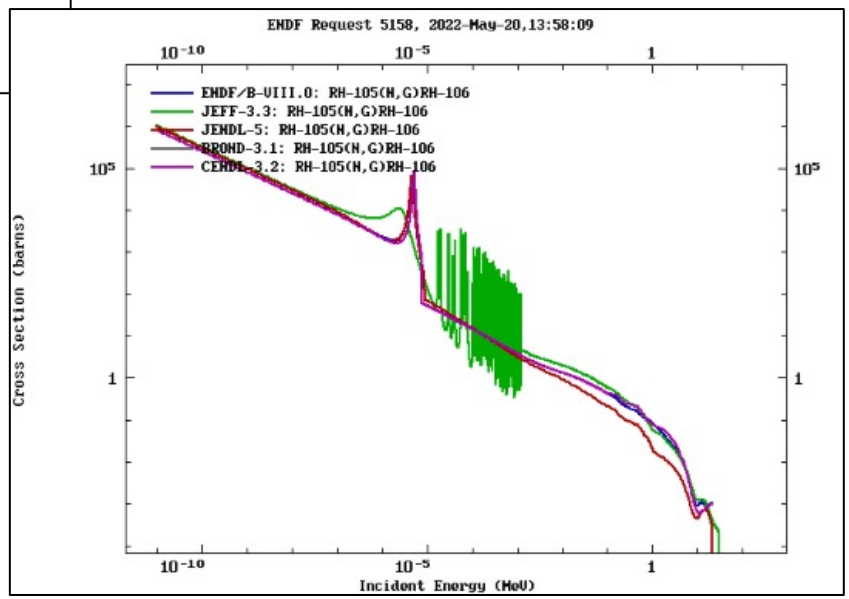
- Evaluated values (red) and compilations (blue) do not come from EXFOR alone



(n_{th},g) sources: Example 2

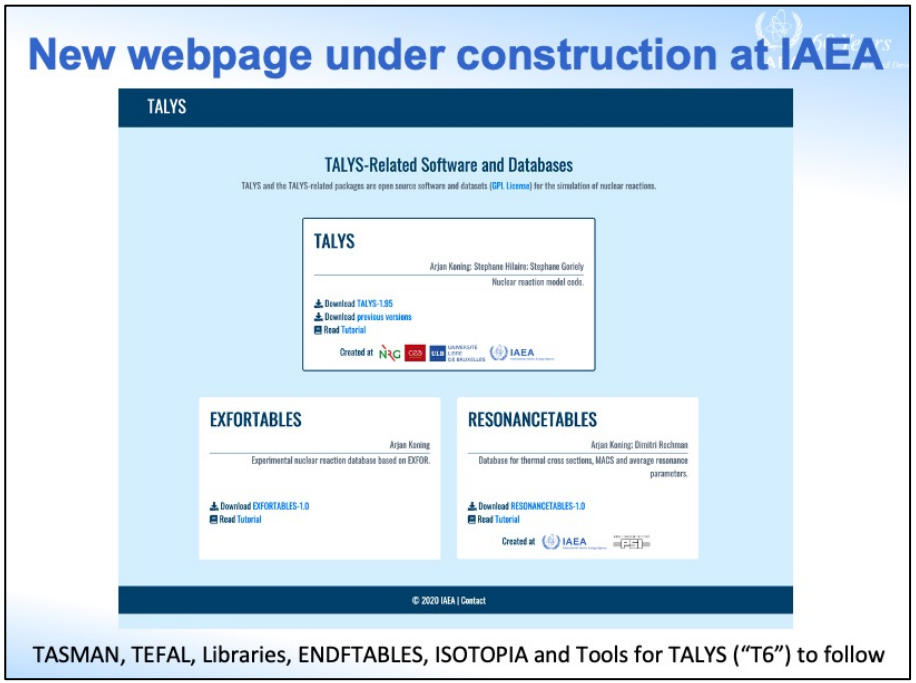
- Evaluated values (red) do not come from EXFOR alone

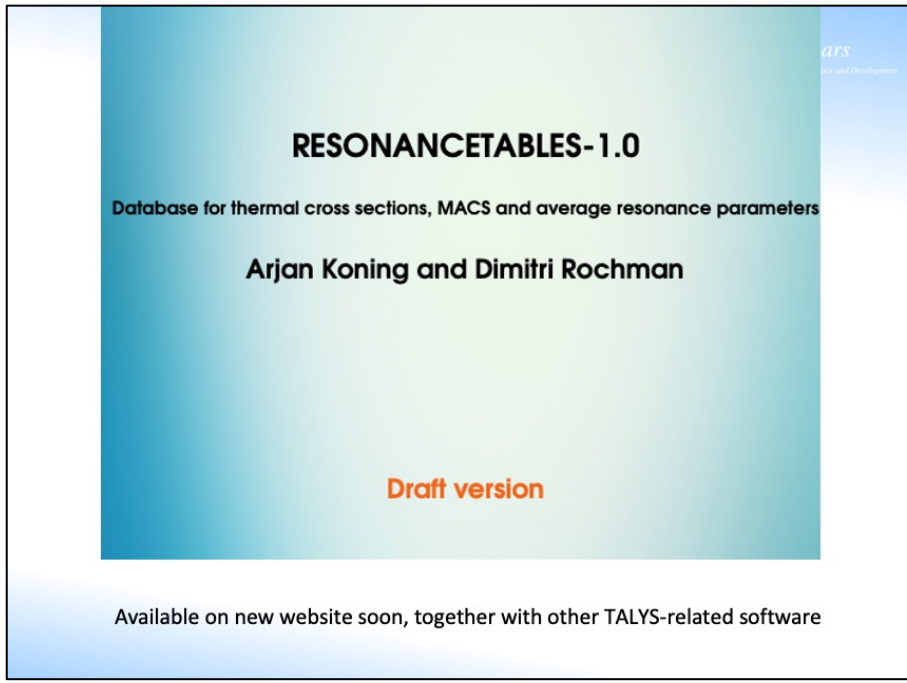




(n_{th},g) Rules

- Rules of selection applied for TENDL and some JEFF fission products
- Traceability
- Scripts based





https://www-nds.iaea.org/talys/

(n_{th},g) Rules

Example: Table with all possible options for thermal capture cross sections

```
62 151   0    1.51400E+04    3.00000E+02   Mugh18                                Sm151
  ripl            1.52000E+04    3.00000E+02   JUKO
  mugh06          1.51700E+04    3.00000E+02   Mugh06
  mugh18          1.51400E+04    3.00000E+02   Mugh18
  sukhoruchkin    1.51700E+04    2.99000E+02   Sukhoruchkin
  exfor           1.20000E+04    0.00000E+00   Melaika_1955_12086003
  exfor           1.51700E+04    3.00000E+02   Mughabghab_2006_V10022001
  exfor           1.50200E+04    5.25000E+02   Marrone_2006_22893007
  cendl3.1        1.51239E+04           CE=    9.98937E-01
  endfb8.0        1.51379E+04           CE=    9.99861E-01
  jeff3.3         1.51294E+04           CE=    9.99300E-01
  jendl4.0        1.51598E+04           CE=    1.00131E+00
  tendl.2019      1.51334E+04           CE=    9.99564E-01
62 152   0    2.06000E+02    3.00000E+00   Mugh18                                Sm152
  ripl            2.06000E+02    1.50000E+01   JUKO
  mugh06          2.06000E+02    6.00000E+00   Mugh06
  mugh18          2.06000E+02    3.00000E+00   Mugh18
  sukhoruchkin    2.06000E+02    6.00000E+00   Sukhoruchkin
  exfor           1.38000E+02    2.76000E+01   Seren_1947_11447096
  exfor           2.00000E+02    6.00000E+00   Pattenden_1958_21325012
  exfor           2.24000E+02    7.00000E+00   Tattersall_1960_20638048
  exfor           2.15000E+02    1.00000E+01   Fehr_1960_12023006
  exfor           2.09000E+02    9.00000E+00   Cabell_1962_20627002
  exfor           2.09100E+02    2.07000E+01   Bernabei_1962_12099002
  exfor           2.06000E+02    6.00000E+00   Mughabghab_2006_V10022041
  exfor           2.04800E+02    6.32832E+00   Karadag_2007_22964002
  exfor           2.38930E+02    1.91100E+01   Nyarko_2010_31698006
  exfor           2.07300E+02    9.40000E+00   Agbemava_2011_31717003
  exfor           2.07000E+02    1.00000E+00   FarinaArbocco_2013_23266134
  exfor           2.12000E+02    8.00000E+00   Nguyen_2017_30843002
  cendl3.1        2.06640E+02           CE=    1.00311E+00
  endfb8.0        2.05946E+02           CE=    9.99738E-01
  jeff3.3         2.05974E+02           CE=    9.99874E-01
  jendl4.0        2.05842E+02           CE=    9.99233E-01
  tendl.2019      2.05971E+02           CE=    9.99859E-01
```

Library values obtained from point wise files (PREPRO's RECENT module)

(n_{th},g) Rules

Order of adoption for thermal cross sections, resonance integrals and MACS

1. Kayzero database
2. Mughabghab 2018 Atlas
3. Sukhoruchkin 2015 Atlas
4. Mughabghab 2006 Atlas
5. RIPL or Kopecky database
6. EXFOR (the most recent value)

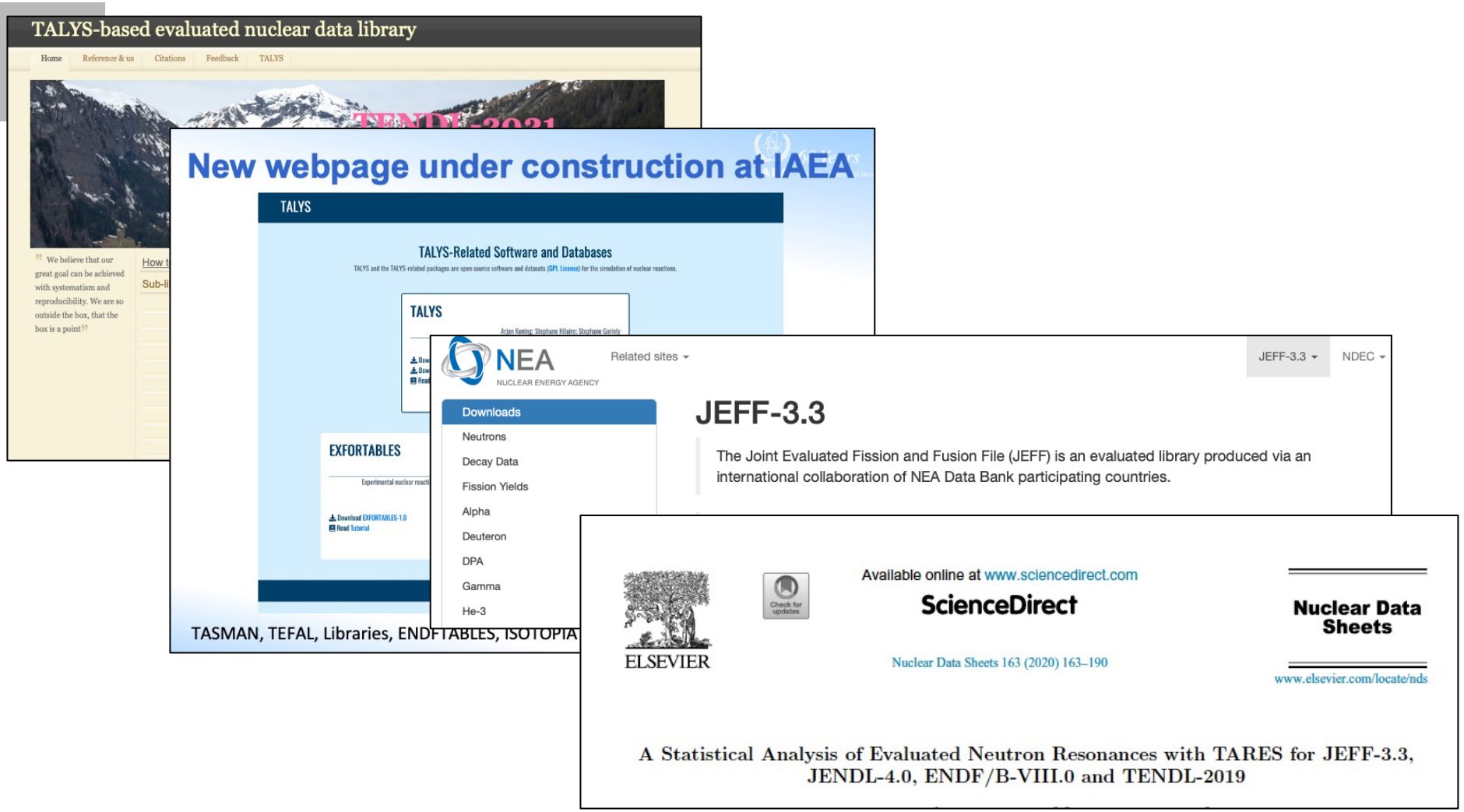
For MACS, the order of adoption is

1. Mughabghab 2018 Atlas
2. Sukhoruchkin 2015 Atlas
3. KADONIS database
4. EXFOR (the most recent value)

Final database: if 1 doesn't exist, we take 2, if it doesn't exist, we take 3, etc.

Implementation and validation

- Different tools were developed, followed by (extensive) testing



Implementation and validation

- Different tools were developed, followed by (extensive) testing

TABLE I. (Color online) Average $\overline{C/E}$ and standard deviation (Std) for each library and different quantities. In the case of the fission cross section, ^{238}U is excluded from the JEFF-3.3 library as thermal fission cross section is zero. Both contributions from MF2 and MF3 are considered. In this table as in the following ones, the term E refers to Ref. [30].

Library	Isotopes	$\overline{C/E}$	Std	Outlier
	Thermal capture cross section			
TARES&TENDL-2019	374	1.000	0.050	3
JEFF-3.3	308	1.045	0.454	4
JENDL-4.0	244	1.021	0.194	12
ENDF/B-VIII.0	282	1.216	3.871	1
	Thermal elastic cross section			
TARES&TENDL-2019	226	0.991	0.075	15
JEFF-3.3	208	1.056	1.398	2
JENDL-4.0	193	1.087	1.398	1
ENDF/B-VIII.0	199	1.138	1.421	1
	Thermal fission cross section			
TARES&TENDL-2019	45	1.003	0.521	2
JEFF-3.3	34	2.310	7.923	0
JENDL-4.0	33	0.971	0.371	4
ENDF/B-VIII.0	33	2.057	6.142	0

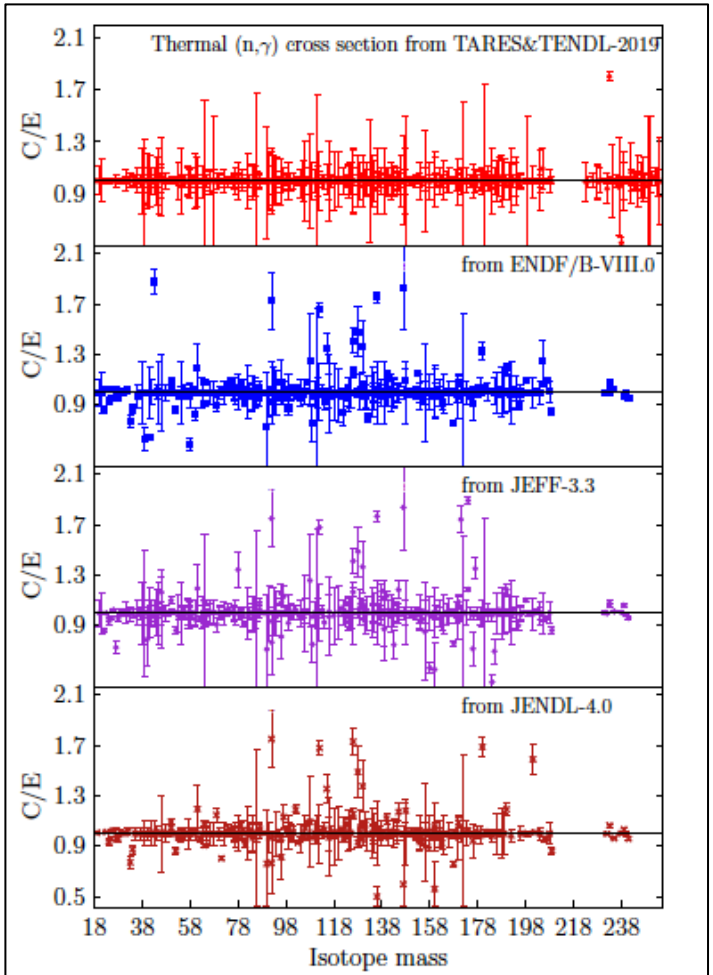
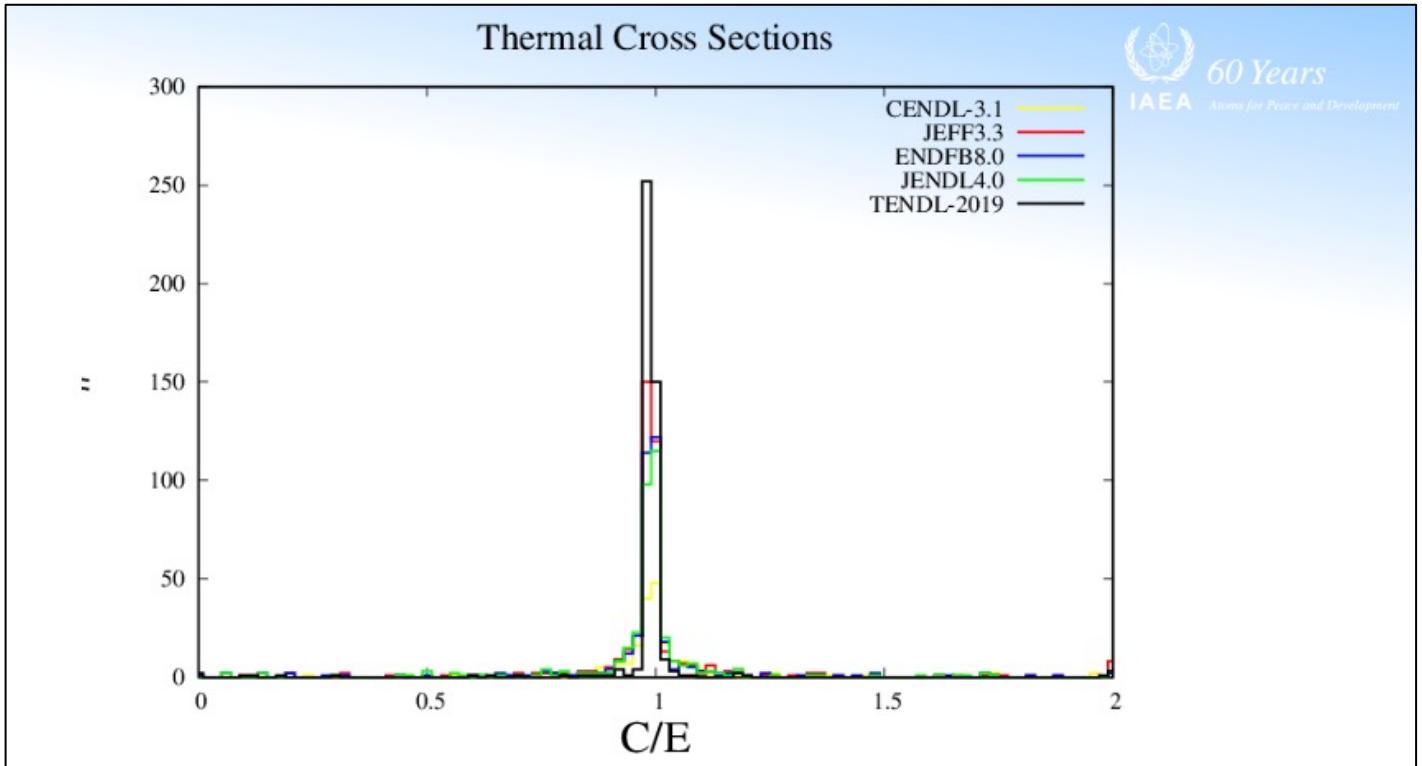


FIG. 8. (Color online) C/E values for the thermal capture cross sections for the various considered libraries. The "E" is from Ref. [30], see Table I for details. The uncertainties are experimental. For other reactions, see Appendix B.

Implementation and validation

- Different tools were developed, followed by (extensive) testing



Lib	F(C/E)	N	N <5%	N < 20%	N < 50%
CENDL-3.1	1.036	201	129(0.642)	177(0.881)	187(0.930)
ENDFB-8.0	1.022	375	284(0.757)	332(0.885)	351(0.936)
JEFF-3.1	1.024	425	315(0.741)	377(0.887)	398(0.936)
JENDL-4.0	1.025	359	269(0.749)	320(0.891)	334(0.930)
TENDL-2019	1.008	446	416(0.933)	431(0.966)	434(0.973)

Remarks on k_0

- K_0 generally good, with some exceptions

Table 3.1: List of isotopes presenting the largest differences between the recommended values and the k_0 neutron activation. For ^{70}Zn, ^{76}Se and ^{190}Os the uncertainty on the resonance integral for the k_0 database is assigned to 10 %, as no value is originally provided.

Isotope	cross section		resonance integral	
	This work	Refs. [7, 29]	This work	Refs. [7, 29]
^{110}Pd	0.30 ± 0.03 b.	0.0137 ± 0.0012 b.	2.18 ± 0.04 b.	0.163 ± 0.023 b.
^{68}Zn	1.07 ± 0.19 b.	0.0701 ± 0.0020 b.	3.06 ± 0.55 b.	0.224 ± 0.007 b.
^{70}Zn	92.3 ± 18.8 mb.	21 ± 1 mb.	0.94 ± 0.16 b.	0.166 ± 0.017 b.
^{76}Se	85.0 ± 8.7 b.	18.9 ± 0.6 b.	39.0 ± 3.4 b.	14.6 ± 1.5 b.
^{190}Os	10.95 ± 1.12 b.	3.48 ± 0.25 b.	39.5 ± 1.9 b.	7.06 ± 0.8 b.

[7] Frans de Corte. "The k_0-standardization method: a move to the optimization of neutron activation analysis". PhD thesis. University of Gent, Belgium, 1987 (cited on page 17).

[29] A. Trkov and V. Radulovic. "Nuclear reactions and physical models for neutron activation analysis". In: *Jour. of Radioanal. Nucl. Chem.* 304 (2015), pages 763–778 (cited on pages 17, 18).

Remarks on (n_{th},g) not measured

- Short-lived fission products, or isotopes for astrophysics.
- What to do ?
  - Rely on systematics (HFR) for resonance parameters,

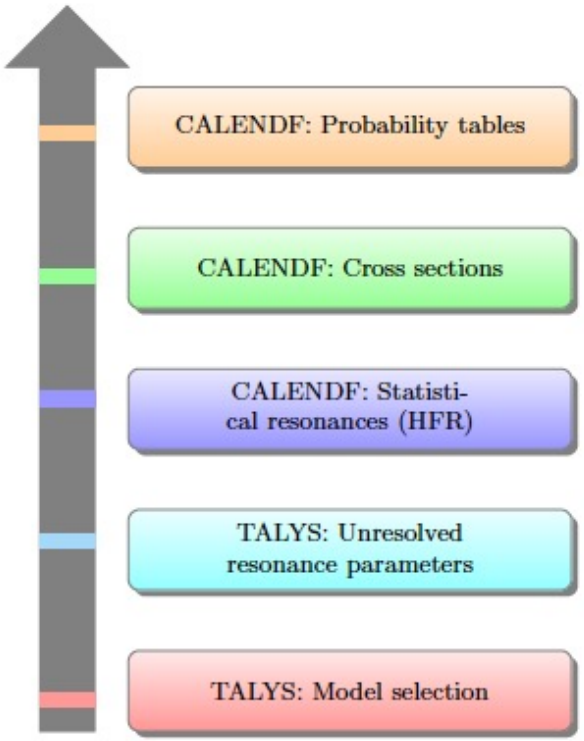
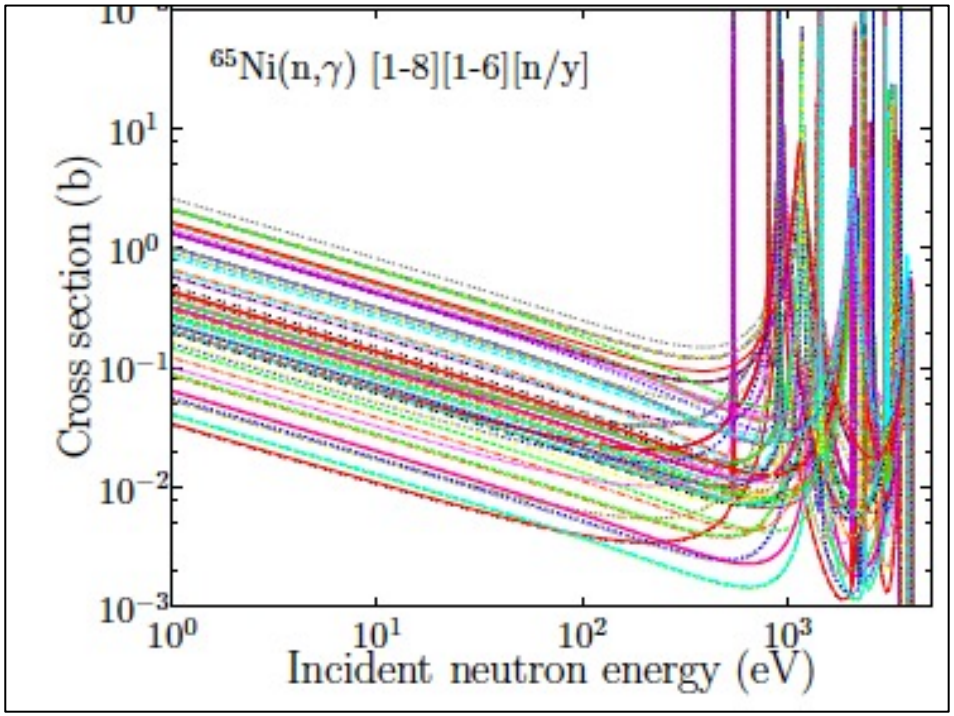
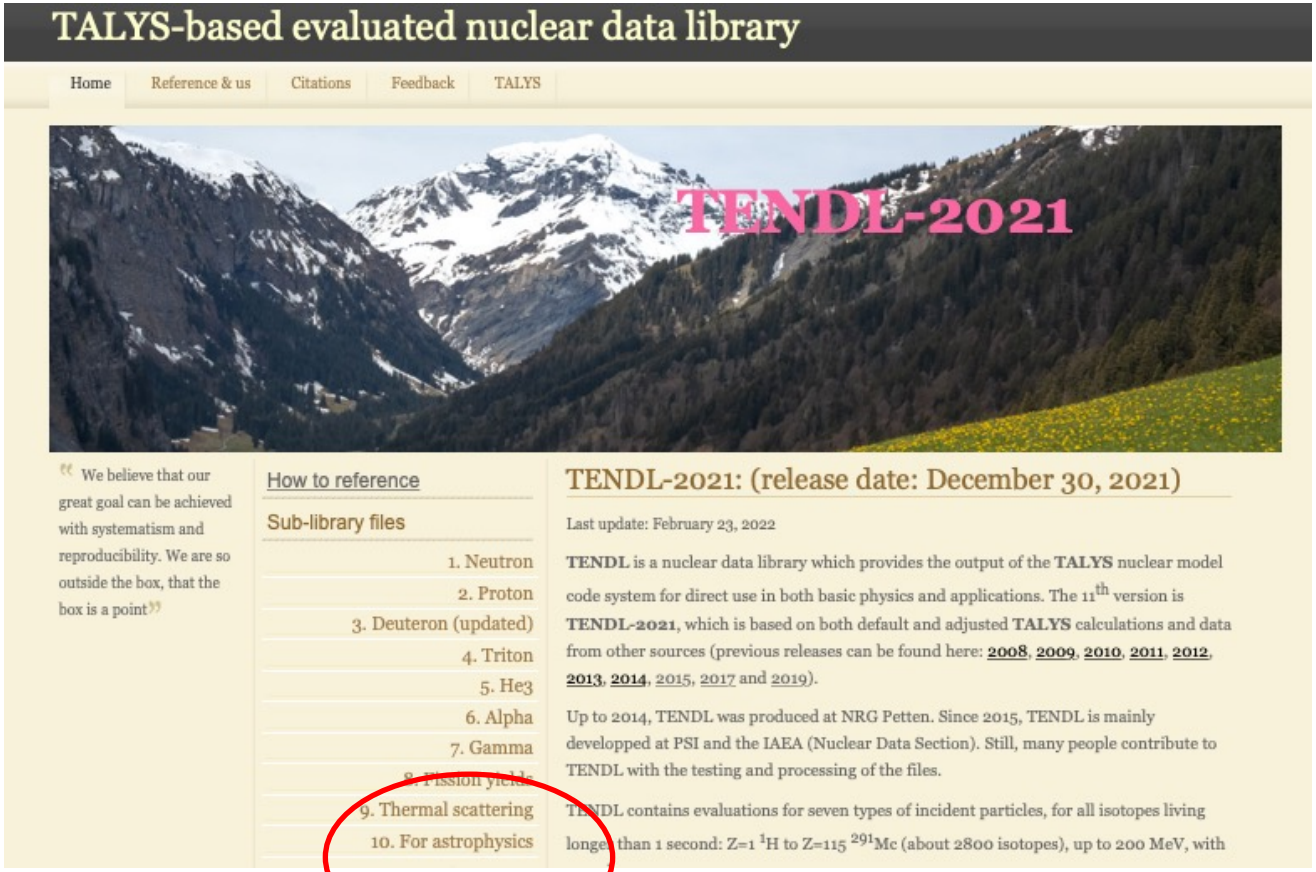


FIG. 18. (Color online) Flow chart for the production of the statistical resonances (HFR) using TALYS and TARES/CALENDF.



Remarks on (n_{th},g) not measured

- Short-lived fission products, or isotopes for astrophysics.
- What to do ?
  - or simply on model variations for average values (thermal, MACS)
  - (work performed with A. Koning, S. Goriely and D. Rochman)



Remarks on (n_{th},g) not measured

TENDL-stars 2021

(n,g) cross sections, reaction rates and MACS for astrophysics

Description

Below are various links to 8892 isotopes for astrophysics applications (capture cross sections, capture rates and MACS).

Different reaction "model sets" were used: "a model set" represents a combination of 7 TALYS models:

1. Gamma strength function (values 8 or 9): either Gogny D1M HFB+QRPA, or SMLO
2. Level density (values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables
3. JLM microscopic optical model potential or KD optical model (values y or n)
4. Gamma strength function for M1 (values 3 or 8): Hartree-Fock BCS tables or Gogny D1M HFB+QRPA
5. Collective enhancement (values y or n): yes or no
6. Width fluctuation (values 0, 1 or 2): Moldauer model, or Hofmann-Richert-Tepel-Weidenmueller model
7. Mass model (values 0, 1, 2 or 3): Duflo-Zuker formula, Moeller table, Goriely HFB-Skyrme table, or HFB-Gogny D1M table (except for known masses, where the experimental value is used)

Each of the set models is named with 7 values, such as "91n3n12" (default TALYS model), or 81n8n12. These values correspond to the ones in the TALYS manual. Quantities are definied such as:

1) XS (n,g) cross sections: capture cross sections from 0.01 eV to 20 MeV (from the TALYS file xs000000.tot)

2) < sigma_v >: reaction rates for all temperatures taking into account the thermal population of the target (from the TALYS file astrorate.g)

3) G(T): normalized partition function (from the TALYS file astrorate.tot)

4) MACS: Maxwellian Averaged (n,g) Cross Sections

Available files

	XS (n,g) cross sections with	< sigma_v > rates with	G(T) with	MACS 30 keV
1. 270 stable isotopes:	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets
2. 3256 isotopes with known mass	12 or 288 model sets	12 or 288 model sets	12 model sets	12 model sets
3. 5366 other isotopes	12 or 288 model sets	12 or 288 model sets	12 model sets	12 model sets

Last update: Wed May 19, 2022

Remarks on (n_{th},g) not measured

```
# File for Tc079 reaction (n,g)  PSI, Switzerland, 03-30-2022 11:27:59 PM
# Reaction calculated with TALYS 1.96
#
#
#
# name of model sets with 7 digits, such as 85y8n01
#                                          |||||||
#                                          ||||||massmodel (0,1,2, or 3)     (0: Duflo-Zuker formula,     1: Moeller table,  2: Goriely HFB-Skyrme table,
#                                          |||||widthmode  (0,1 or 2)        (0: no width fluctuation,    1: Moldauer model, 2: Hofmann-Richert-Tepel-Weidenmueller mo
#                                          ||||colenhance  (y, n)            (y: (yes) explicit collective enhancement of the level density)
#                                          |||strengthM1   (3, 8)            (3: Hartree-Fock BCS tables, 8:Gogny D1M HFB+QRPA
#                                          ||jlmomp        (y, n)            (y: (yes) JLM microscopic optical model potential)
#                                          |ldmodel        (1, 2, 5)         (1: Constant temperature + Fermi gas model,  2: Back-shifted Fermi gas model,
#                                          strength        (8, 9)            (8: Gogny D1M HFB+QRPA,      9: SMLO
#
#  Default TALYS model: 91n3n12
#
# Number of model sets: 288
#
# energy (MeV)    Mean        Std         Median      MAD         min         max         91n3n12 (  1)  85y8n00 (  2)  85y8n01 (  3)  85y8n02 (  4)  85y8n03 (  5)
1.00000E-11    6.008e+06   5.170e+06   4.512e+06   3.538e+06   8.238e+05   1.640e+07   8.739e+06      1.177e+07      9.226e+06      8.739e+06      1.640e+07
2.53000E-08    1.194e+05   1.028e+05   8.972e+04   7.036e+04   1.638e+04   3.261e+05   1.737e+05      2.340e+05      1.834e+05      1.737e+05      3.261e+05
2.00000E-07    4.249e+04   3.657e+04   3.190e+04   2.501e+04   5.825e+03   1.160e+05   6.180e+04      8.323e+04      6.524e+04      6.180e+04      1.160e+05
1.00000E-06    3.440e-05   5.947e-05   5.766e-06   3.917e-06   5.283e-07   1.946e-04   3.102e-06      3.223e-06      8.354e-06      5.108e-06      1.798e-04
1.00000E-05    1.108e-05   1.871e-05   2.186e-06   1.520e-06   2.085e-07   6.152e-05   1.102e-06      1.373e-06      3.322e-06      2.033e-06      5.684e-05
1.00000E-04    4.138e-06   5.661e-06   1.574e-06   1.069e-06   1.973e-07   1.942e-05   7.319e-07      1.554e-06      3.204e-06      1.965e-06      1.795e-05
2.00000E-04    3.427e-06   3.867e-06   1.889e-06   1.249e-06   2.427e-07   1.372e-05   8.189e-07      1.979e-06      3.958e-06      2.428e-06      1.268e-05
5.00000E-04    3.119e-06   2.469e-06   2.248e-06   1.328e-06   3.493e-07   8.662e-06   1.090e-06      2.921e-06      5.713e-06      3.507e-06      8.003e-06
1.00000E-03    3.327e-06   2.331e-06   2.881e-06   1.670e-06   4.763e-07   9.227e-06   1.444e-06      4.033e-06      7.822e-06      4.802e-06      5.646e-06
2.00000E-03    3.939e-06   3.064e-06   3.645e-06   1.932e-06   6.532e-07   1.265e-05   1.973e-06      5.631e-06      1.088e-05      6.677e-06      3.980e-06
5.00000E-03    5.492e-06   5.034e-06   3.070e-06   2.046e-06   4.329e-07   1.957e-05   3.047e-06      8.818e-06      1.699e-05      1.043e-05      2.500e-06
1.00000E-02    7.396e-06   7.274e-06   4.288e-06   3.258e-06   3.033e-07   2.737e-05   4.258e-06      1.239e-05      2.385e-05      1.465e-05      1.754e-06
2.00000E-02    1.012e-05   1.033e-05   5.971e-06   5.104e-06   2.114e-07   3.813e-05   5.932e-06      1.733e-05      3.336e-05      2.051e-05      1.226e-06
3.00000E-02    1.215e-05   1.257e-05   7.205e-06   6.290e-06   1.706e-07   4.604e-05   7.161e-06      2.098e-05      4.039e-05      2.486e-05      9.924e-07
5.00000E-02    1.517e-05   1.585e-05   9.011e-06   8.314e-06   1.296e-07   5.764e-05   8.966e-06      2.637e-05      5.081e-05      3.132e-05      7.583e-07
1.00000E-01    1.964e-05   2.067e-05   1.160e-05   1.113e-05   8.842e-08   7.436e-05   1.158e-05      3.437e-05      6.634e-05      4.107e-05      5.252e-07
2.00000E-01    2.251e-05   2.375e-05   1.317e-05   1.289e-05   6.040e-08   8.412e-05   1.313e-05      3.968e-05      7.684e-05      4.801e-05      3.690e-07
5.00000E-01    1.712e-05   1.805e-05   9.936e-06   9.789e-06   3.800e-08   6.499e-05   9.578e-06      3.054e-05      5.982e-05      3.862e-05      2.506e-07
8.00000E-01    1.096e-05   1.152e-05   6.237e-06   6.124e-06   3.030e-08   4.218e-05   5.873e-06      1.960e-05      3.892e-05      2.611e-05      2.134e-07
1.00000E+00    5.994e-02   1.364e-02   5.690e-02   9.890e-03   3.770e-02   9.118e-02   5.021e-02      9.111e-02      6.864e-02      5.678e-02      6.722e-02
1.20000E+00    1.150e-02   7.182e-03   1.427e-02   3.070e-03   8.911e-08   2.149e-02   1.532e-02      2.148e-02      5.344e-07      1.733e-02      1.548e-02
1.60000E+00    3.778e-02   1.439e-02   4.065e-02   1.021e-02   1.245e-02   6.052e-02   4.459e-02      6.049e-02      2.111e-02      5.532e-02      4.428e-02
1.80000E+00    2.457e-02   2.761e-02   1.413e-02   9.925e-03   2.194e-08   8.462e-02   2.937e-08      1.984e-02      8.462e-02      9.715e-08      1.460e-02
2.00000E+00    5.281e-02   1.102e-02   5.307e-02   9.235e-03   3.444e-02   7.549e-02   4.456e-02      7.548e-02      6.301e-02      5.870e-02      5.623e-02
2.50000E+00    5.049e-02   9.442e-03   5.141e-02   8.050e-03   3.438e-02   6.872e-02   4.375e-02      6.872e-02      5.951e-02      5.848e-02      5.146e-02
3.00000E+00    4.650e-02   7.474e-03   4.529e-02   6.570e-03   3.349e-02   6.010e-02   4.211e-02      6.010e-02      5.326e-02      5.458e-02      4.529e-02
3.50000E+00    4.155e-02   5.647e-03   4.038e-02   4.680e-03   3.185e-02   5.114e-02   3.973e-02      5.114e-02      4.586e-02      4.826e-02      3.875e-02
4.00000E+00    3.659e-02   4.282e-03   3.611e-02   3.275e-03   2.932e-02   4.516e-02   3.707e-02      4.311e-02      3.878e-02      4.148e-02      3.288e-02
5.00000E+00    3.129e-02   5.311e-03   3.113e-02   3.985e-03   2.267e-02   4.206e-02   4.202e-02      3.117e-02      3.133e-02      4.007e-02      2.404e-02
6.00000E+00    2.477e-02   4.381e-03   2.363e-02   3.145e-03   1.747e-02   3.518e-02   3.513e-02      2.365e-02      2.327e-02      2.985e-02      1.851e-02
7.00000E+00    2.006e-02   3.688e-03   1.945e-02   2.550e-03   1.403e-02   2.905e-02   2.899e-02      1.878e-02      1.795e-02      2.295e-02      1.483e-02
8.00000E+00    1.649e-02   3.154e-03   1.634e-02   2.205e-03   1.149e-02   2.413e-02   2.404e-02      1.523e-02      1.414e-02      1.816e-02      1.217e-02
1.00000E+01    6.177e-03   6.431e-03   4.397e-03   4.397e-03   2.713e-10   1.759e-02   1.722e-02      5.266e-08      9.482e-03      1.225e-02      8.625e-10
1.20000E+01    5.312e-03   5.483e-03   4.161e-03   4.161e-03   2.465e-10   1.384e-02   1.314e-02      3.649e-08      9.213e-03      8.959e-03      6.727e-10
1.40000E+01    2.127e-03   3.779e-03   0.000e+00   1.375e-08   1.251e-10   1.103e-02   1.468e-08      2.660e-08      7.121e-03      2.864e-08      3.336e-10
1.60000E+01    6.749e-03   1.458e-03   6.202e-03   1.329e-03   4.472e-03   9.422e-03   9.039e-03      5.762e-03      6.016e-03      5.888e-03      4.731e-03
1.80000E+01    6.063e-03   1.314e-03   5.557e-03   1.188e-03   4.001e-03   8.454e-03   8.131e-03      5.171e-03      5.399e-03      5.296e-03      4.228e-03
2.00000E+01    5.418e-03   1.178e-03   4.960e-03   1.057e-03   3.576e-03   7.534e-03   7.344e-03      4.596e-03      4.811e-03      4.783e-03      3.762e-03
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Conclusion

- There is a need for international recommendations on (n_{th},g), RIPL-like,
- Need of clear rules, traceability,
- Need of accessibility in a computer format (and eventually reports/papers)
- (n_{th},el), I_g, RP are also important,
- (n_{th},g) for 8892 isotopes can be needed.

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PSI

Wir schaffen Wissen – heute für morgen