IAEA
60 Years
Atoms for Peace and Development

Level density validation for and with TALYS

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Contents

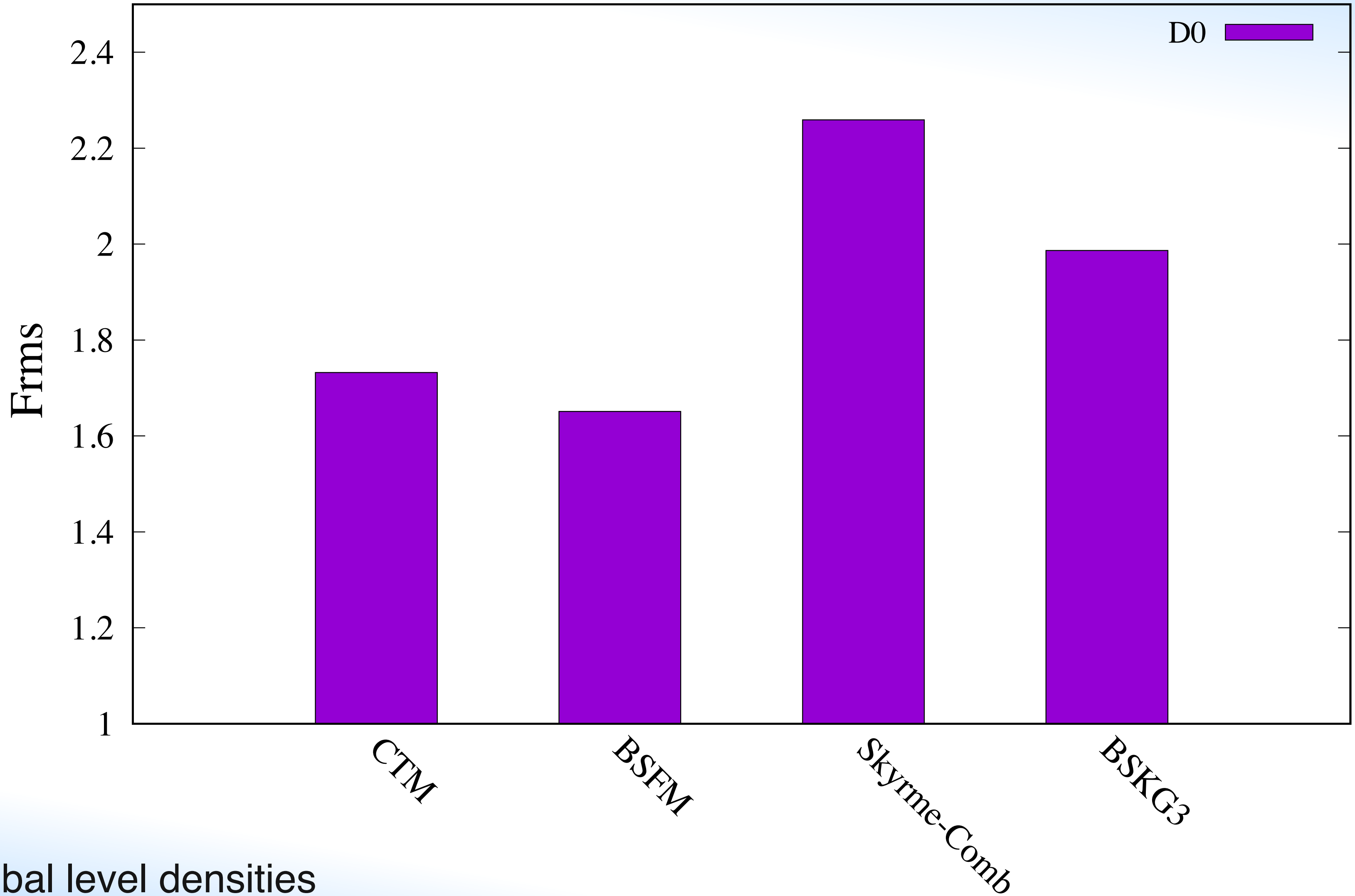
- Some basic level density validation
- Optimisation to discrete levels and D0
- Indirect level density validation
- Impact on TALYS cross section calculations

TALYS level density models

ldmodel 1: Constant Temperature + Fermi gas model (CTM)
ldmodel 2: Back-shifted Fermi gas Model (BFM)
ldmodel 3: Generalised Superfluid Model (GSM)
ldmodel 4: Skyrme-Hartree-Fock-Bogolyubov level densities from numerical tables
ldmodel 5: Skyrme-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 6: Temperature-dependent Gogny-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 7: BSKG3 - Skyrme-Hartree-Fock-Bogolyubov triaxial combinatorial level densities from numerical tables
ldmodel 8: QRPA level densities from numerical tables

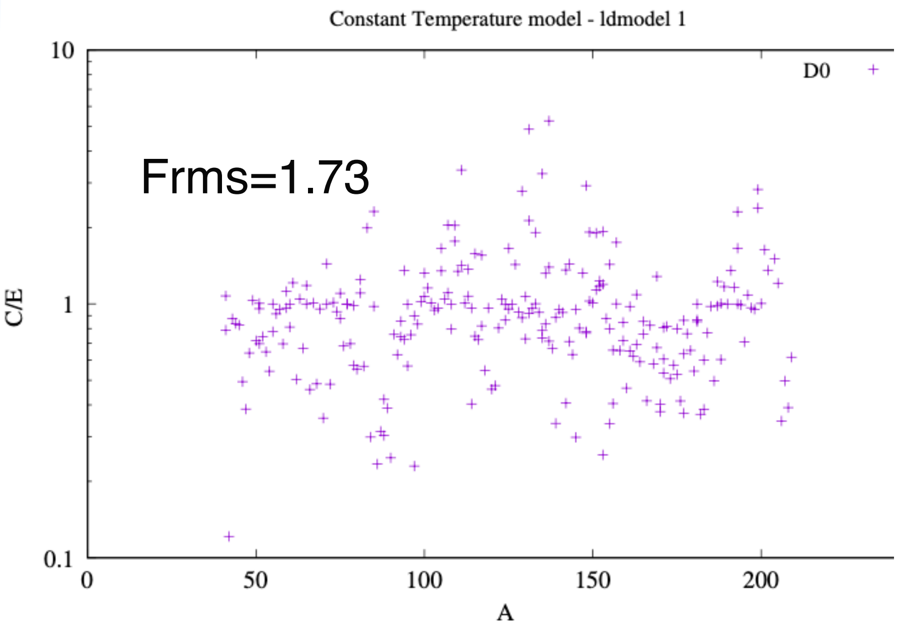
Best level density models (averaged over all TALYS applications):
1, 2, 7 and sometimes 5. The big promise is 8!

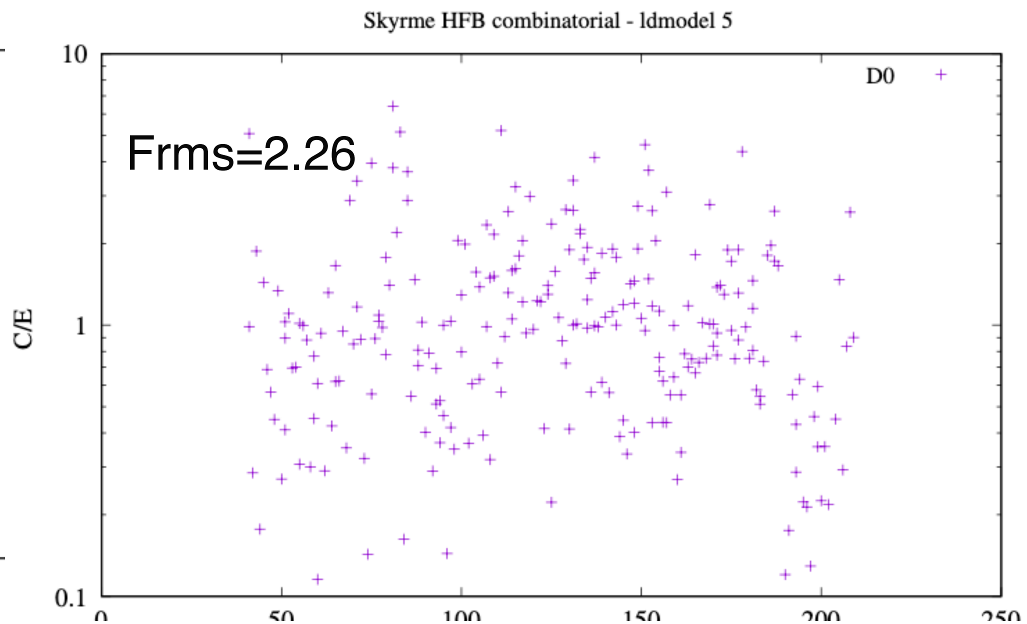
TALYS Average s-wave resonance width (D0) vs. experiment

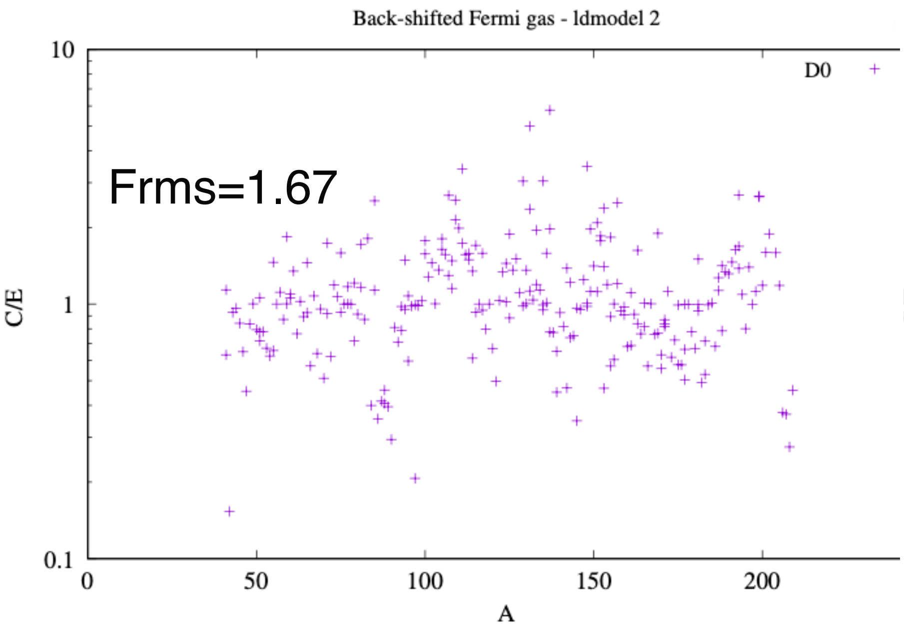


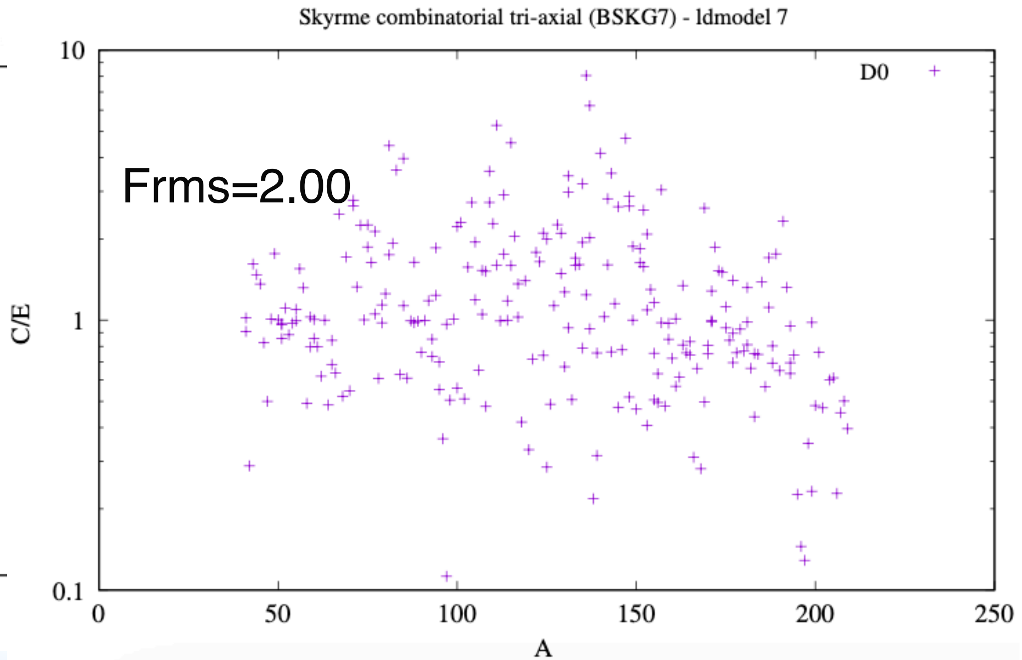
Global level densities
Nuclides with experimental D0 data: 300 (RIPL-3)

Global level density validation with D0









Suspicious for all LD models: e.g. K42, Zr97

Parameter adjustment

By default, TALYS considers the best nominal level density ρ_{nom} adjusted to the discrete level scheme and D_0, whenever available. However, for adjustment purposes, flexibility can be achieved either by varying directly all the related parameters or through a scaling function, i.e.

$$\rho(E_x, J, \pi) = \exp(c\sqrt{E_x - \delta})\rho_{nom}(E_x - \delta, J, \pi) \quad (230)$$

where $c = 0$ and $\delta = 0$ correspond to unaltered nominal level densities. The "pairing shift" δ simply implies obtaining the level density from the table or formula at a different energy. The parameter c plays a role similar to that of the level density parameter a within the phenomenological models (see Eq. 223). Adjusting c and δ together gives adjustment flexibility at both low and higher energies and allows the user to adjust level densities for cross section fitting.

Eq. (230) appropriate for Fermi gas range but not for constant T range

Should be extended by adjustment of the spin distribution (is already in latest version of TALYS)

Is applicable to both microscopic and analytic LD's

TALYS keywords:
C: ctable(Z,A)
δ: ptable(Z,A)

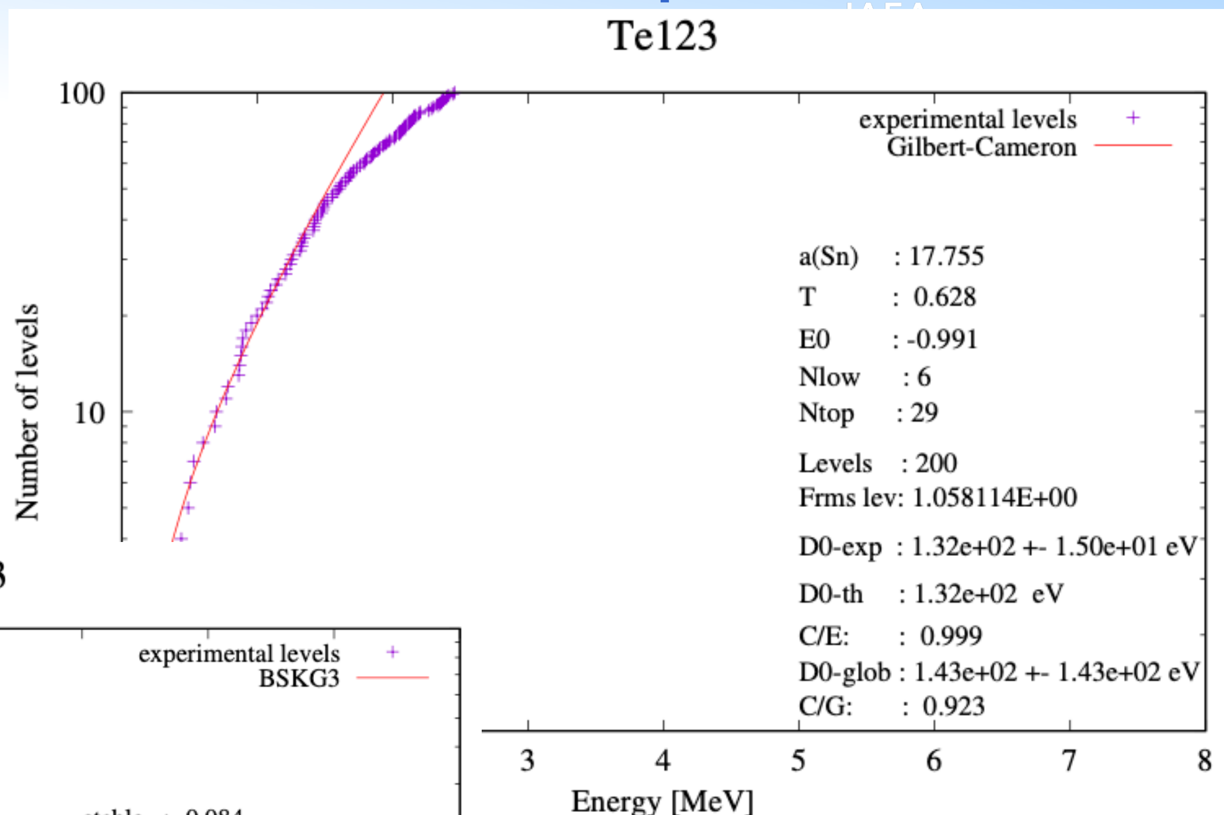
Te-123: Gilbert-Cameron versus BSKG3 - experimental D0

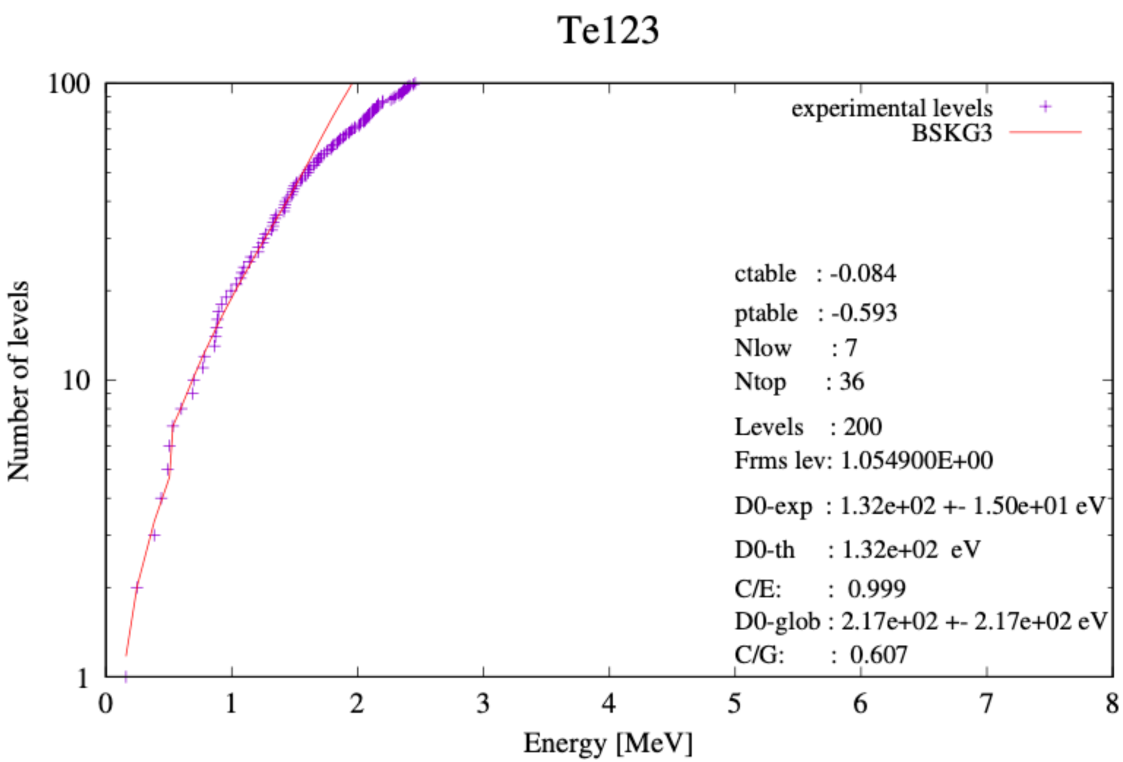
Minimize:

$$\chi^2_{\text{global}} = \sum_{i=1}^{N} \chi^2_{D,i} + \chi^2_{\text{lev},i}\,.$$

$$\chi^2_{\text{lev},i} = \sum_{k=N_L^i}^{N_U^i} \frac{(N^i_{\text{cum}}(E_k) - k)^2}{k},$$

$$\chi^2_{D,i} = \left(\frac{D^{\text{theo}}_{0,i} - D^{\text{exp}}_{0,i}}{\Delta D^{\text{exp}}_{0,i}} \right)^2,$$

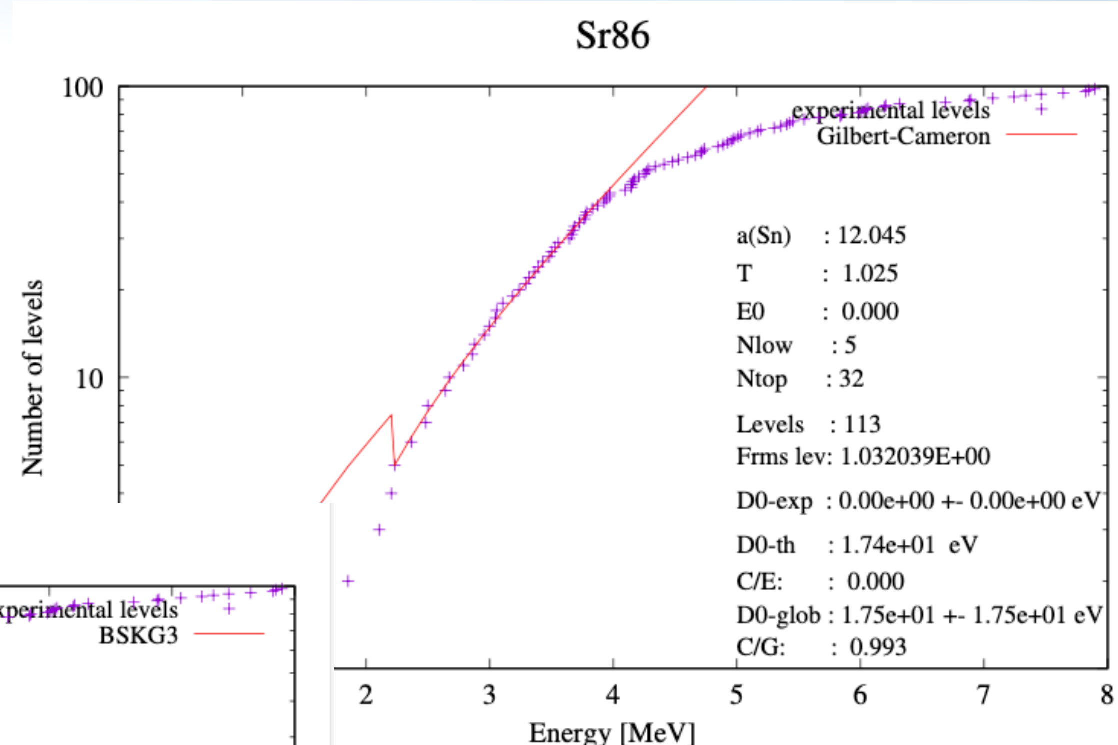


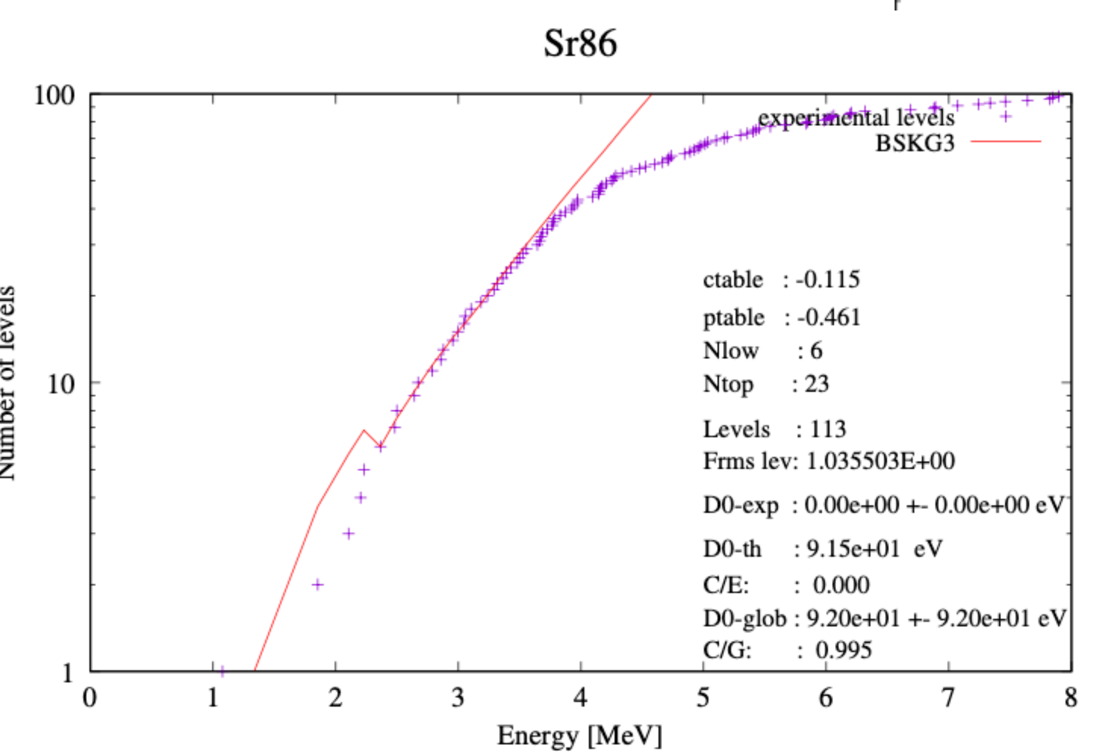


Optimize ctable, ptable, Nlow (NL) and Ntop (NU) at the same time

Sr-86: Gilbert-Cameron versus BSKG3 - no experimental D0

Use D0 estimate from global level density with unc. 100% to constrain discrete level fit





Note: Many technological important nuclides have no exp. D0.
For example, Cu64,66 have while Cu63,65 have not. In those cases, (n,γ) is better constrained than (n,n’)

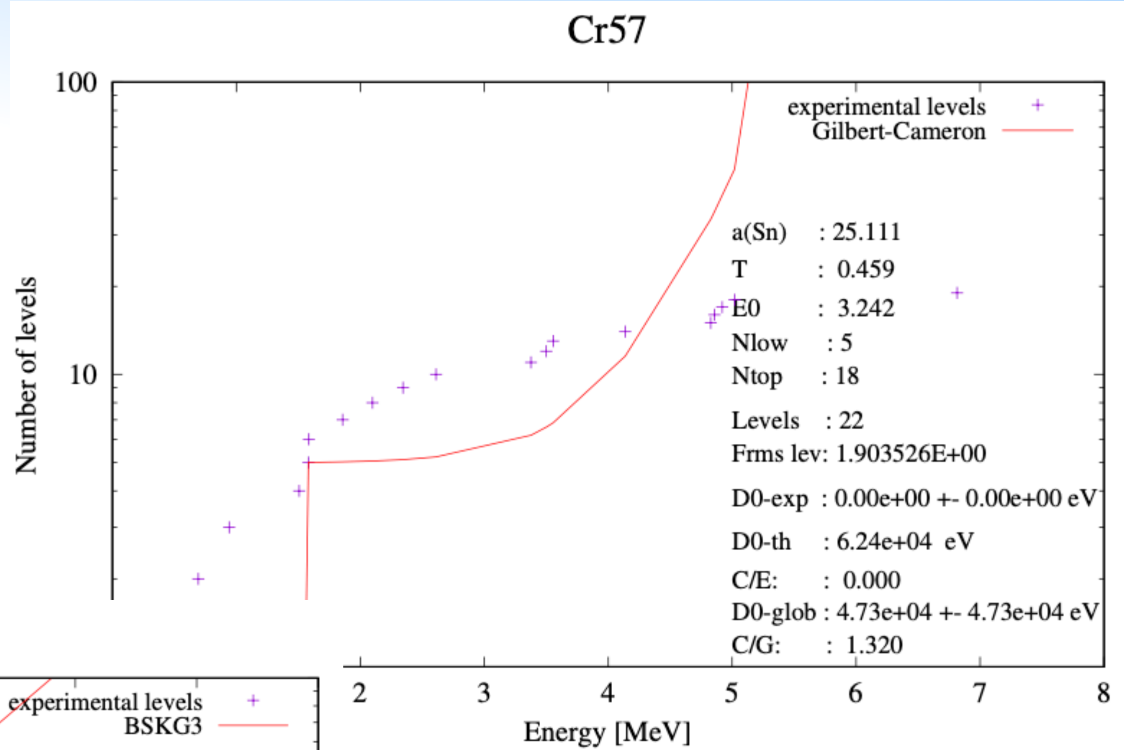
Use clean discrete level database

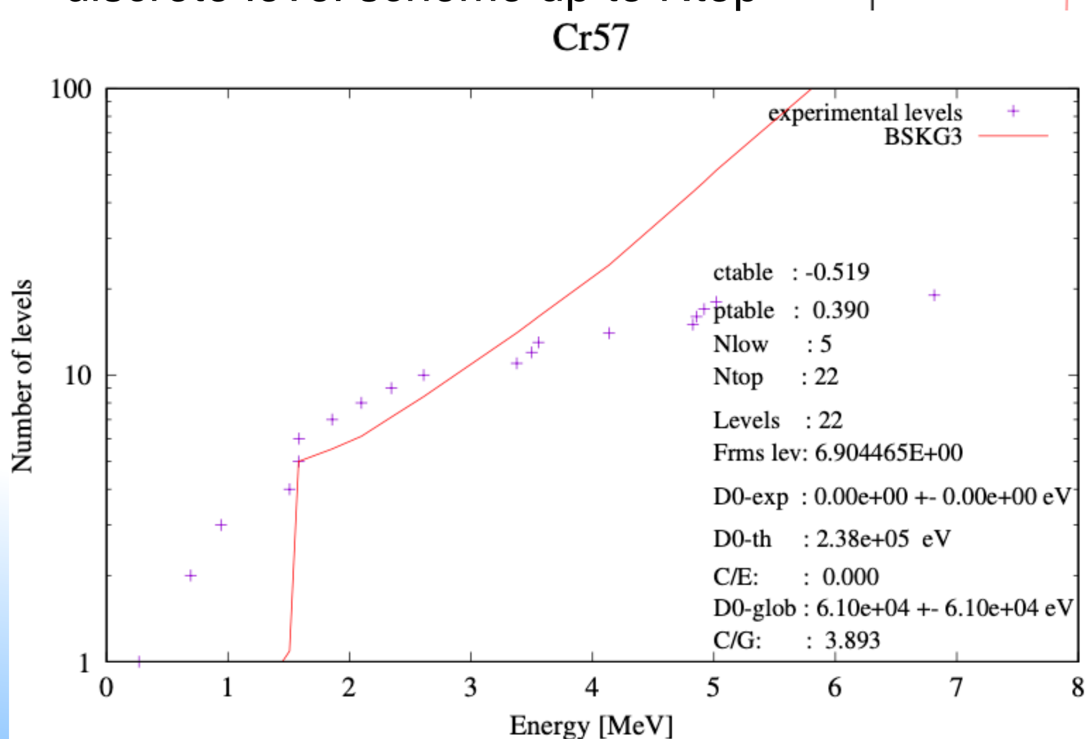
RIPL discrete level file:

1496 nuclides with > 15 levels

~200 rejected because of huge deviation from any level density model (Frms, ctable, ptable)

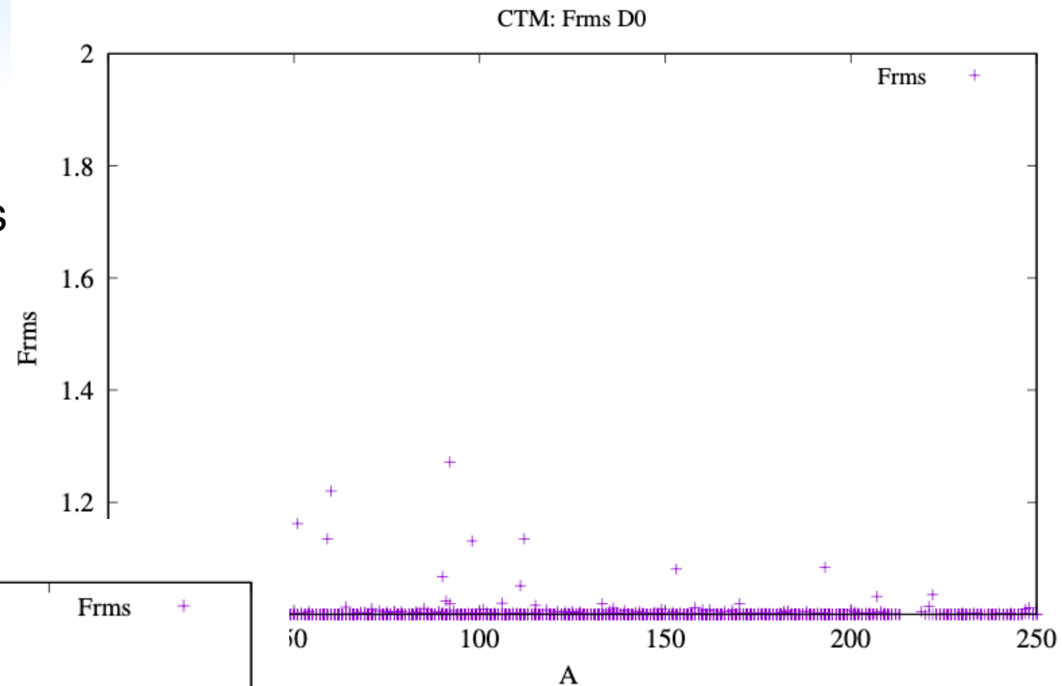
~1300 nuclides with usable discrete level scheme up to Ntop

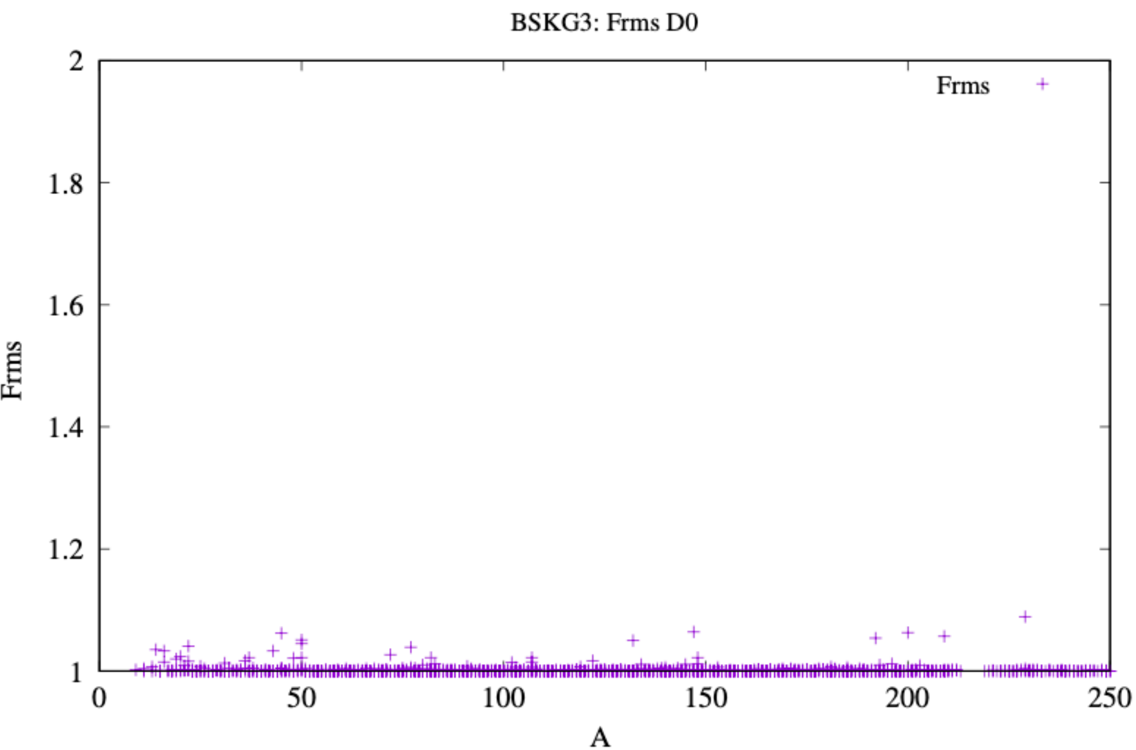




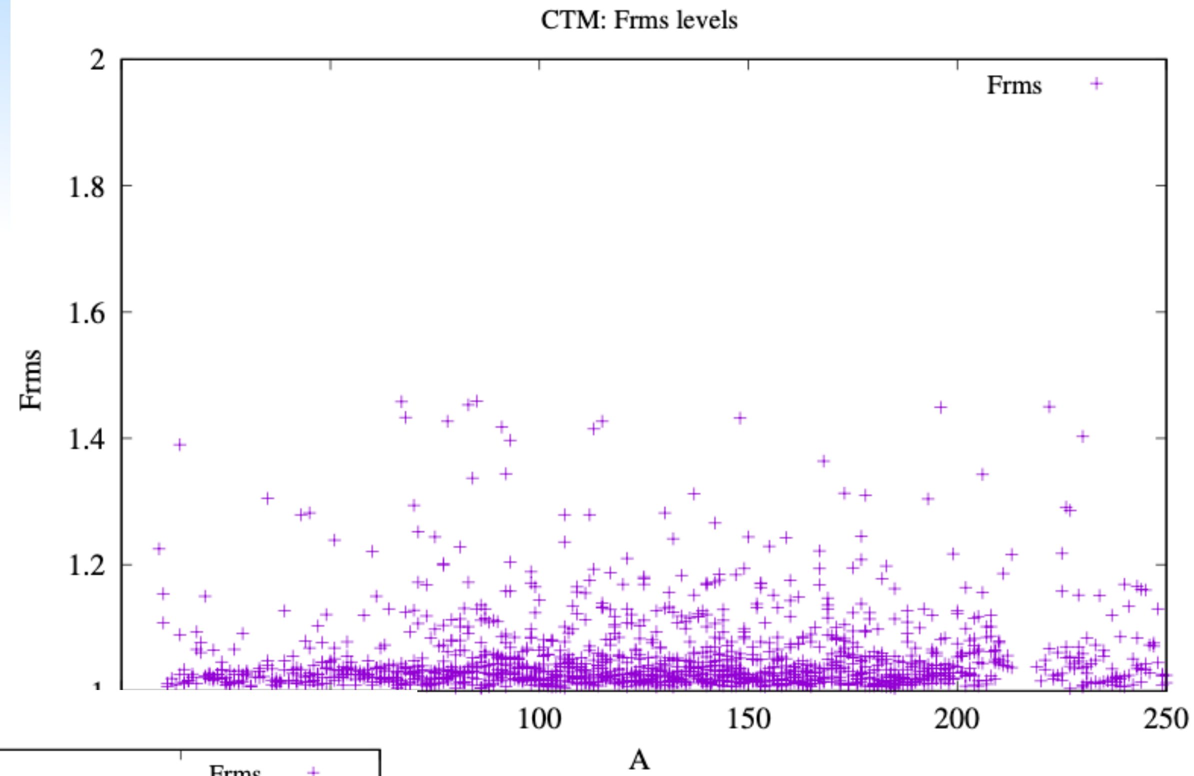
Adjusted level densities- D0

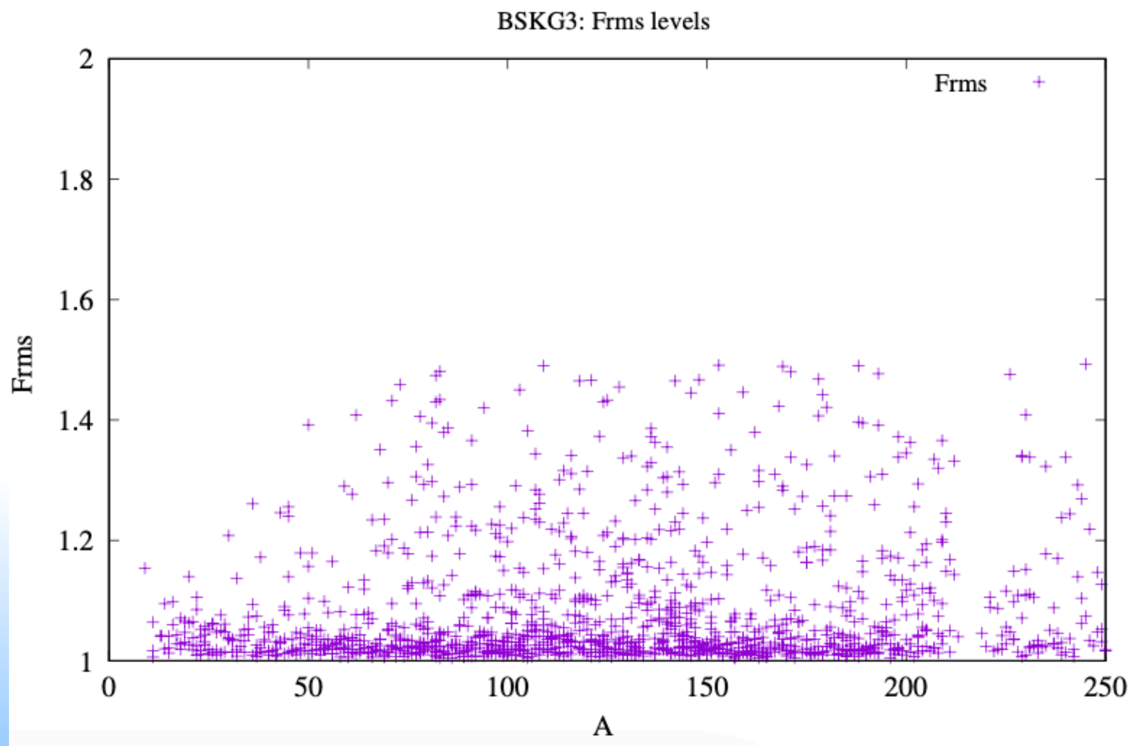
No perfect fit because of simultaneous adjustment to discrete levels





Adjusted level densities - Discrete levels

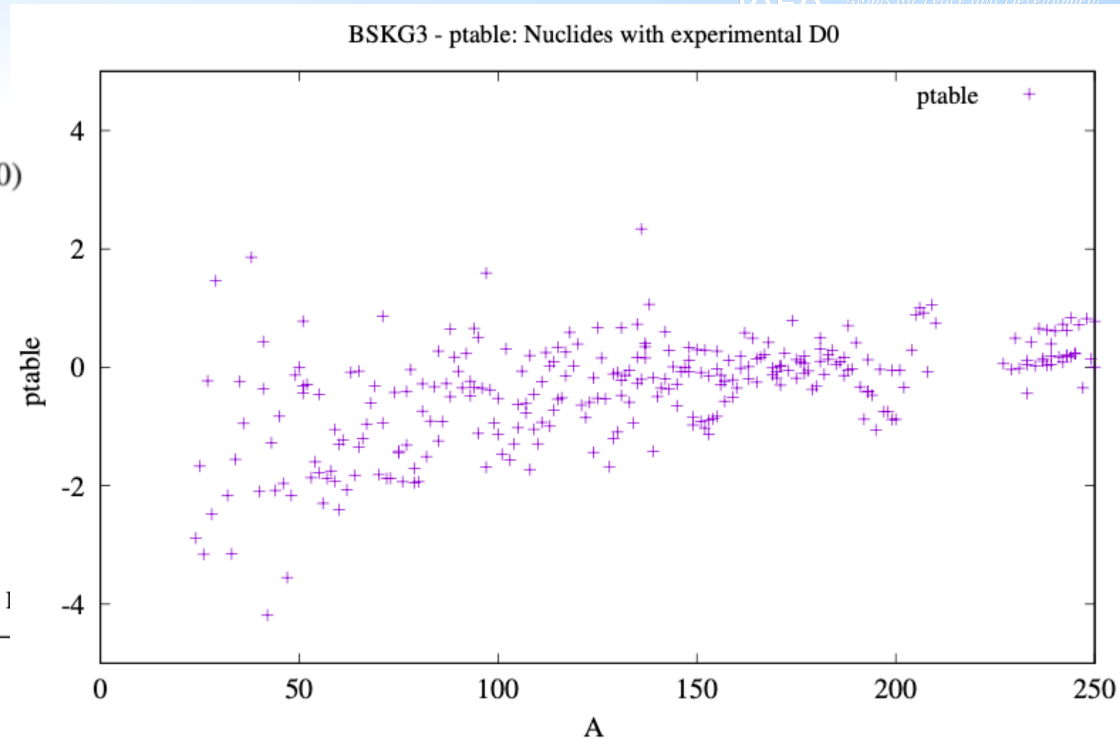


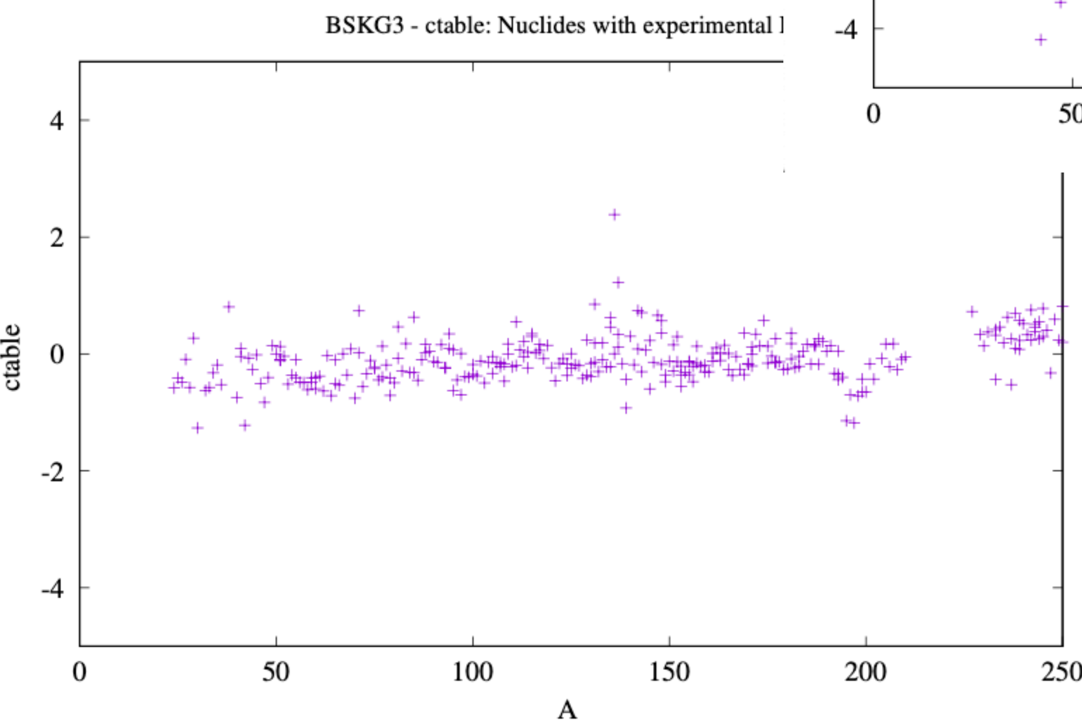


Still to do:
Compare global BSKG3 with global CTM (i.e. global formula for T and E0)

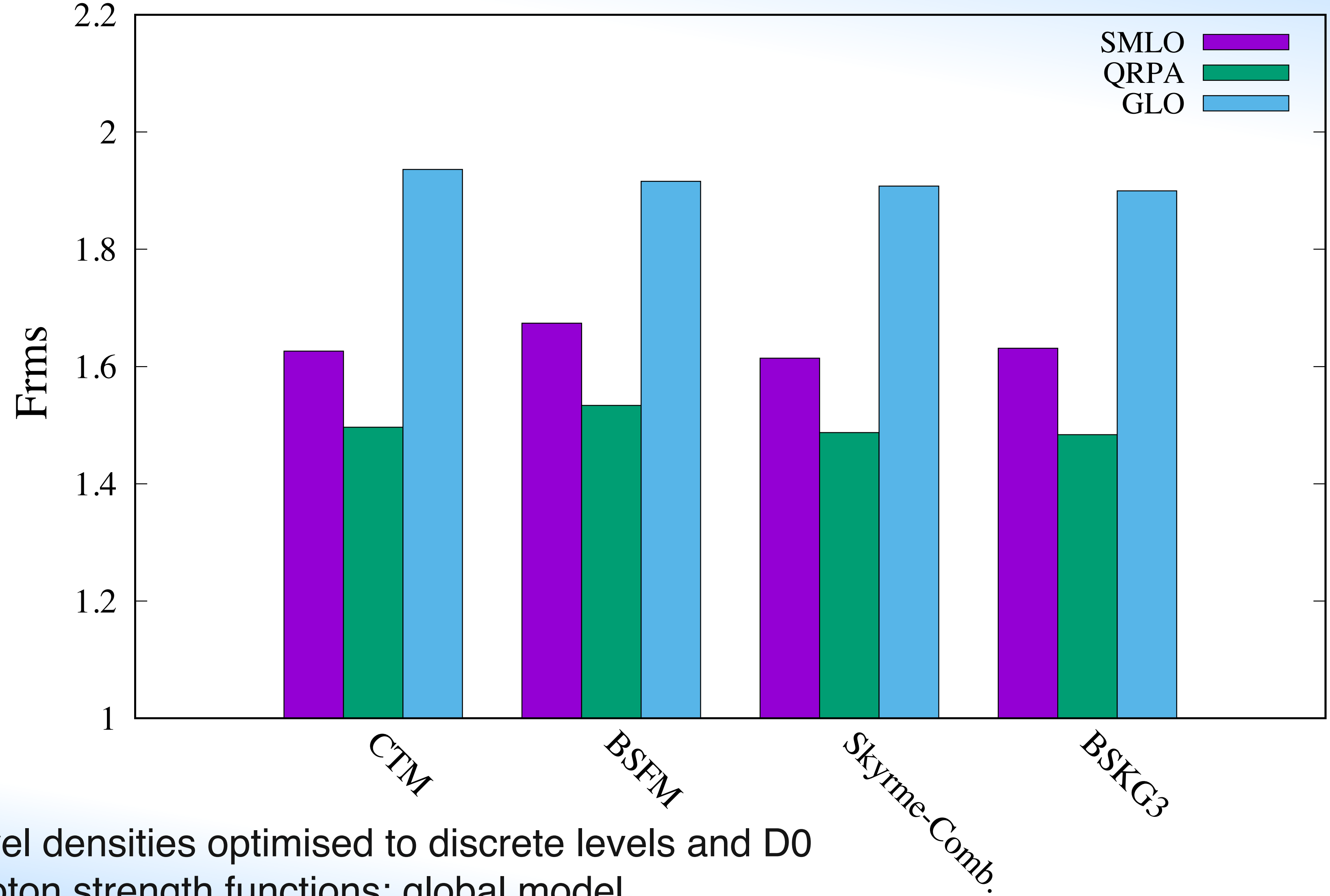
BSKG3 level density parameters adjusted to D0 and discrete levels

$$\rho(E_x, J, \pi) = \exp(c\sqrt{E_x - \delta})\rho_{nom}(E_x - \delta, J, \pi) \qquad (230)$$



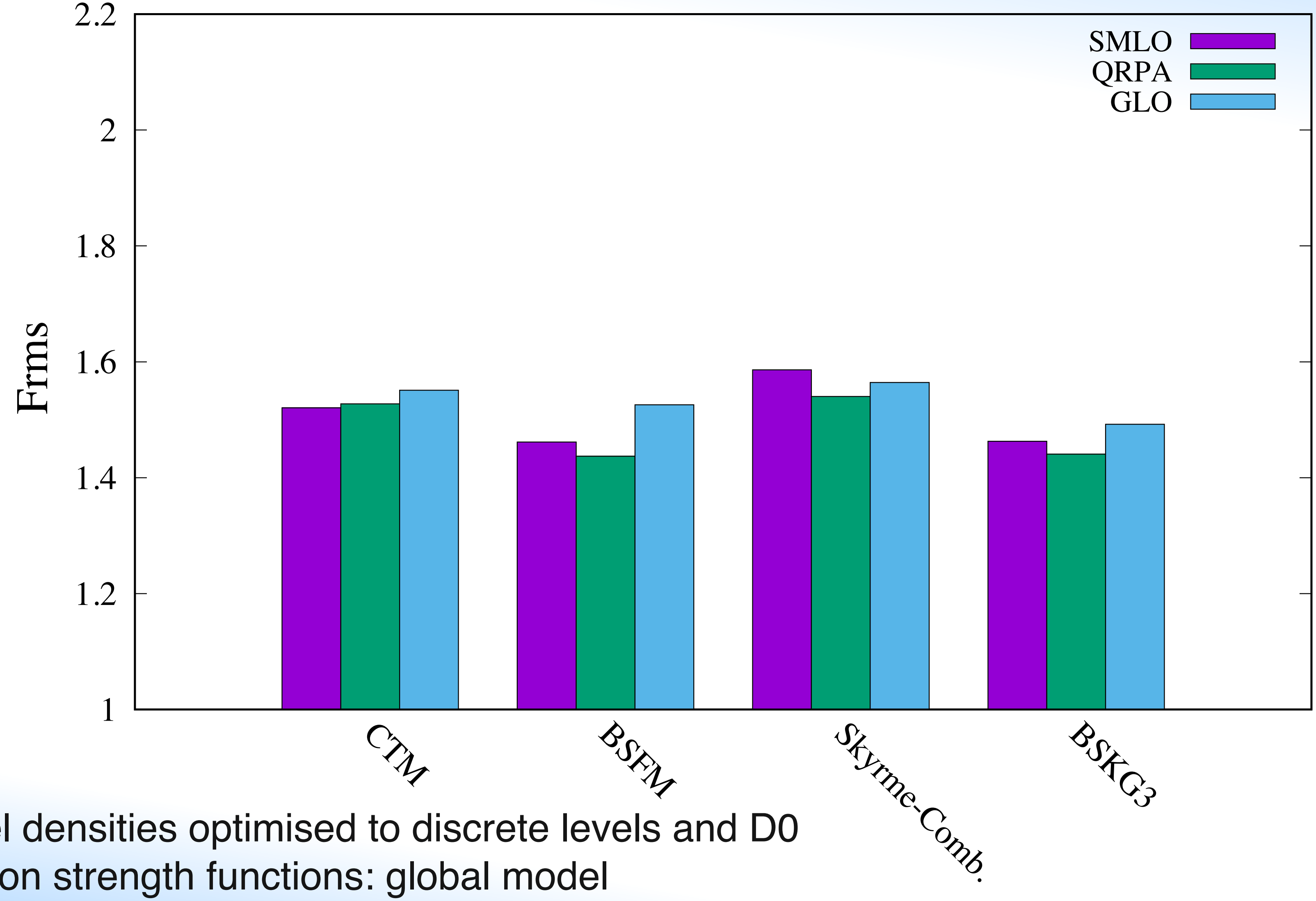


TALYS Average radiative width vs. experiment



Level densities optimised to discrete levels and D0
Photon strength functions: global model
Nuclides with experimental <Gg> data: 228

TALYS Maxwellian Averaged cross sections vs. experiment



Level densities optimised to discrete levels and D0
Photon strength functions: global model
Nuclides with experimental MACS data: 277

Normalisation of inelastic scattering to high-lying discrete levels

- Suppose:
  - Nlow = 4
  - Ntop = 20
  - Ncum starts to exceed exp. discrete levels above Ntop
  - For inelastic scattering to the first 40 levels:
    - Weight in HF for level 1 to Ntop : 1
    - Weight in HF for levels (Ntop + 1) to 40: (Ncum(Eexp (level 40)) - Ntop)/(40 -Ntop)

Goodness-of-fit: Frms with experimental uncertainty

$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2}$$

Frms = 1.40 means "~40% off"

$$\varepsilon_{rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}\ln r_i\right]$$

Erms = 1. means "no model bias"

Instead of

$$r_i = \frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}},$$

Usual C/E value

we use

$$\begin{aligned} r_i &= 1-\left(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1\right)\mathrm{erf}\left(\frac{x}{\sqrt{2}}\right) \quad \text{if} \quad \sigma^i_{\rm th} < \sigma^i_{\rm exp}, \\ &= 1+\left(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1\right)\mathrm{erf}\left(\frac{x}{\sqrt{2}}\right) \quad \text{if} \quad \sigma^i_{\rm th} > \sigma^i_{\rm exp}, \\ &= 1 \quad \text{if} \quad \sigma^i_{\rm th} = \sigma^i_{\rm exp}. \end{aligned}$$

C/E value including uncertainties

$$x = \frac{\sigma^i_{\rm th} - \sigma^i_{\rm exp}}{\delta\sigma^i_{\rm exp}}$$

Parameter optimisation up to 20 MeV

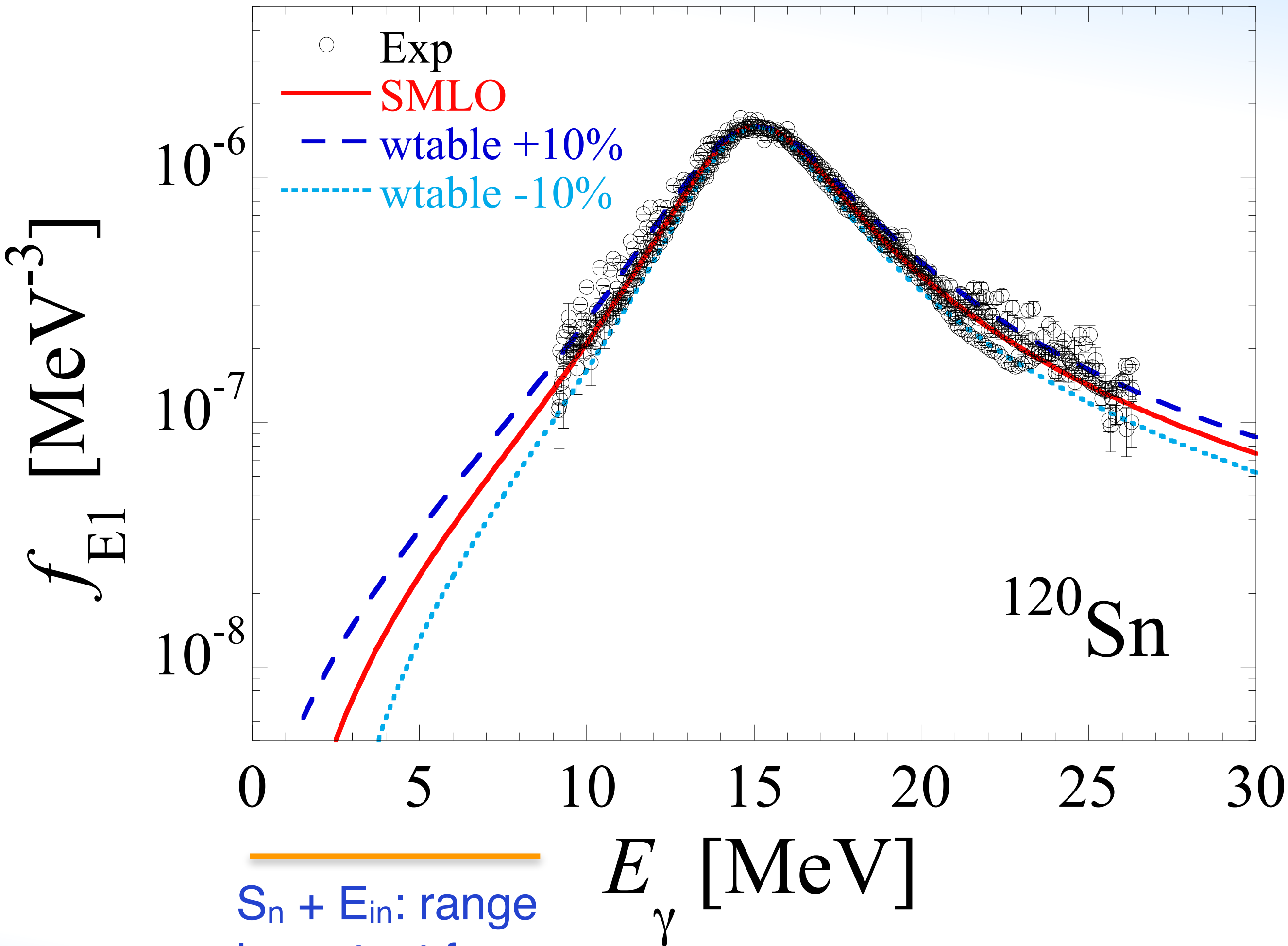
- Use TASMAN: Nelder-Mead optimisation
  - Multi-dimensional parameter landscape not too wild
  - 20 TALYS runs per parameter usually enough
- (n,gamma):
  - PSF: wtable of compound nucleus
- (n,n'), (n,2n), (n,p) and (n,np)
  - rvadjust p, gadjust(0,0), gadjust(0,1), gadjust(1,0)
- (n,alpha)
  - rvadjust a, cstrip a
- Isomer versus ground state:
  - Risomer of the final nuclide
  - S2adjust of final nuclide

Experimental data

- TALYS/TENDL methodology requires **all** EXFOR to be available instantaneously
- Best current option (for AK): EXFORtables - directory structured database
- All data normalised to latest standards/monitors
- Outlier assignment:
  - 23444 cross section data sets
  - 10969 declared inlier
  - 1975 declared outlier
  - Still need to put 23444 JSON files on IAEA-github

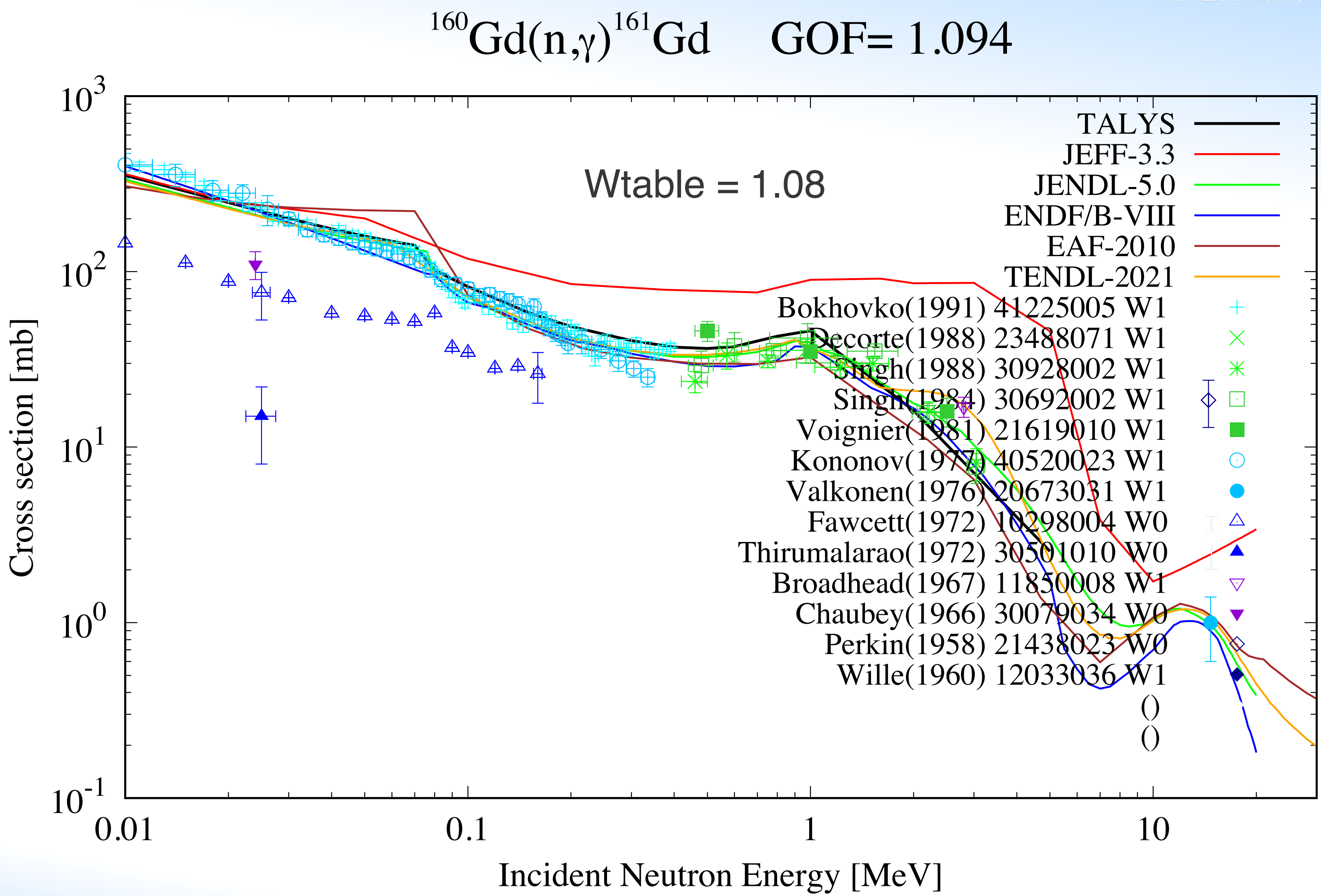
```
/Users/koning/quality/json> cat 12033007.json
{
    "Subentry"    : "12033007",
    "Author"      : "Wille",
    "Year "       : 1960,
    "Projectile"  : "n",
    "Target Z"    :   57,
    "Target A"    :  139,
    "Target state": "0",
    "Reaction"    : "(n,x)",
    "Final Z"     :   55,
    "Final A"     :  136,
    "Final state" : "g",
    "Quantity"    : "Cross section",
    "X4 Reaction" : "57-LA-139(N,A)55-CS-136-G,,SIG",
    "MF"          :    3,
    "MT"          :  107,
    "Evaluations" :
    [
        {
        "Evaluator"   : "Arjan Koning",
        "Date"        : "2022-12-13",
        "Weight"      :    0,
        "Comment"     : [
                        " Excluded from evaluation: graphical outlier"
                        ]
        },
        {
        "Evaluator"   : "Arjan Koning (2020)",
        "Date"        : "2012-06-30",
        "Weight"      :   -1,
        "Comment"     : [
                        "NEA quality score: R2"
                        ]
        },
        {
        "Evaluator"   : "Natalia Dzysiuk (2018)",
        "Date"        : "2018-03-24",
        "Weight"      :    0,
        "Comment"     : [
                        " wrong half-life, inconsistent time of irradiation"
                        ]
        }
    ]
}
```

Adjusting (n,γ) cross sections with PSF width parameter



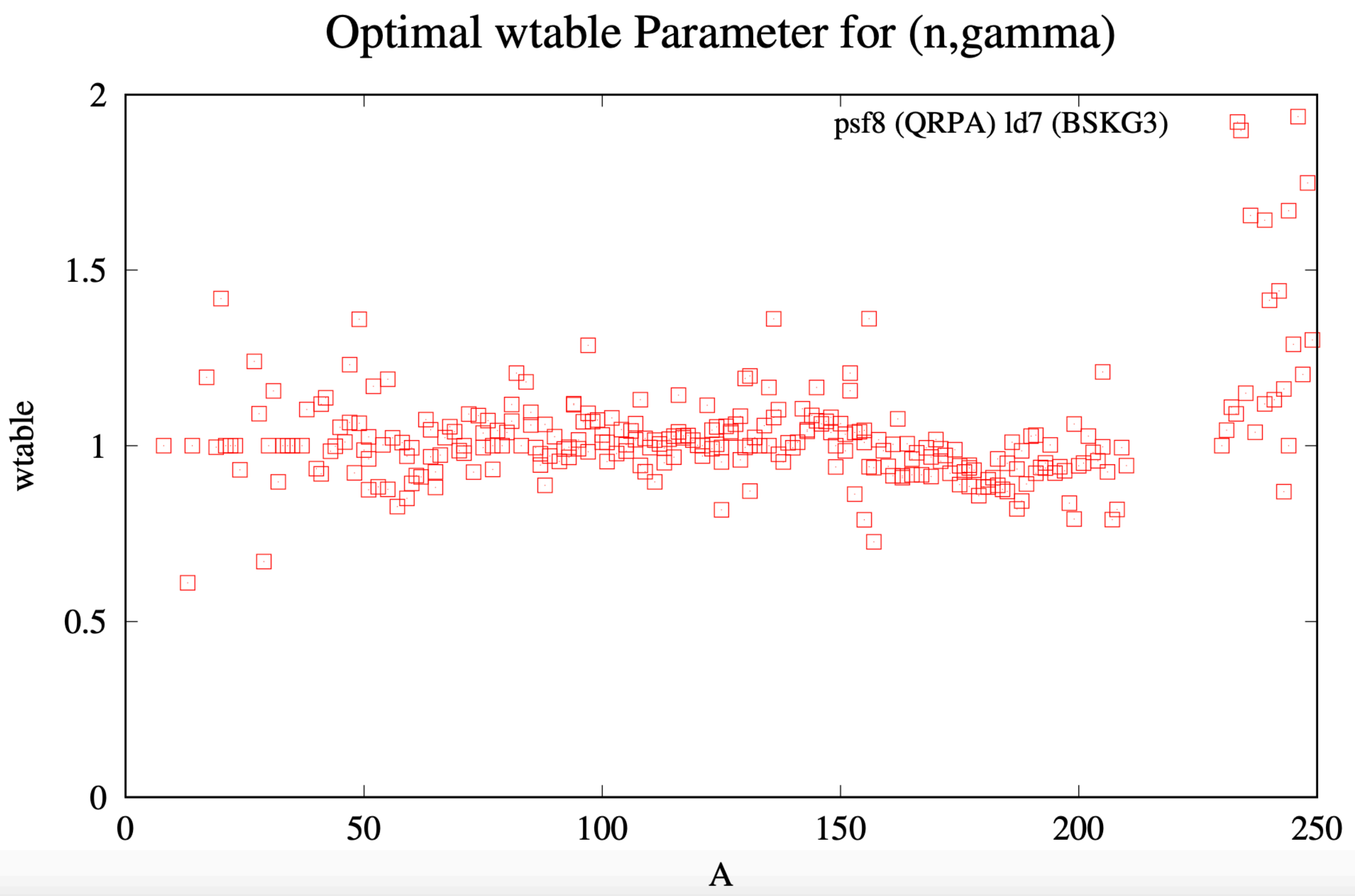
S_n + E_{in}: range important for (n,γ)

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



^{160}Gd(n,γ)^{161}Gd GOF= 1.094
Wtable = 1.08
TALYS
JEFF-3.3
JENDL-5.0
ENDF/B-VIII
EAF-2010
TENDL-2021
Bokhovko(1991) 41225005 W1
Decorte(1988) 23488071 W1
Singh(1988) 30928002 W1
Singh(1984) 30692002 W1
Voignier(1981) 21619010 W1
Kononov(1977) 40520023 W1
Valkonen(1976) 20673031 W1
Fawcett(1972) 10298004 W0
Thirumalarao(1972) 30501010 W0
Broadhead(1967) 11850008 W1
Chaubey(1966) 30079034 W0
Perkin(1958) 21438023 W0
Wille(1960) 12033036 W1
()
()
Cross section [mb]
Incident Neutron Energy [MeV]

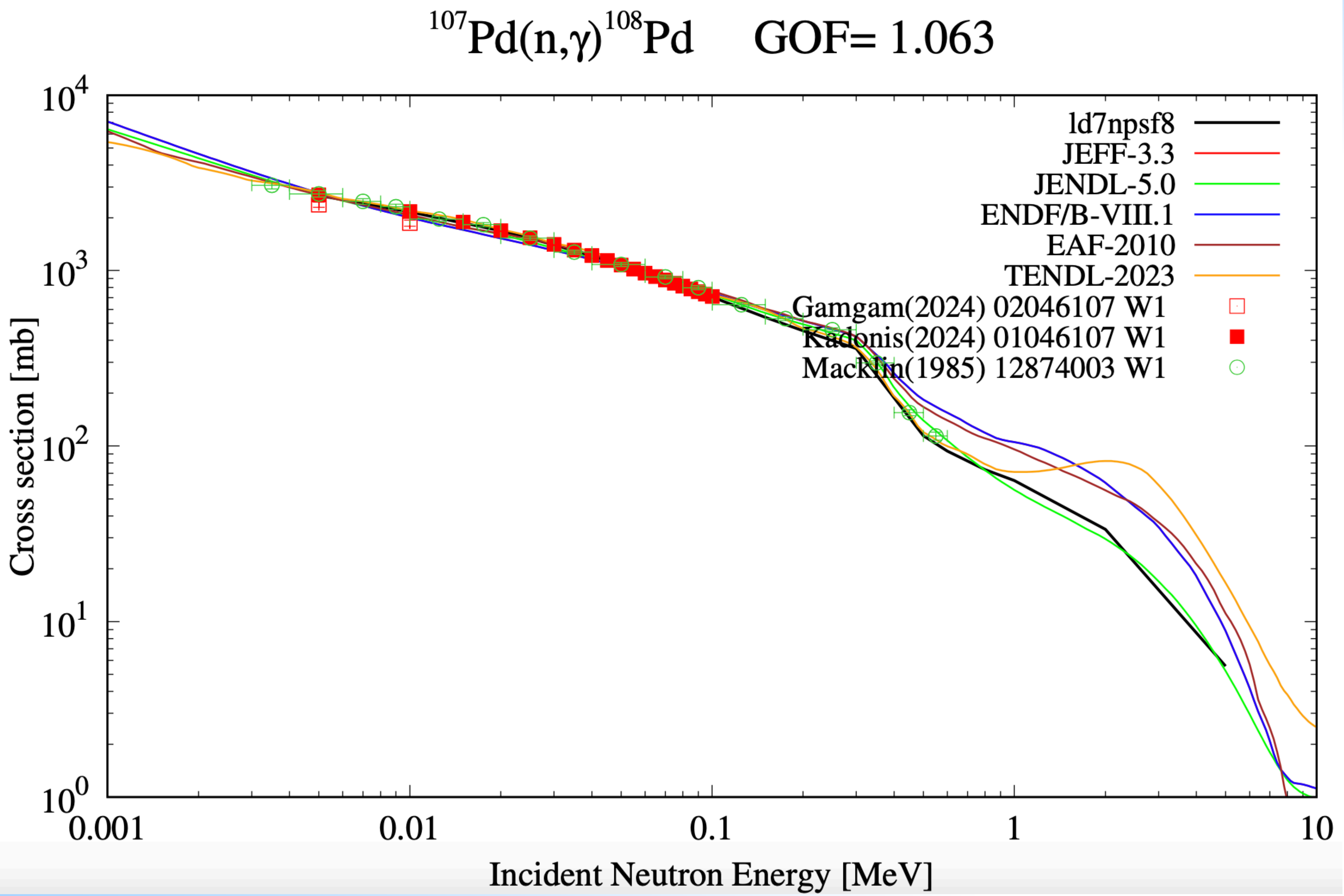
Current optimal combination of level density and photon strength function



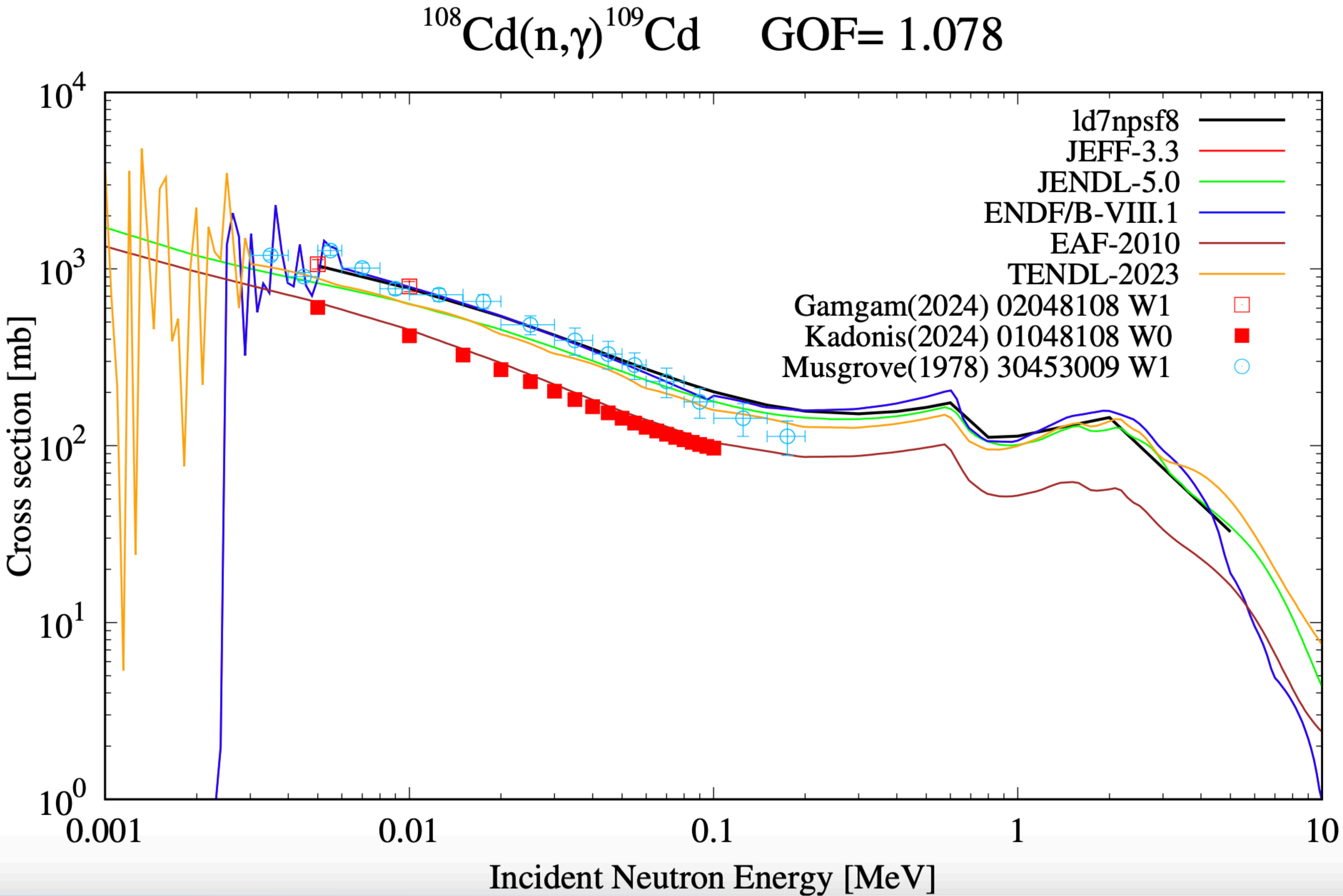
Unify all (n,γ) data

- EXFOR for cross sections, excluding outliers
- Pseudo-data created from perfect TALYS fit to average radiative width $\Gamma\gamma$ (one point)
  - Gives a value for wtable, one for each LD model
  - Use the LD spread of calculated cross sections as uncertainty
  - Use this to create pseudo-exp. cross sections at 5 and 10 keV
- Pseudo-data created from perfect TALYS fit to Maxwellian Averaged Cross Section from Astral/Kadonis database (one point)
  - Gives a value for wtable, one for each LD model
  - Use the LD spread of calculated cross sections as uncertainty
  - Use this to create pseudo-exp. cross sections between 5 and 100 keV
- Use pseudo-exp. data in the same fit as normal exp. cross sections
- Outlier detection for average radiative width and MACS

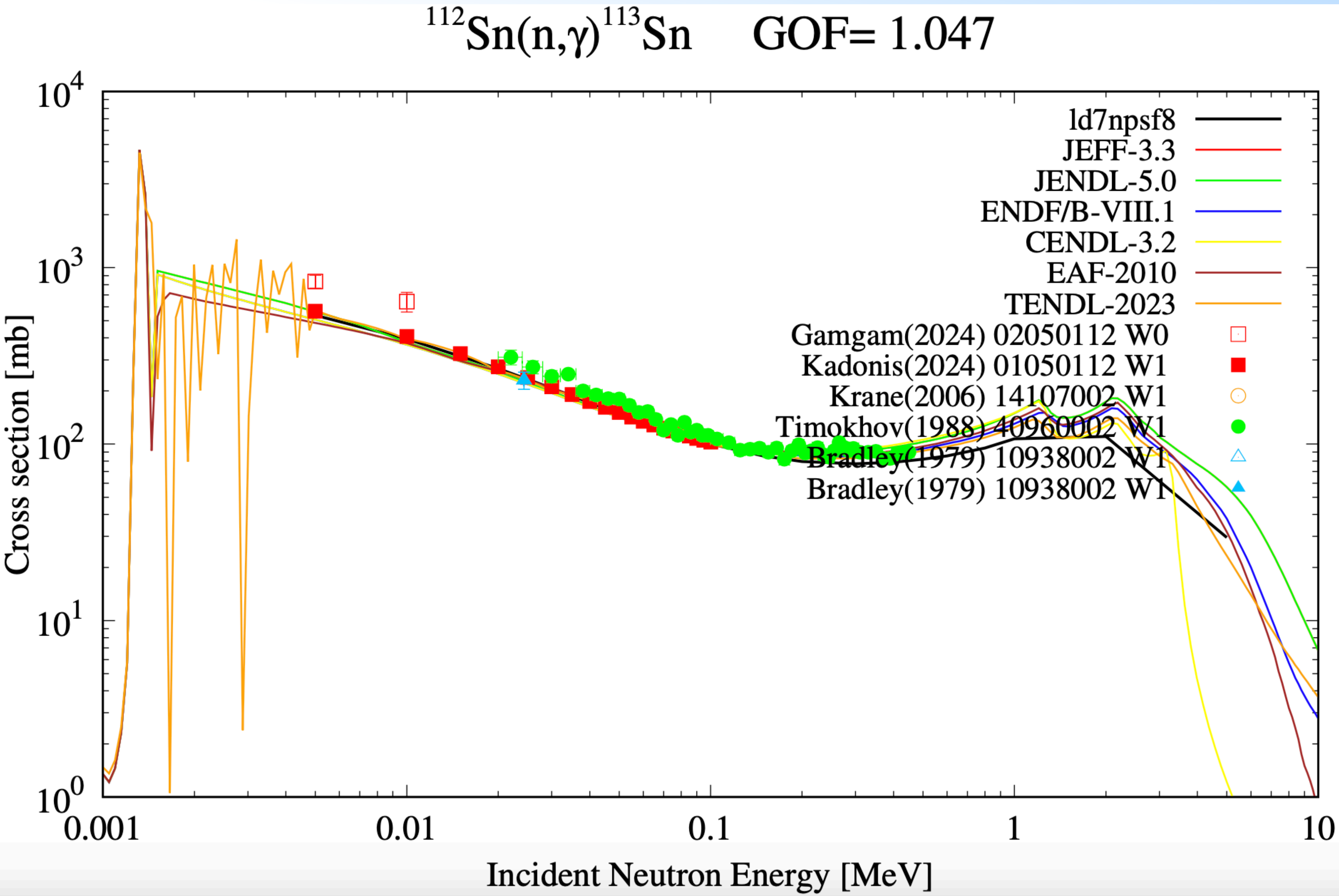
Typical case



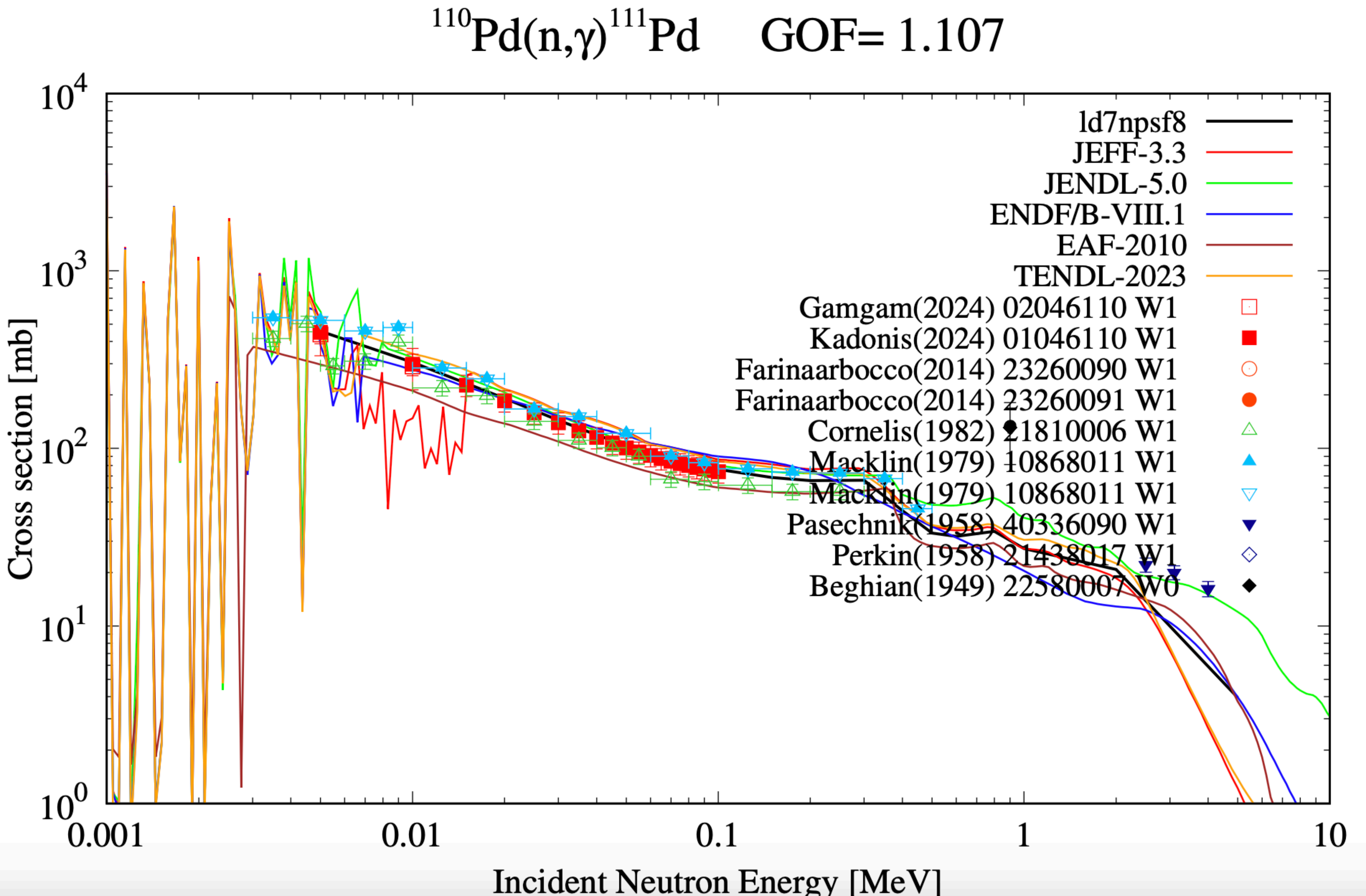
Example: MACS considered an outlier



Example: Average radiative width Γγ considered an outlier



…but usually: (n,γ) cross sections, MACS and Γγ are consistent



Outliers for TENDL (n,γ) evaluation

8 isotopes with MACS from Astral/Kadonis considered as outlier:
Cr-50, Cu-63,65, Br-81, Cd-106,108, Sm-148,154

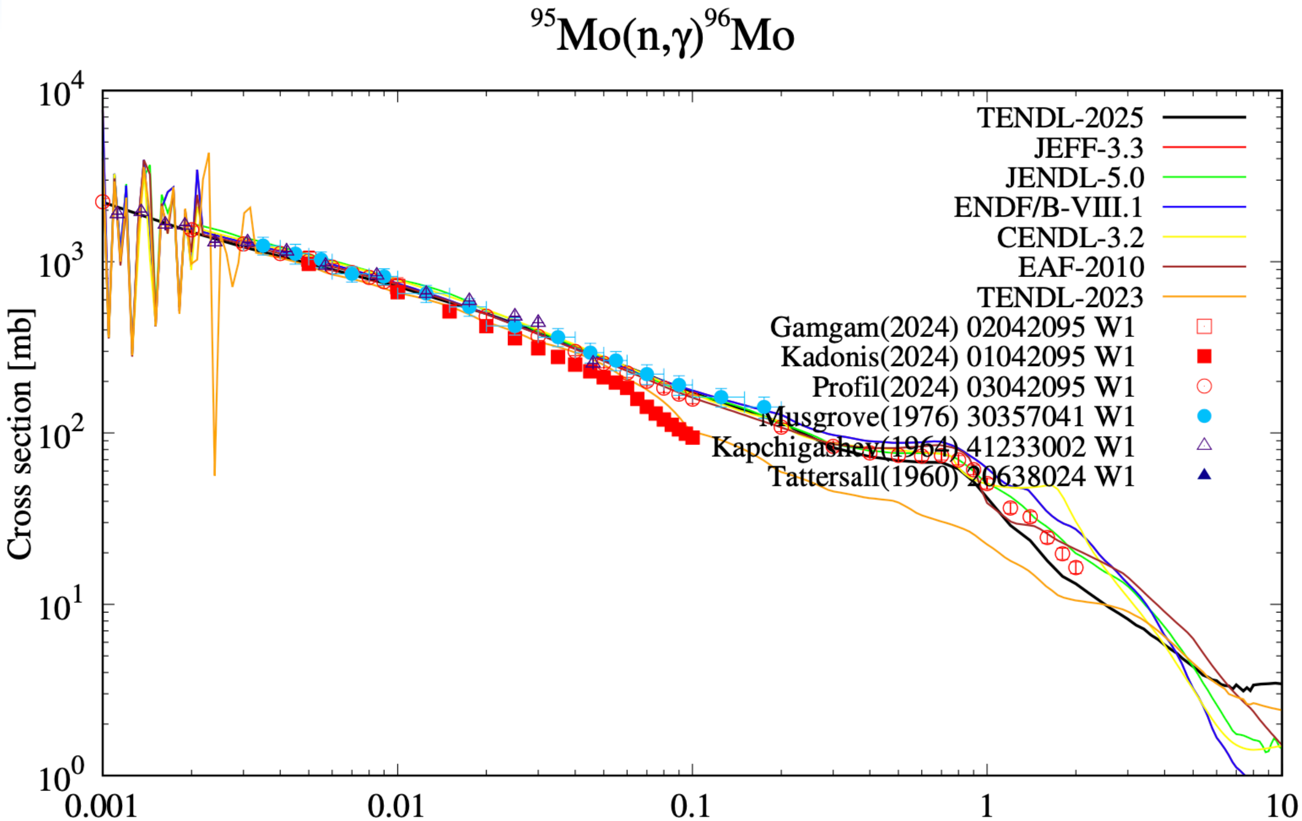
36 isotopes with Γγ considered as outlier:
Ca-40,42,44,……Hg-198

My notebook of remaining cases to solve

```
Gd157 0.3 - 1 MeV too low, discrete levels seem OK
Hf177 very weird peak at 2 MeV
Hf178 weird peak at 2 MeV
Hf180 0.5 - 1 MeV too high
In115 - totally too high , suppress fit for g, m, n
Lu175 around 1 MeV too low?
Mo95 0.1 - 1 MeV too low  solved after removing discrete levels for target
Mo97 0.2 - 1 MeV too low esp compared to Profil data?  solved after removing discrete levels for target
Pb208 rather high at few MeV
Rh103 too low, also for g and m
Sb123 isomeric ratio check m, n
Se80(n,gamma) too high above 0.3 MeV
Tc99(n,gamma) low above 0.1 MeV
Te122 too high above 0.2 MeV
W183 0.3 - 1 MeV too low
W184 0.2 - 2 MeV too high
W186 0.6 - 2 MeV too low
Xe132 low (why?) NOT in BATCH, adopted LD1

Interesting: Os187 has exp peak at 2 MeV, which only Hf177, 178 and Ir191 have for TALYS
```

RIPL discrete level scheme important



JENDL-5

RIPL-3

Removing levels has large effect

3. Level scheme of Mo- 95

No.	Ex(MeV)	J	PI
0	0.00000	5/2	+
1	0.20412	3/2	+
2	0.76580	7/2	+
3	0.78620	1/2	+
4	0.82063	3/2	+
5	0.94768	9/2	+
6	1.03927	1/2	+
7	1.05676	5/2	+
8	1.07372	7/2	+
9	1.09200	3/2	+
10	1.30259	1/2	+

42	95	587	142	
0	0.000000	2.5	1	0
1	0.059300	2.5	1	1
2	0.204116	1.5	1	1
3	0.526600	3.5	1	1
4	0.765803	3.5	1	2
5	0.786201	0.5	1	2
6	0.820628	1.5	1	3

TALYS: YANDF structure for level density tables

```
# header:
#   title: Tc100 level density
#   source: TALYS-2.1
#   user: Arjan Koning
#   date: 2025-03-16
#   format: YANDF-0.3
# residual:
#   Z: 43
#   A: 100
#   nuclide: Tc100
# parameters:
#   fission barrier: 0
#   ldmodel keyword: 5
#   level density model: Hilaire-Goriely Skyrme
#   Rhotot(Sn) [MeV^-1]:  5.853849E+05
#   number of excited levels: 100
#   Nlow: 4
#   Ntop: 20
#   ctable: -2.774200E-01
#   ptable: -7.658300E-01
#   experimental D0 [eV]:  1.400000E+01
#   experimental D0 unc. [eV]:  1.200000E+00
#   global D0 [eV]:  1.552358E+01
#   global D0 unc. [eV]:  1.552358E+01
#   theoretical D0 [eV]:  1.400057E+01
#   Chi-2 D0:  2.266164E-07
#   C/E D0:  1.000041E+00
#   Frms D0:  1.000000E+00
#   Erms D0:  1.000000E+00
#   C/G D0:  9.018906E-01
#   Chi-2 per level:  3.017535E-01
#   Frms per level:  1.085027E+00
#   Erms per level:  9.867235E-01
#   average deviation per level:  9.097415E-01
# quantity:
#   type: total level density
#   datablock:
#     columns: 5
#     entries: 100
##       E            Level      N_cumulative      Total_LD        Exp_LD
##     [MeV]           []             []          [MeV^-1]       [MeV^-1]
   1.721500E-01      1            6.617190E+00   3.843851E+01   2.434613E+01
   2.006700E-01      2            7.973864E+00   4.756921E+01   2.712600E+01
   2.234700E-01      3            9.119342E+00   5.024027E+01   3.003404E+01
   2.439500E-01      4            4.000000E+00   5.261105E+01   3.129988E+01
   2.635600E-01      5            5.069006E+00   5.451331E+01   3.282015E+01
   2.875200E-01      6            6.426341E+00   5.665005E+01   6.515430E+01
```

TALYS: YANDF structure for level density tables (continued

```
   1.337886E+01   98             1.523974E+08   1.050405E+08   8.190800E+01
   1.340840E+01   99             1.555245E+08   1.058847E+08   8.619006E+01
   1.341446E+01  100             1.561730E+08   1.068775E+08   8.400032E+01
# quantity:
#   type: level density
#   Parity: 1
#   datablock:
#     columns: 46
#     entries: 60
##       E              T          N_cumulative   rho_observed    rho_total       J=  0.0        J=  1.0        J=  2.0        J=  3.0        J=
##     [MeV]          [MeV]            []          [MeV^-1]       [MeV^-1]       [MeV^-1]       [MeV^-1]       [MeV^-1]       [MeV^-1]       [MeV^
   2.500000E-01   1.260320E-01   5.796660E+00   2.318664E+01   1.825597E+02   3.585640E+00   1.627511E+00   3.348752E+00   4.174334E+00   3.29328
   5.000000E-01   1.782361E-01   1.713370E+01   4.534817E+01   3.602382E+02   4.761246E+00   2.537095E+00   8.701150E+00   9.146145E+00   6.12500
   7.500000E-01   2.182937E-01   3.445288E+01   6.927672E+01   5.969662E+02   4.232631E+00   4.561946E+00   1.243222E+01   1.145301E+01   1.16785
   1.000000E+00   2.520639E-01   6.016666E+01   1.028551E+02   9.447372E+02   5.115467E+00   6.270041E+00   1.736999E+01   1.528264E+01   1.72572
   1.250000E+00   2.818160E-01   9.745163E+01   1.491399E+02   1.394366E+03   7.494006E+00   8.438171E+00   2.481481E+01   2.138929E+01   2.39625
   1.500000E+00   3.087140E-01   1.507815E+02   2.133197E+02   2.085454E+03   8.870983E+00   1.104404E+01   3.204881E+01   3.188046E+01   3.42707
   1.750000E+00   3.334492E-01   2.398582E+02   3.563066E+02   3.393921E+03   1.715721E+01   2.029018E+01   5.705436E+01   5.608946E+01   5.54769
   2.000000E+00   3.564722E-01   3.786460E+02   5.551513E+02   5.332528E+03   3.258583E+01   3.121616E+01   7.965952E+01   8.152479E+01   8.99207
   2.250000E+00   3.780958E-01   5.766601E+02   7.920561E+02   7.885057E+03   4.089179E+01   4.254385E+01   1.059822E+02   1.068730E+02   1.32057
   2.500000E+00   3.985480E-01   8.661532E+02   1.157973E+03   1.167979E+04   5.470546E+01   6.008087E+01   1.581076E+02   1.506591E+02   1.85131
   2.750000E+00   4.180007E-01   1.270419E+03   1.617062E+03   1.679721E+04   7.123441E+01   8.416255E+01   2.125417E+02   1.904085E+02   2.57280
   3.000000E+00   4.365875E-01   1.871772E+03   2.405414E+03   2.493661E+04   1.161081E+02   1.241326E+02   3.206979E+02   2.977931E+02   3.64993
   3.250000E+00   4.544147E-01   2.777212E+03   3.621758E+03   3.762182E+04   1.686231E+02   1.851064E+02   4.892593E+02   4.531126E+02   5.55986
   3.500000E+00   4.715684E-01   4.060326E+03   5.132458E+03   5.440375E+04   2.296449E+02   2.424268E+02   6.500207E+02   6.166148E+02   7.88627
   3.750000E+00   4.881197E-01   5.860460E+03   7.200535E+03   7.784309E+04   3.117330E+02   3.326349E+02   8.781214E+02   8.543216E+02   1.07589
   4.000000E+00   5.041278E-01   8.369131E+03   1.003469E+04   1.102539E+05   4.084593E+02   4.592863E+02   1.208004E+03   1.151217E+03   1.47033
   4.250000E+00   5.196431E-01   1.183226E+04   1.385252E+04   1.545771E+05   5.381581E+02   6.204632E+02   1.631866E+03   1.533443E+03   1.99980
   4.500000E+00   5.347083E-01   1.673149E+04   1.959691E+04   2.198914E+05   7.612924E+02   8.622344E+02   2.291828E+03   2.164213E+03   2.80428
   4.750000E+00   5.493605E-01   2.364849E+04   2.766801E+04   3.125566E+05   1.073460E+03   1.195285E+03   3.208619E+03   3.045447E+03   3.92193
   5.000000E+00   5.636320E-01   3.308268E+04   3.773675E+04   4.317026E+05   1.435622E+03   1.590123E+03   4.267314E+03   4.082115E+03   5.24686
   5.500000E+00   5.911422E-01   6.764582E+04   6.912628E+04   8.118315E+05   2.515590E+03   2.768054E+03   7.447311E+03   7.198621E+03   9.30679
   6.000000E+00   6.174279E-01   1.299661E+05   1.246405E+05   1.499615E+06   4.322644E+03   4.760361E+03   1.285440E+04   1.245189E+04   1.64812
   6.500000E+00   6.426393E-01   2.400801E+05   2.202281E+05   2.709263E+06   7.257842E+03   8.003221E+03   2.179324E+04   2.109689E+04   2.84621
   7.000000E+00   6.668984E-01   4.289382E+05   3.777161E+05   4.749472E+06   1.195355E+04   1.310064E+04   3.591688E+04   3.487535E+04   4.71245
   7.500000E+00   6.903054E-01   7.452751E+05   6.326739E+05   8.135029E+06   1.930163E+04   2.109368E+04   5.793707E+04   5.646387E+04   7.66990
```

TALYS: YANDF structure for level density tables (continued

```
# quantity:
#   type: spin distribution
#   Excitation energy [MeV]:   1.500000E+00
#   datablock:
#     columns: 3
#     entries: 41
##      Spin         R (parity -)    R (parity +)
##       []               []              []
        0.0          1.484985E-02    4.158540E-02
        1.0          1.340520E-01    5.177226E-02
        2.0          1.078400E-01    1.502384E-01
        3.0          1.920713E-01    1.494492E-01
        4.0          1.325488E-01    1.606543E-01
        5.0          1.663892E-01    1.311657E-01
        6.0          8.049695E-02    1.189196E-01
        7.0          8.090085E-02    7.919571E-02
        8.0          4.160250E-02    7.000232E-02
        9.0          2.835019E-02    2.467863E-02
       10.0          1.195156E-02    1.545182E-02
       11.0          4.236779E-03    4.008278E-03
       12.0          1.744799E-03    2.218526E-03
       13.0          1.640285E-03    1.047288E-03
```

TALYS ‘best’ fits

- 337 nuclides with ‘best parameter’ files
  - ldmodel 7 (BSKG3): 239 nuclides
  - ldmodel 2 (BSFG): 33 nuclides
  - ldmodel 1 (Gilbert-Cameron): 65 nuclides
- Examples:

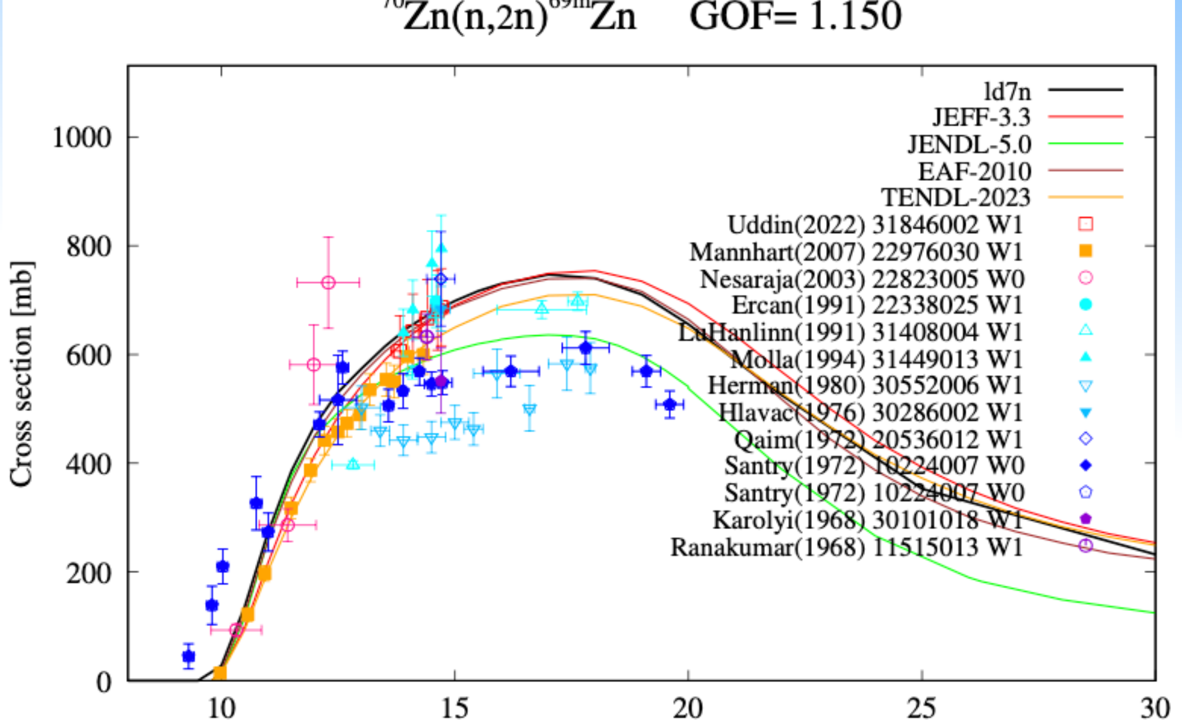
```
# n+ Se76 Adjusted parameters from fitting
ldmodel 7
rvadjust n 1. 0.01 3. 1.5 1.03
rvadjust     p     1.08864
gadjust       34  77     1.04523
gadjust       34  76     0.96539
gadjust       33  76     1.20759
wtable        34  77     1.05313 e1
```

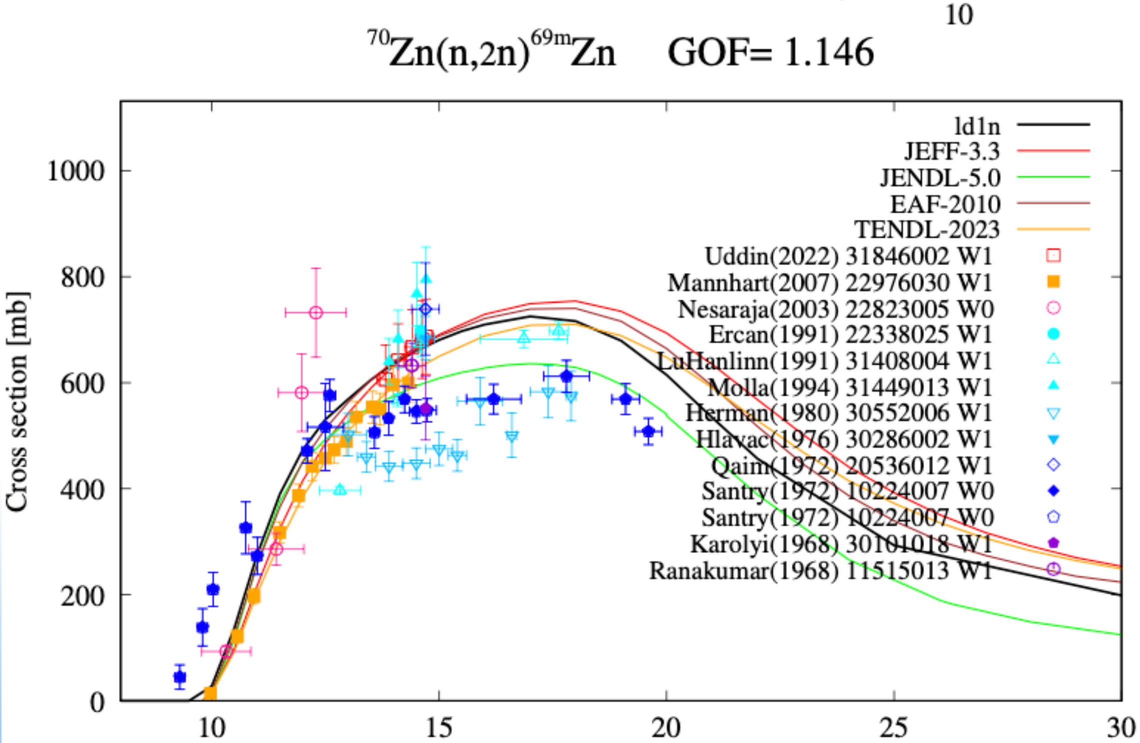
(n,γ), (n,n’), (n,p), (n,2n), (n,3n)

```
# n+Te126 Adjusted parameters from fitting
ldmodel 7
rvadjust     p     0.98233
gadjust       52 127     1.10863
gadjust       52 126     0.94201
gadjust       51 126     0.92631
s2adjust      51 126     1.18843 0
risomer       51 126     3.96631
s2adjust      52 125     1.08452 0
risomer       52 125     3.41970
wtable        52 127     1.04572 e1
s2adjust      52 127     0.50121 0
risomer       52 127     3.35422
rvadjust     a     1.04077
cstrip       a     1.34119
s2adjust      50 123     1.36835 0
risomer       50 123     1.15880
```

(n,γ), (n,n’), (n,p), (n,2n), (n,3n), (n,α) + isomers

Similar performance of ld1 (CTM) and ld7 (BSKG3)





To be done: numerical GOF comparison for all nuclides and reaction channels until minimal GOF satisfies the eye or vice versa

Summary

- CTM, BSFG and BSKG3 seem to be of similar quality:
  - D0 validation
  - $\Gamma\gamma$ validation
  - (n,γ) and MACS validation
  - All other open channels up to 20 MeV (more compensation from OMP, pre-equilibrium etc models of course)
- Validation to D1 still needs to be done
- Oslo method not yet included in this scheme.
- Currently, no level density parameter adjustment is used in cross section fitting, only the LD model is a parameter. This is too strict.
- All LD models give similar fits to discrete levels and D0, after parameter adjustment. It is the spin distribution which makes the big difference in Hauser-Feshbach calculations, leading to different shapes in the excitation functions (good for BSKG3!).
- More precise evaluations, i.e. declaring more EXFOR outliers, will give more meaningful results for the quality of level density models.

60 Years

IAEA

Atoms for Peace and Development

Thank you!

IAEA 60 Years

Atoms for Peace and Development

(Towards an evaluation of) compilation of D0, D1, Γγ and MACS evaluations and compilations

Arjan Koning, IAEA

Dimitri Rochman, PSI

Shin Okumura, IAEA

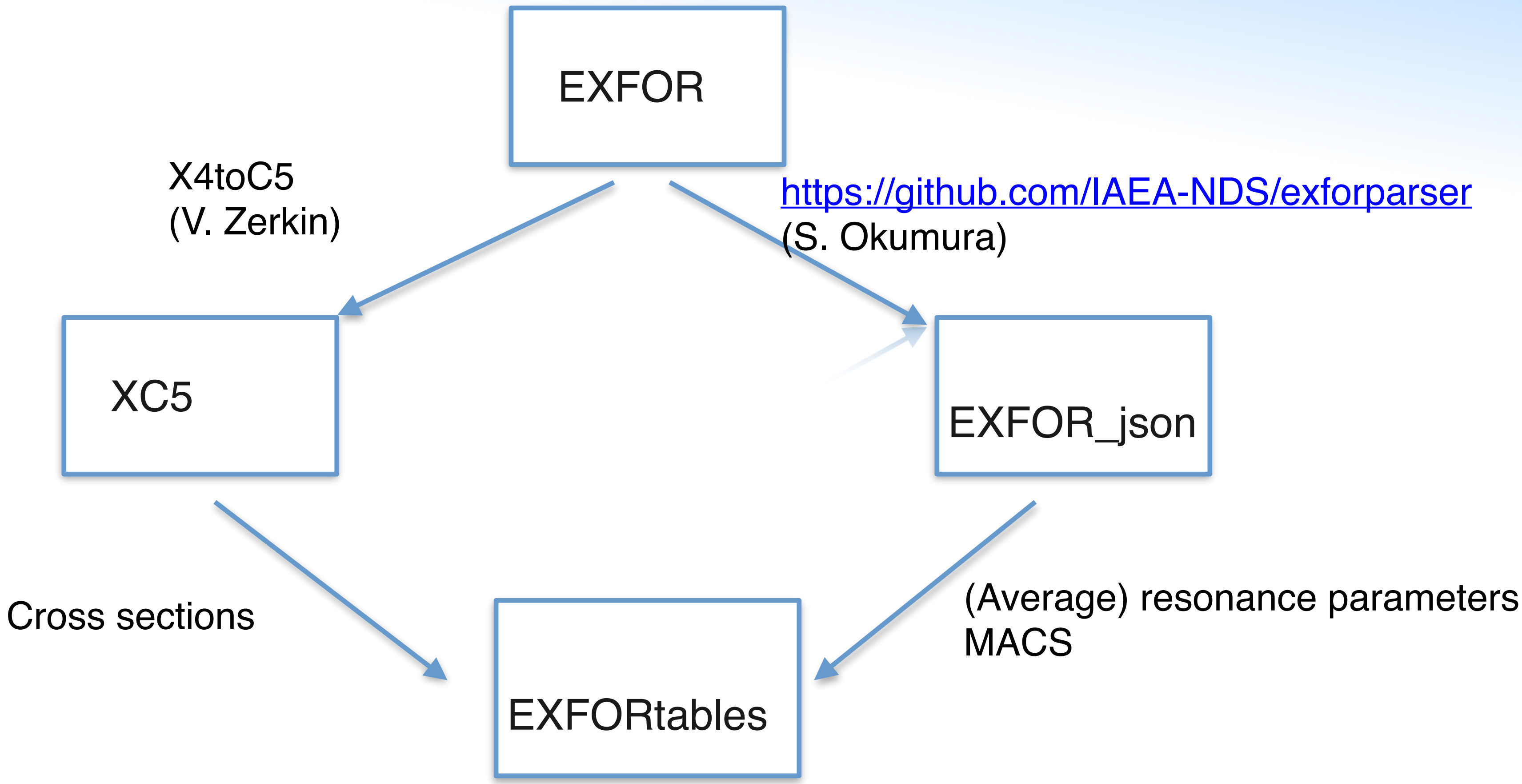
Objective

- To do the dirty ground work for experts who are qualified to produce **the** evaluated value:
  - Find and/or digitise all available evaluations/compilations
  - Try to mine all relevant data from EXFOR
  - Reproduce the value from the major nuclear data libraries for reference
- Produce unified formatted databases with clear metadata and data
- Do this for all
  - thermal cross sections:(n,tot), (n,el), (n,γ), (n,f), (n,p), (n,α),
  - resonance integrals: Ig and If,
  - strength functions: S0, S1, R,
  - **Average resonance parameters: D0, D1, Γγ,**
  - **Maxwellian averaged cross sections: MACS**

Example: D0

- Sources:
  - RIPL-2
  - RIPL-3
  - Atlas 2016 (Mughabghab)
  - EXFOR
  - TARES (Rochman):
    - D0, D1, $\Gamma\gamma$ estimated from individual resonances
    - All individual resonance parameters from major NDL's and Mughabghab and Sukhoruchkin Atlas
- Current rule for D0 (until someone knows better): RIPL-3 > RIPL-2 > Atlas > EXFOR

Computational access to EXFOR



All data in directory structured organisation

D0: one file per nuclide with all available information

YANDF format

```
# header:
#   title: Ta181 D0 resonance data
#   source: Resonancetables
#   date: 2025-03-23
# target:
#   Z: 73
#   A: 181
#   nuclide: Ta181
# reaction:
#   type: D0
# parameters:
#   selected value [eV]:  4.200000E+00
#   selected value uncertainty [eV]:  3.000000E-01
#   selected value source: RIPL-3
#   number of values: 14
#   average value [b]:  7.305685E+00
#   relative standard deviation [%]:     132.892517
# quantity:
#   type: Compilation
#   average value:  4.190000E+00
#   relative standard deviation [%]:       0.337518
# datablock:
#   columns: 8
#   entries: 3
##    Author                        Type          Year          Value        dValue       Reference       Ratio
##      []              []           []            []           [eV]          [eV]            []            []
      RIPL-2                Compilation           2000    4.200000E+00  3.000000E-01          97I      1.000000
      RIPL-3                Compilation           2009    4.200000E+00  3.000000E-01          97I      1.000000
      Mughabghab_2016       Compilation           2016    4.170000E+00  4.000000E-02                   0.992857
# quantity:
#   type: EXFOR
#   average value:  8.390000E+00
#   relative standard deviation [%]:     134.663437
# datablock:
#   columns: 8
#   entries: 10
##    Author                        Type          Year          Value        dValue       Reference       Ratio
##      []              []           []            []           [eV]          [eV]            []            []
      I.A.Radkevich         EXFOR                 1956    8.800000E+00  0.000000E+00    40382-049      2.095238
      J.S.Desjardins        EXFOR                 1960    4.350000E+00  0.000000E+00    11948-010      1.035714
      S.P.Kapchigashev      EXFOR                 1966    4.200000E+01  5.000000E+00    40778-084     10.000000
      T.Y.Byoun             EXFOR                 1973    4.300000E+00  0.000000E+00    10577-040      1.023810
      V.S.Shorin            EXFOR                 1975    2.900000E+00  0.000000E+00    41330-010      0.690476
      T.S.Belanova          EXFOR                 1975    4.210000E+00  9.800000E-01    40430-006      1.002381
      G.Hacken              EXFOR                 1978    4.170000E+00  4.000000E-02    10673-003      0.992857
      V.P.Vertebnyy         EXFOR                 1983    4.300000E+00  3.000000E-01    40881-002      1.023810
      I.Tsubone             EXFOR                 1983    4.770000E+00  0.000000E+00    21957-003      1.135714
      I.Tsubone             EXFOR                 1987    4.100000E+00  1.400000E-01    22109-004      0.976191
# quantity:
#   type: Nuclear data library
#   average value:  5.809590E+00
#   relative standard deviation [%]:       0.000000
# datablock:
#   columns: 8
#   entries: 1
##    Author                        Type          Year          Value        dValue       Reference       Ratio
##      []              []           []            []           [eV]          [eV]            []            []
      TARES                 NDL                   2025    5.809590E+00  0.000000E+00                   1.383236
```

D1: one file per nuclide with all available information

```
# header:
#   title: Mo098 D1 resonance data
#   source: Resonancetables
#   date: 2025-03-23
# target:
#   Z: 42
#   A: 98
#   nuclide: Mo098
# reaction:
#   type: D1
# parameters:
#   selected value [eV]:  2.900000E+02
#   selected value uncertainty [eV]:  3.000000E+01
#   selected value source: RIPL-3
#   number of values: 6
#   average value [b]:  3.094467E+02
#   relative standard deviation [%]:      11.928135
# quantity:
#   type: Compilation
#   average value:  2.886667E+02
#   relative standard deviation [%]:       0.653216
# datablock:
#   columns: 8
#   entries: 3
##    Author                         Type           Year           Value        dValue        Reference        Ratio
##      []              []            []             []            [eV]          [eV]           []              []
      RIPL-2                  Compilation           2000     2.900000E+02  6.000000E+01           96I      1.000000
      RIPL-3                  Compilation           2009     2.900000E+02  3.000000E+01           07I      1.000000
      Mughabghab_2016         Compilation           2016     2.860000E+02  1.400000E+01                    0.986207
# quantity:
#   type: EXFOR
#   average value:  3.400000E+02
#   relative standard deviation [%]:      14.705882
# datablock:
#   columns: 8
#   entries: 2
##    Author                         Type           Year           Value        dValue        Reference        Ratio
##      []              []            []             []            [eV]          [eV]           []              []
      K.E.Remley              EXFOR                 2018     3.900000E+02  2.000000E+01     14676-009      1.344828
      K.E.Remley              EXFOR                 2018     2.900000E+02  2.500000E+01     14676-009      1.000000
# quantity:
#   type: Nuclear data library
#   average value:  3.106800E+02
#   relative standard deviation [%]:       0.000000
# datablock:
#   columns: 8
#   entries: 1
##    Author                         Type           Year           Value        dValue        Reference        Ratio
##      []              []            []             []            [eV]          [eV]           []              []
      TARES                   NDL                   2025     3.106800E+02  0.000000E+00                    1.071310
```

Γγ: one file per nuclide with all available information

```
# header:
#   title: Nd143 gamgam resonance data
#   source: Resonancetables
#   date: 2025-03-23
# target:
#   Z: 60
#   A: 143
#   nuclide: Nd143
# reaction:
#   type: gamgam
# parameters:
#   selected value [eV]:  8.600000E-02
#   selected value uncertainty [eV]:  9.000001E-03
#   selected value source: RIPL-3
#   number of values: 8
#   average value [b]:  7.897911E-02
#   relative standard deviation [%]:      10.082768
# quantity:
#   type: Compilation
#   average value:  8.206666E-02
#   relative standard deviation [%]:       6.778119
# datablock:
#   columns: 8
#   entries: 3
##    Author                       Type           Year          Value        dValue        Reference         Ratio
##      []             []           []             []           [eV]          [eV]            []              []
      RIPL-2                  Compilation         2000     8.600000E-02  9.000001E-03          96I        1.000000
      RIPL-3                  Compilation         2009     8.600000E-02  9.000001E-03          06M        1.000000
      Mughabghab_2016         Compilation         2016     7.420000E-02  1.800000E-03                     0.862791
# quantity:
#   type: EXFOR
#   average value:  7.850000E-02
#   relative standard deviation [%]:      11.588156
# datablock:
#   columns: 8
#   entries: 4
##    Author                       Type           Year          Value        dValue        Reference         Ratio
##      []             []           []             []           [eV]          [eV]            []              []
      Karzhavina              EXFOR               1969     7.600000E-02  1.100000E-02     40113015        0.883721
      Alves                   EXFOR               1969     7.200000E-02  1.000000E-02     20688021        0.837209
      Tellier                 EXFOR               1971     9.400000E-02  5.000000E-02     20121008        1.093023
      Barry                   EXFOR               2006     7.200000E-02  1.000000E-03     14093002        0.837209
# quantity:
#   type: Nuclear data library
#   average value:  7.163290E-02
#   relative standard deviation [%]:       0.000000
# datablock:
#   columns: 8
#   entries: 1
##    Author                       Type           Year          Value        dValue        Reference         Ratio
##      []             []           []             []           [eV]          [eV]            []              []
      TARES                   NDL                 2025     7.163290E-02  0.000000E+00                     0.832941
```

MACS: one file per nuclide with all available information

```
# header:
#   title: Ge074(n,g) MACS
#   source: Resonancetables
#   date: 2025-03-23
# target:
#   Z: 32
#   A: 74
#   nuclide: Ge074
# reaction:
#   type: (n,g)
# observables:
#   selected value [b]:  3.586053E-02
#   selected value uncertainty [b]:  1.518720E-03
#   selected value source: Astral
#   number of values: 12
#   average value [b]:  3.965035E-02
#   relative standard deviation [%]:      31.133821
# quantity:
#   type: Compilation spectrum-averaged
#   average value:  3.901513E-02
#   relative standard deviation [%]:       9.041577
# datablock:
#   columns: 9
#   entries: 4
##    Author                      Type          Year          Value          dValue        Reference        Ratio         Spectrum
##      []              []          []            []            [b]            [b]            []             []             []
      Kadonis                Compilation        2000      3.760000E-02   3.900000E-03                  1.048506   MXW
      Sukhoruchkin           Compilation        2015      4.500000E-02   5.000000E-03                  1.254862   MXW
      Mughabghab_2016        Compilation        2016      3.760000E-02   3.900000E-03                  1.048506   MXW
      Astral                 Compilation        2020      3.586053E-02   1.518720E-03                  1.000000   MXW
# quantity:
#   type: EXFOR
#   average value:  3.650000E-02
#   relative standard deviation [%]:      47.945206
# datablock:
#   columns: 9
#   entries: 2
##    Author                      Type          Year          Value          dValue        Reference        Ratio         Spectrum
##      []              []          []            []            [b]            [b]            []             []             []
      Macklin                EXFOR              1957      5.400000E-02   8.000000E-03   11399014       1.505834
      Anand                  EXFOR              1979      1.900000E-02   6.000000E-03   30390005       0.529830
# quantity:
#   type: EXFOR spectrum-averaged
#   average value:  4.940835E-02
#   relative standard deviation [%]:      19.413013
# datablock:
#   columns: 9
#   entries: 2
##    Author                      Type          Year          Value          dValue        Reference        Ratio         Spectrum
##      []              []          []            []            [b]            [b]            []             []             []
      Walter                 EXFOR              1984      5.900000E-02   7.000000E-03   220370262      1.645263   MXW
      Marganiec              EXFOR              2009      3.981670E-02   4.101700E-03   14237002       1.110321   MXW
# quantity:
#   type: Nuclear data library
#   average value:  3.698175E-02
#   relative standard deviation [%]:      36.829266
# datablock:
#   columns: 9
#   entries: 4
##    Author                      Type          Year          Value          dValue        Reference        Ratio         Spectrum
##      []              []          []            []            [b]            [b]            []             []             []
      cendl3.2               NDL                2019      1.347600E-02   0.000000E+00                  0.375789      MXW
      jendl5.0               NDL                2021      4.576000E-02   0.000000E+00                  1.276055      MXW
      tendl.2023             NDL                2023      4.293100E-02   0.000000E+00                  1.197166      MXW
      endfb8.1               NDL                2024      4.576000E-02   0.000000E+00                  1.276055      MXW
```

Accumulated results:D0


```
# header:
#   title: D0 resonance data
#   source: Resonancetables
#   date: 2025-03-23
# reaction:
#   type: D0
# quantity:
#   type: resonance data
# datablock:
#   columns: 8
#   entries: 346
```


## Z	A	Liso	Value	dValue	Reference	#Experiments	Nuclide
## []	[]	[]	[eV]	[eV]	[]	[]	[]
9	19	0	1.600000E+05	4.000000E+04	RIPL-2	1	F019
11	23	0	1.000000E+05	2.000000E+04	RIPL-3	1	Na023
12	0	0	1.000000E+05	0.000000E+00	J.B.Garg	1	Mg000
12	24	0	4.800000E+05	7.000000E+04	RIPL-3	0	Mg024
12	25	0	5.000000E+04	1.000000E+04	RIPL-3	0	Mg025
12	26	0	2.100000E+05	8.000000E+04	RIPL-3	0	Mg026
13	27	0	5.500000E+04	6.000000E+03	RIPL-3	1	Al027
14	0	0	1.800000E+03	0.000000E+00	K.Tsukada	2	Si000
14	28	0	3.320000E+05	3.500000E+04	RIPL-3	2	Si028
14	29	0	1.930000E+05	2.200000E+04	RIPL-3	0	Si029
14	30	0	2.250000E+05	3.000000E+04	RIPL-3	0	Si030
15	31	0	5.000000E+04	1.200000E+04	RIPL-3	1	P031
16	0	0	5.000000E+04	0.000000E+00	J.B.Garg	3	S000
16	32	0	1.900000E+05	6.000000E+04	RIPL-3	6	S032
16	33	0	2.100000E+04	1.000000E+04	RIPL-3	2	S033
16	34	0	1.100000E+05	4.000000E+04	RIPL-3	1	S034
17	0	0	3.500000E+03	0.000000E+00	J.B.Garg	3	Cl000
17	35	0	2.300000E+04	6.000000E+03	RIPL-3	0	Cl035
17	37	0	1.500000E+04	4.000000E+03	RIPL-3	0	Cl037
18	40	0	5.200000E+04	4.700000E+03	RIPL-3	2	Ar040
19	0	0	2.500000E+03	0.000000E+00	J.B.Garg	1	K000
19	39	0	1.300000E+04	3.000000E+03	RIPL-3	0	K039
19	40	0	8.400000E+02	9.000000E+01	Mughabghab_2016	1	K040

Accumulated results: MACS

```
# header:
#   title: (n,g) MACS
#   source: Resonancetables
#   date: 2025-03-23
# reaction:
#   type: (n,g)
# quantity:
#   type: MACS
# datablock:
#   columns: 9
#   entries: 306
```

## Z	A	Liso	Value	dValue	Reference	#Experiments	Nuclide	Spectrum
## []	[]	[]	[b]	[b]	[]	[]	[]	[]
1	1	0	2.540000E-04	2.000000E-05	Kadonis	0	H001	MXW
1	2	0	3.000000E-06	2.000000E-07	Kadonis	0	H002	MXW
2	3	0	7.600001E-06	6.000001E-07	Kadonis	2	He003	MXW
3	7	0	4.200000E-05	3.000000E-06	Kadonis	2	Li007	MXW
4	9	0	9.079392E-06	4.273056E-07	Astral	2	Be009	MXW
6	12	0	1.540000E-05	1.000000E-06	Kadonis	1	C012	MXW
6	13	0	2.812424E-05	6.453618E-06	Astral	3	C013	MXW
6	14	0	8.480000E-06	5.700000E-07	Kadonis	0	C014	MXW
7	14	0	4.100000E-05	6.000000E-05	Kadonis	0	N014	MXW
7	15	0	5.800000E-06	6.000001E-07	Kadonis	0	N015	MXW
8	16	0	3.800000E-05	4.000000E-06	Kadonis	2	O016	MXW
8	18	0	8.900000E-06	8.000000E-07	Kadonis	1	O018	MXW
9	19	0	3.200000E-03	1.000000E-04	Kadonis	8	F019	MXW
10	20	0	1.190000E-04	1.100000E-05	Kadonis	0	Ne020	MXW
10	21	0	1.500000E-03	9.000000E-04	Kadonis	0	Ne021	MXW
10	22	0	5.800000E-05	4.000000E-06	Kadonis	6	Ne022	MXW
11	23	0	1.518547E-03	1.399371E-05	Astral	6	Na023	MXW
12	24	0	3.300000E-03	4.000000E-04	Kadonis	0	Mg024	MXW
12	25	0	6.400000E-03	4.000000E-04	Kadonis	0	Mg025	MXW
12	26	0	1.260000E-04	9.000000E-06	Kadonis	1	Mg026	MXW
13	27	0	3.740000E-03	3.000000E-04	Kadonis	6	Al027	MXW
14	0	0	1.300000E-02	4.000000E-03	Gibbons	1	Si000	
14	28	0	1.420000E-03	1.300000E-04	Kadonis	0	Si028	MXW
14	29	0	6.580000E-03	6.600001E-04	Kadonis	0	Si029	MXW
14	30	0	1.820000E-03	3.300000E-04	Kadonis	2	Si030	MXW
15	31	0	1.740000E-03	9.000001E-05	Kadonis	0	P031	MXW
16	0	0	2.500000E-02	8.000000E-03	Gibbons	1	S000	

Summary

IAEA 60 Years Atoms for Peace and Development

- Effort to compile all evaluations and compilations into the same structure. IAEA-NDS has:
  - All known compilations (we think/hope)
  - The capability to mine data from EXFOR
  - The capacity to extract data from nuclear data libraries (for reference)
  - All individual resonance parameters from NDL's and Atlases.
- Provide the most complete starting point for evaluation.
- For recommended values we rely on experts.

IAEA

60 Years

Atoms for Peace and Development

Thank you!