IAEA 60 Years
Atoms for Peace and Development

Feedback on JEFF-4T5 with emphasis on the TENDL files

Arjan Koning, IAEA, Vienna
Dimitri Rochman, PSI, Villigen

Contents

- TENDL approach
- Thermal and resonance range for JEFF4-T5
- Fast neutron capture cross sections
- Other cross sections
- Summary

Building blocks of TENDL

- Complete automated Resonance Parameter system including covariance data:
    - TARES-1.6 (DR)
    - Latest recommendations from last 2 JEFF meetings included
    - Tested for format and basic physics errors and declared correct (AK)
- EXFOR database
    - Entire database renomalized to the latest standards and monitors
    - Based on Viktor Zerkin's XC5 database and Shin Okumura's Data Explorer
    - 11 500 experimental cross section sets validated, 2050 data sets declared outlier (needed for automatic optimisation)
- Latest version of TALYS, version 2.1 (right now GitHub only)
    - Contains new 'best' model parameter database from automated fitting with TASMAN
        - Czendes global optimization based on Boender-Rinnooy Kan-Timmer-Stougie stochastic method
        - Dimension reduction, only optimize the most sensitive model parameters ("Occam's razor")
- One superscript: autotalys -element Sn -mass 117 -Ltarget 000 -Liso 000 -proj n -bins 60 -high -endf -njoy -residual -isomer -levels -recoil -covar -binsrand 60 -plot -subfission -nomcnp -tasmanfile /Users/koning/tasman/misc/tasman.tendl2023 -tarwork -nofit -best -ntalys 20 -sdefault -s20 -s60 -acf -eaf -mt

TENDL in JEFF4-T5

- 111 nuclides, of 35 materials, not from TENDL: H, He, Li, Be, B, C, N, O, F, Al, Si, Cl, Cr, Mn, Fe, Cu, Rh, Sn, Gd, Hf, Ta, W, Au, Pb, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm
- For the right reasons:
  - No reproducible system yet for light nuclides
  - Model failure for structural nuclides (Cr, Fe, Cu etc.) up to a few MeV, need Gaussian Processes for model defects
  - Systematic approach can not yet outperform the manual evaluation of nuclides with strong sensitivity to crit-safety tests
  - Consistent approach for actinides not yet ready
- For the wrong reasons:
  - Sn, and maybe Gd could come from latest TENDL (meanwhile Sn included)

JEFF4-T5 versus TENDL-2023.2 (in JEFF4-T4)

- TENDL-2025: Reproduction of exp. with horizontal nuclear data evaluation:
  - Towards global agreement for exp./evaluated 'one-point values' : thermal c.s. , RI, MACS etc.
  - Fully automated parameter optimisation below 20 MeV for cross sections
  - In the range from F - Bi: ~ 80 individual reaction channels (of which 16 (n,γ)) still unsatisfactory due to model defects. The rest is competitive with or better than the other NDL's.
  - Globally matching (n,γ) Profil data (though Gilles Noguere found interpolation problems)
- TENDL-2023: Missing several 10s of isomers (JCS, FISPACT), for isomers above 10th discrete level, solved
- TENDL-2023: For several nuclides MF9/MT102 branching ratio for neutron capture to isomer, extrapolation error at low energies: 1.e-22 below 10 eV (discovered by ANL and ORNL), mostly solved
- TENDL-2023: (Tim Ware) unrealistic high photon yields at lowest energies for many nuclides in MT107, solved
- TENDL-2023: (n,α) generally too high above 14 MeV due to bug in implementation of knock-out mechanism, solved

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

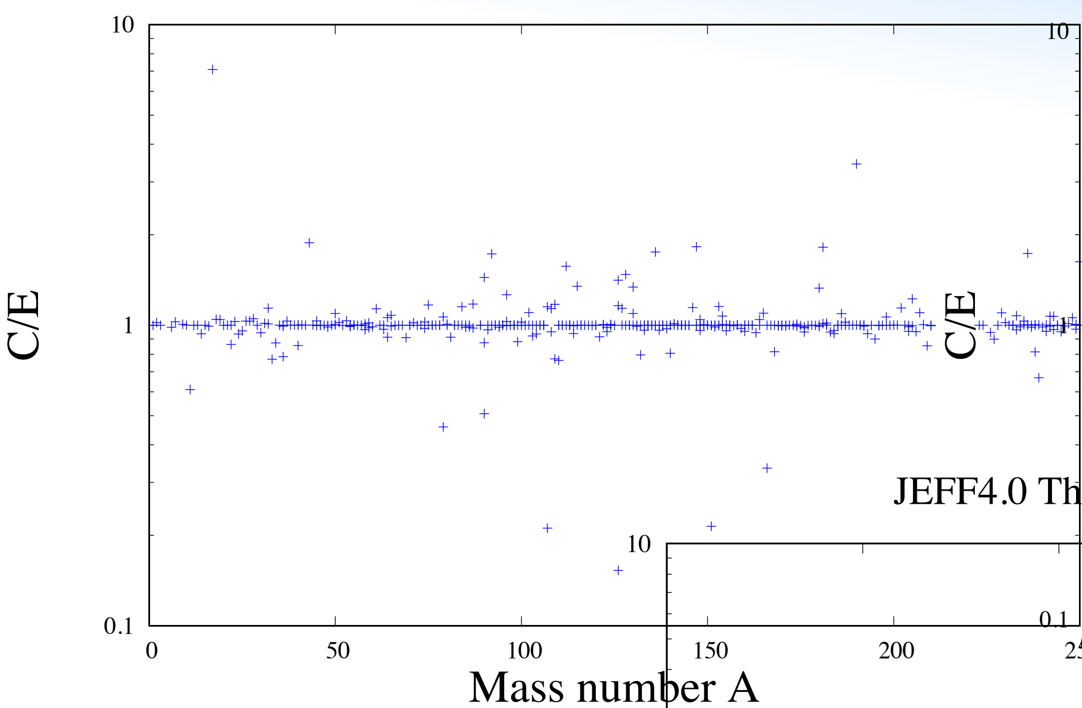
we use

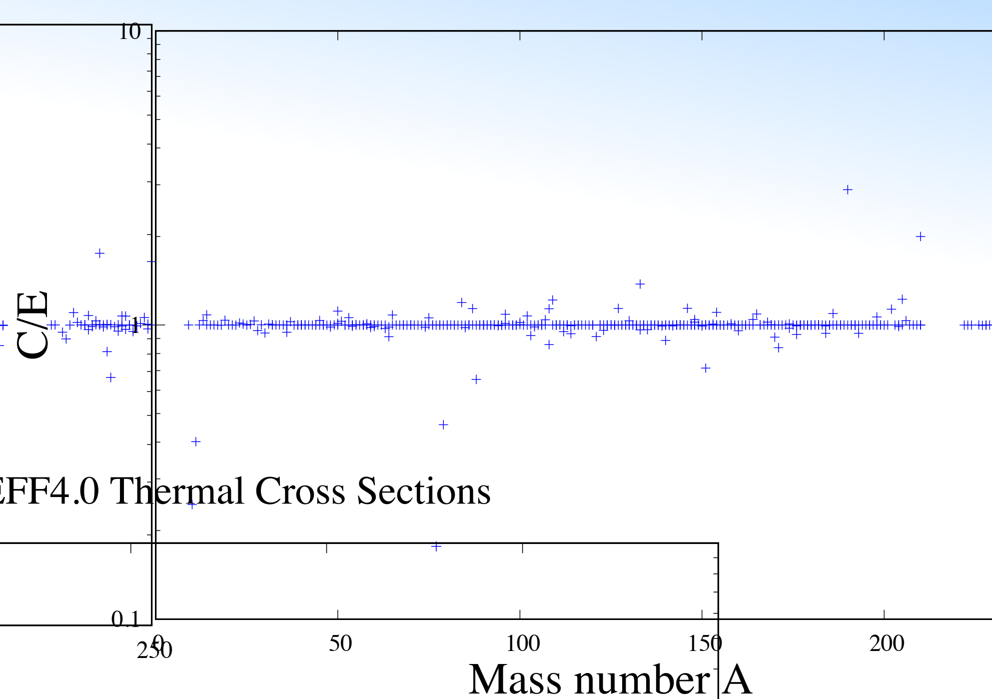
$$\begin{aligned} r_i &= 1-(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1){\rm erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} < \sigma^i_{\rm exp}, \\ &= 1+(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1){\rm erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} > \sigma^i_{\rm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

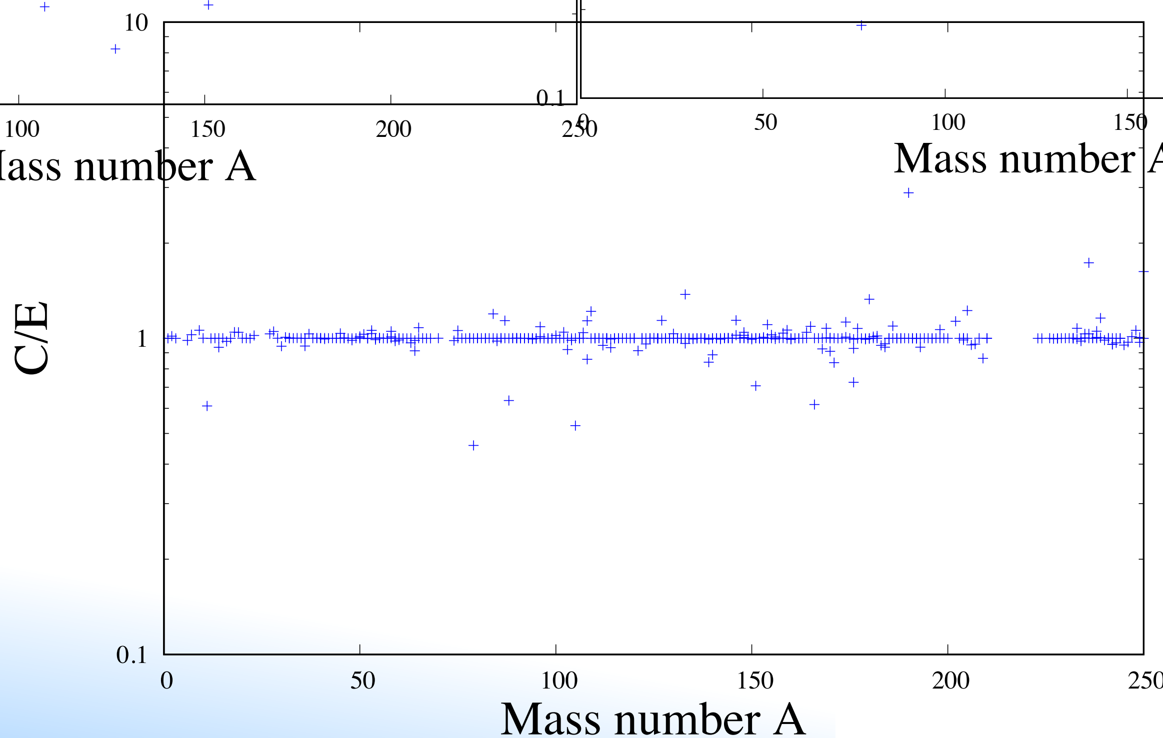
C/E value including uncertainties

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

NDL's versus Atlas-2016 thermal capture cross sections

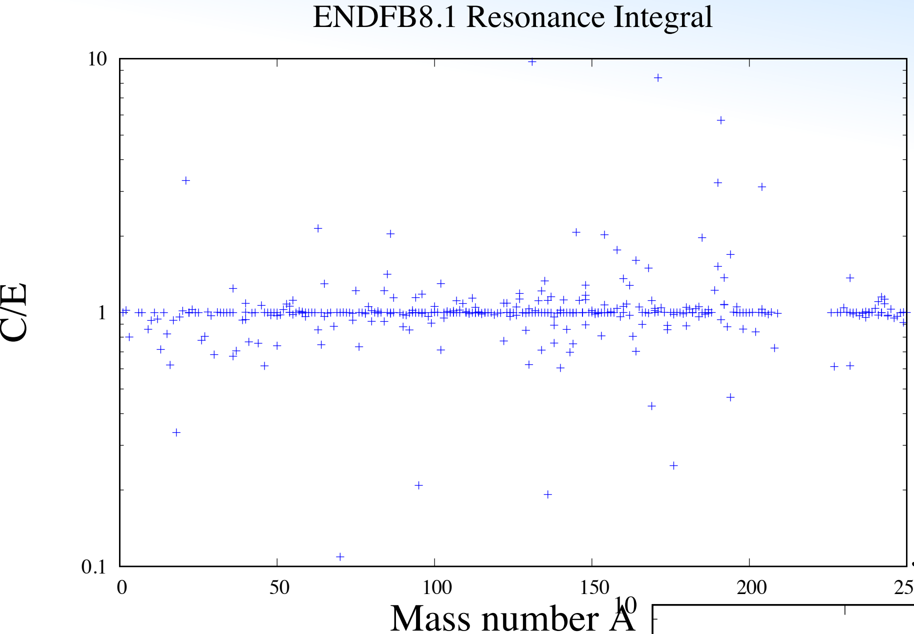


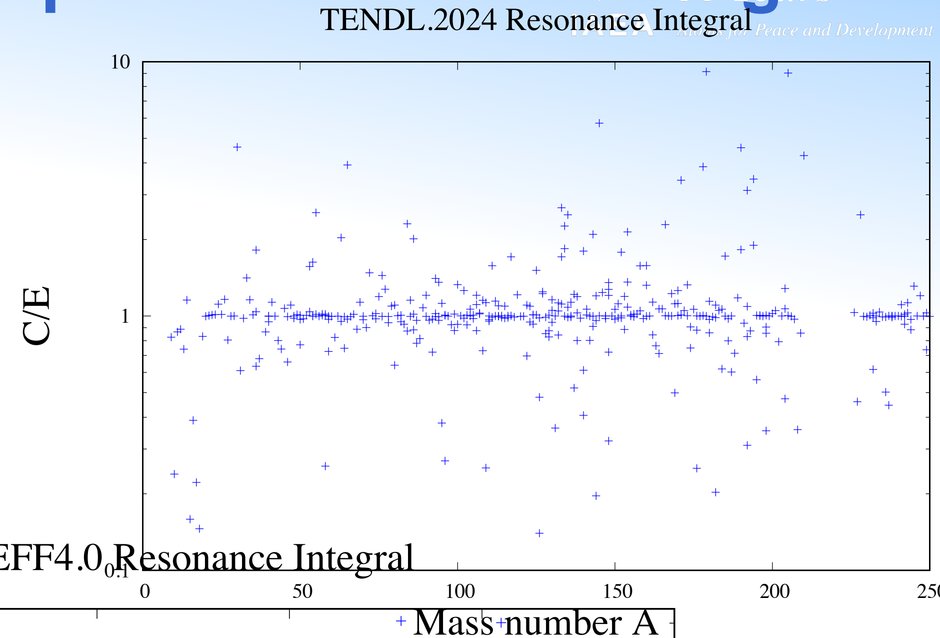


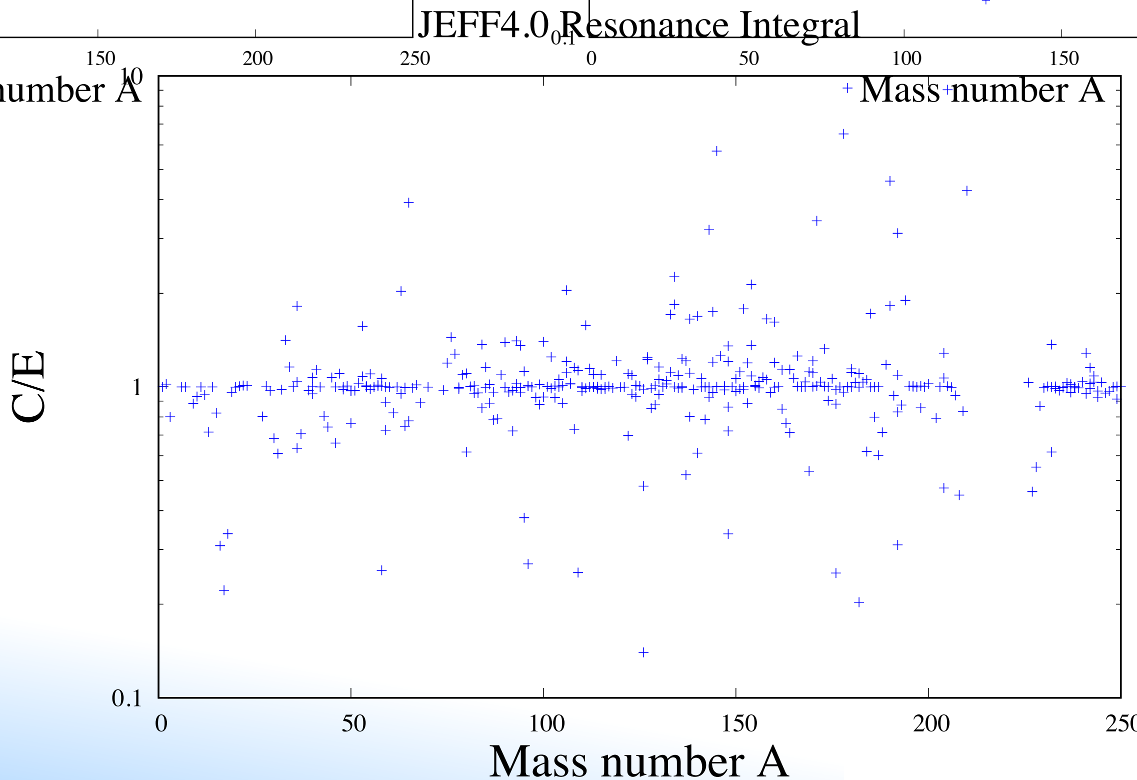


	Frms
CENDL-3.2:	1.034
JENDL-5.0:	1.020
ENDF/B8.1:	1.021
TENDL-2025:	1.011
JEFF-3.3:	1.024
JEFF-4.0:	1.015

NDL's versus Atlas-2016 capture resonance integrals

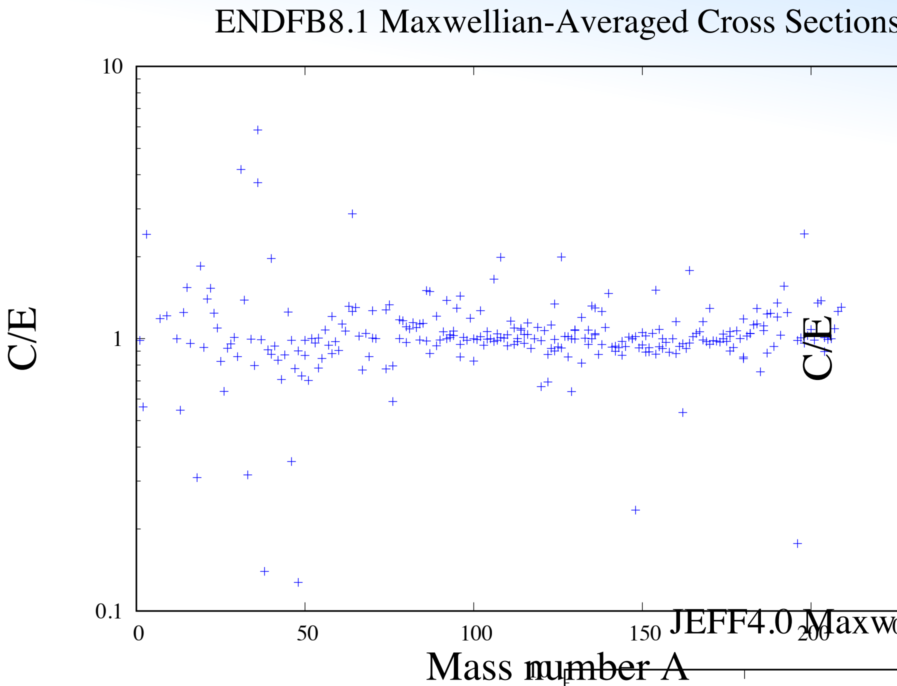


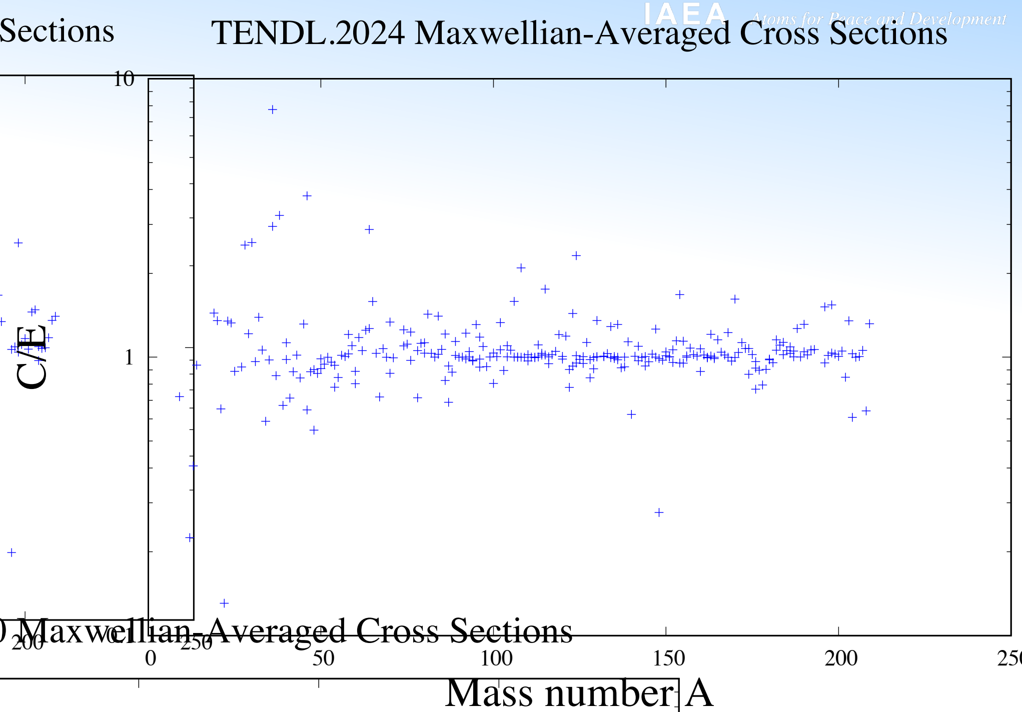


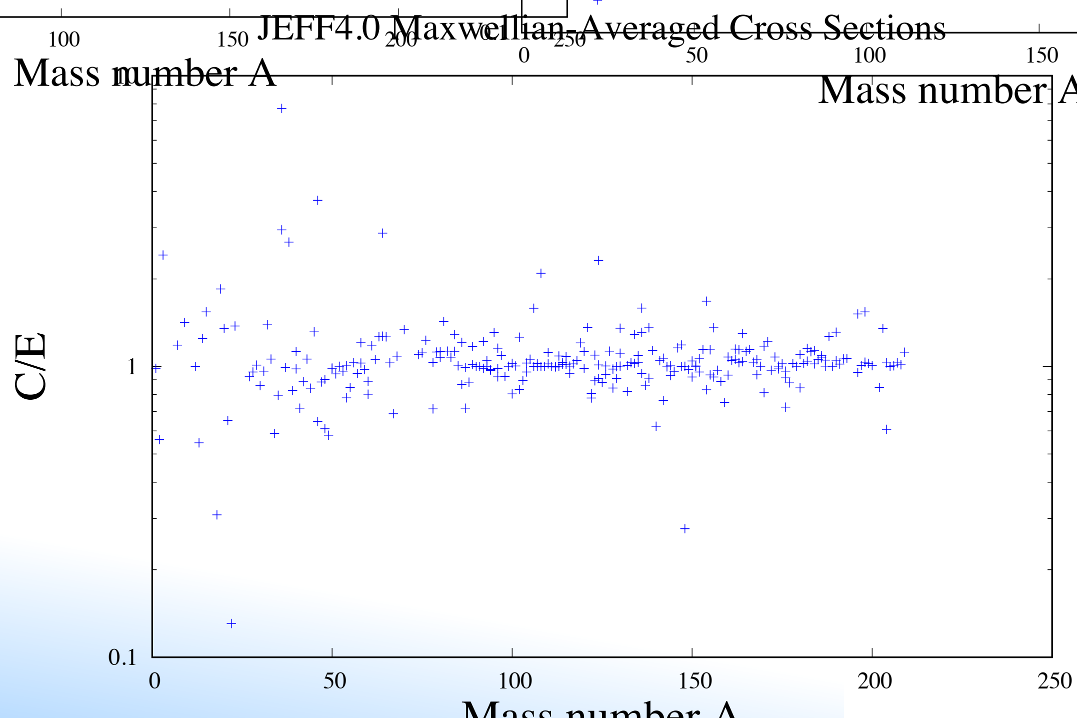


	Frms
CENDL-3.2:	1.034
JENDL-5.0:	1.038
ENDF/B8.1:	1.030
TENDL-2025:	1.045
JEFF-3.3:	1.038
JEFF-4.0:	1.043

NDL's versus Astral/Kadonis MACS at 30 keV







	Frms
CENDL-3.2:	1.069
JENDL-5.0:	1.064
ENDF/B8.1:	1.064
TENDL-2025:	1.052
JEFF-3.3:	1.076
JEFF-4.0:	1.062

Required: Evaluated databases - “evaluation of compilations and evaluations”

- Thermal energy
  - (n,tot)
  - (n,el)
  - (n,γ)
  - (n,f)
  - (n,p)
  - (n,α)
  - nubar: total, prompt and delayed
- Average resonance parameters
  - D0, D1, S0, S1, Γγ
- Maxwellian-Averaged Cross Sections
  - (n,γ) at 30 keV
- Sources: RIPL-3, Atlas-2006,2016 (Mughabgahab), Atlas-Sukhoruchkin, EXFOR
  - A lot of this is in TARES (DR)

Thermal capture cross sections, one file per nuclide

YANDF format

```
# header:
#   title: Pm147(n,g) thermal cross section
#   source: Resonancetables
#   date: 2025-04-11
# target:
#   Z: 61
#   A: 147
#   nuclide: Pm147
# reaction:
#   type: (n,g)
# observables:
#   selected value [b]:  1.684000E+02
#   selected value uncertainty [b]:  3.500000E+00
#   selected value source: Mughabghab_2016
#   number of values: 11
#   average value [b]:  1.622885E+02
#   relative standard deviation [%]:      20.750515
# quantity:
#   type: Compilation
#   average value:  1.722667E+02
#   relative standard deviation [%]:       3.174320
# datablock:
#   columns: 10
#   entries: 3
##    Author              Type          Year          Value        dValue     Reference       Ratio       Spectrum       Energy
##     []         []       []           []            [b]           [b]          []            []           []          [MeV]
      RIPL-3            Compilation     2004     1.800000E+02  2.000000E+01              1.068884                  2.530000E-08
      Mughabghab_2006   Compilation     2006     1.684000E+02  3.500000E+00              1.000000                  2.530000E-08
      Mughabghab_2016   Compilation     2016     1.684000E+02  3.500000E+00              1.000000                  2.530000E-08
```

Rochman

```
# quantity:
#   type: Compilation spectrum-averaged
#   average value:  1.680000E+02
#   relative standard deviation [%]:       0.000000
# datablock:
#   columns: 10
#   entries: 1
##    Author              Type          Year          Value        dValue     Reference       Ratio       Spectrum       Energy
##     []         []       []           []            [b]           [b]          []            []           []          [MeV]
      Sukhoruchkin      Compilation     2015     1.680000E+02  3.000000E+00              0.997625   MXW            2.530000E-08
```

Okumura

```
# quantity:
#   type: EXFOR spectrum-averaged
#   average value:  1.300000E+02
#   relative standard deviation [%]:      53.846153
# datablock:
#   columns: 10
#   entries: 2
##    Author              Type          Year          Value        dValue     Reference       Ratio       Spectrum       Energy
##     []         []       []           []            [b]           [b]          []            []           []          [MeV]
      G.W.Parker        EXFOR           1947     6.000000E+01  0.000000E+00  12149-002-0  0.356295   MXW            2.530000E-08
      D.Bidinosti       EXFOR           1959     2.000000E+02  5.000000E+01  12010-004-0  1.187649   SPA            2.530000E-08
```

Koning

```
# quantity:
#   type: Nuclear data library
#   average value:  1.680746E+02
#   relative standard deviation [%]:       0.275154
# datablock:
#   columns: 10
#   entries: 5
##    Author              Type          Year          Value        dValue     Reference       Ratio       Spectrum       Energy
##     []         []       []           []            [b]           [b]          []            []           []          [MeV]
      cendl3.2          NDL             2019     1.676970E+02  0.000000E+00              0.995825                  2.530000E-08
      jendl5.0          NDL             2021     1.676970E+02  0.000000E+00              0.995825                  2.530000E-08
      tendl.2023        NDL             2023     1.686410E+02  0.000000E+00              1.001431                  2.530000E-08
      endfb8.1          NDL             2024     1.676970E+02  0.000000E+00              0.995825                  2.530000E-08
      jeff4.0           NDL             2025     1.686410E+02  0.000000E+00              1.001431                  2.530000E-08
```

Γ_γ: 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
```

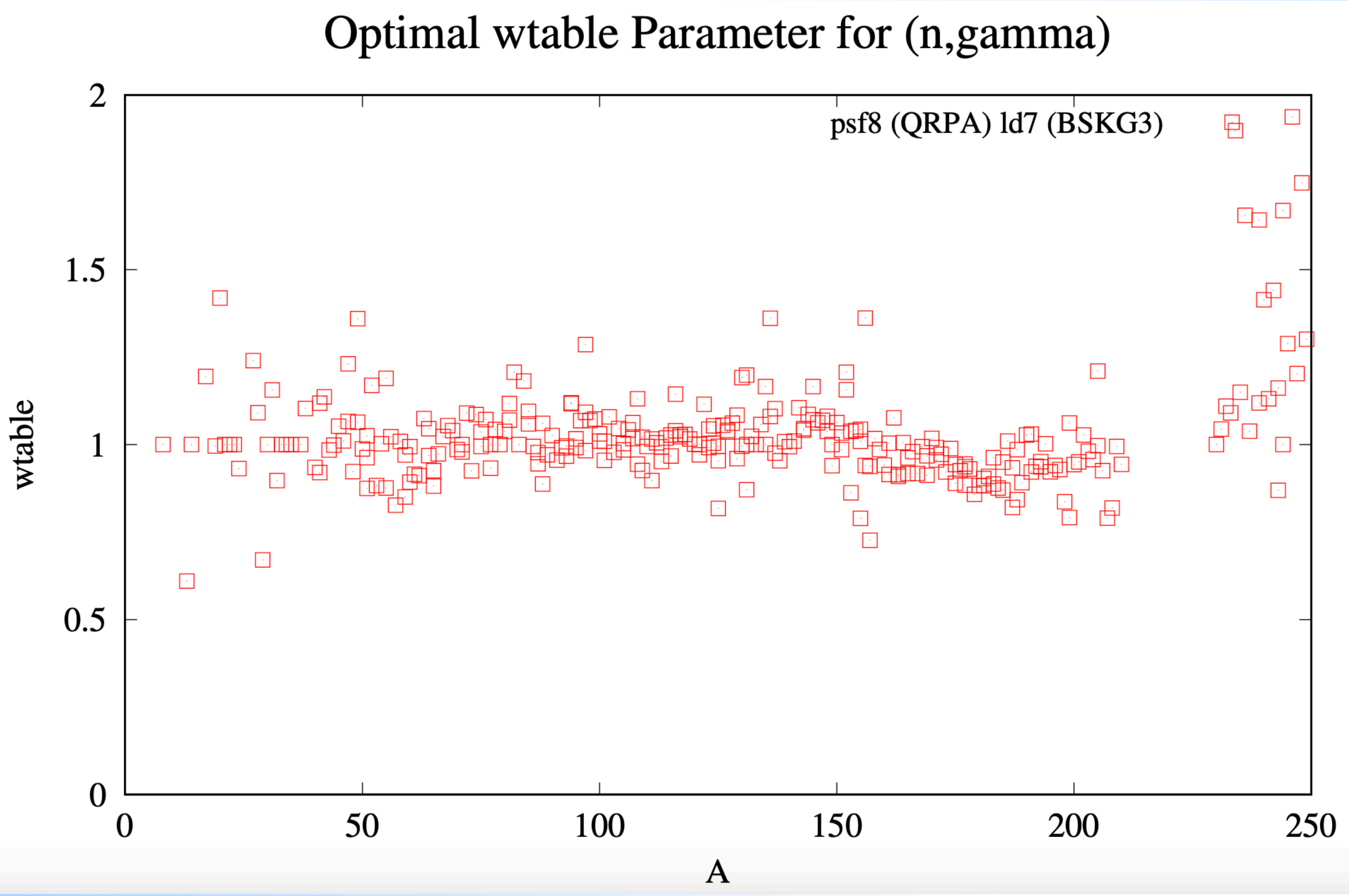
Parameter optimisation in fast range

- Use TASMAN for parameter optimisation
    - Multi-dimensional parameter landscape not too wild
    - 20 TALYS runs per parameter
- (n,γ):
    - Photon strength function: wtable(0,0) of compound nucleus
- (n,n'), (n,2n), (n,p) and (n,np):
    - Optical model: rvadjust p
    - Pre-equilibrium: gadjust(0,0), gadjust(1,0), gadjust(0,1)
- (n,α):
    - Optical model: rvadjust a
    - Pre-equilibrium: cstrip a
- Isomer versus ground state:
    - Discrete levels: Risomer of the final nuclide
    - Level density s2adjust (level density spin distribution) of final nuclide

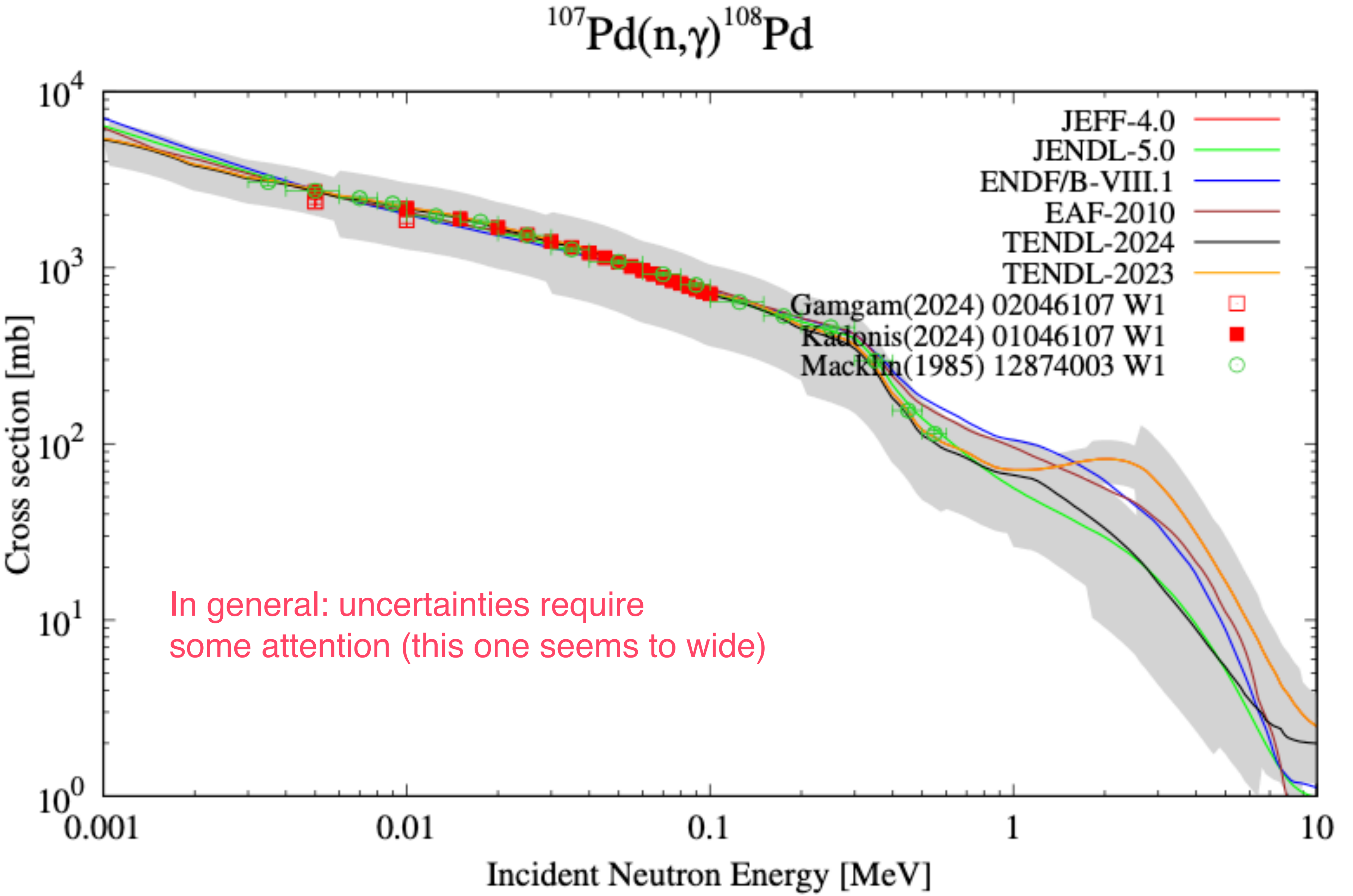
Unify all (n,γ) data

- EXFOR for cross sections, excluding outliers
- Pseudo-data created from perfect TALYS fit to average radiative width Γ_γ (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

Current optimal combination of level density and photon strength function

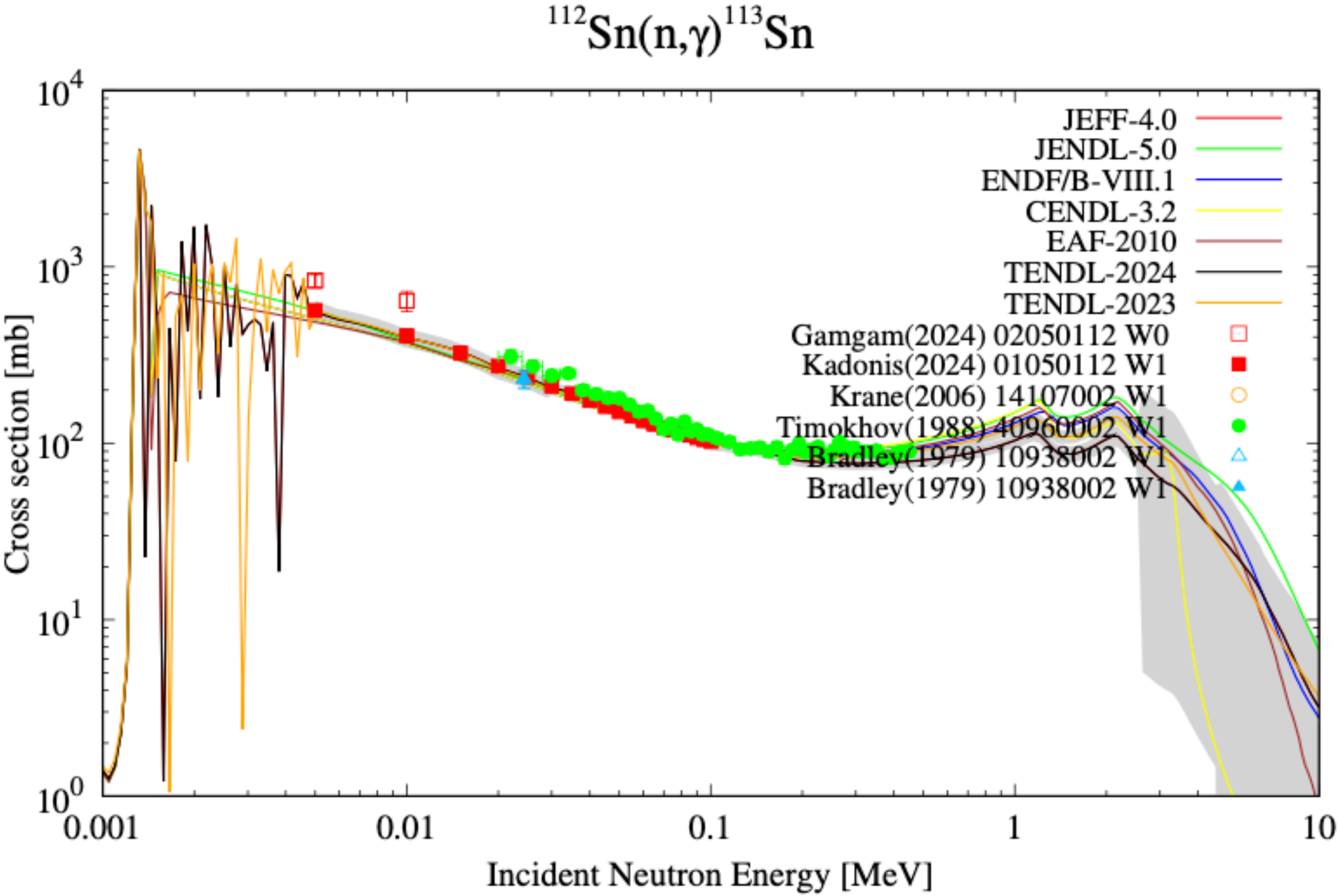


Typical case

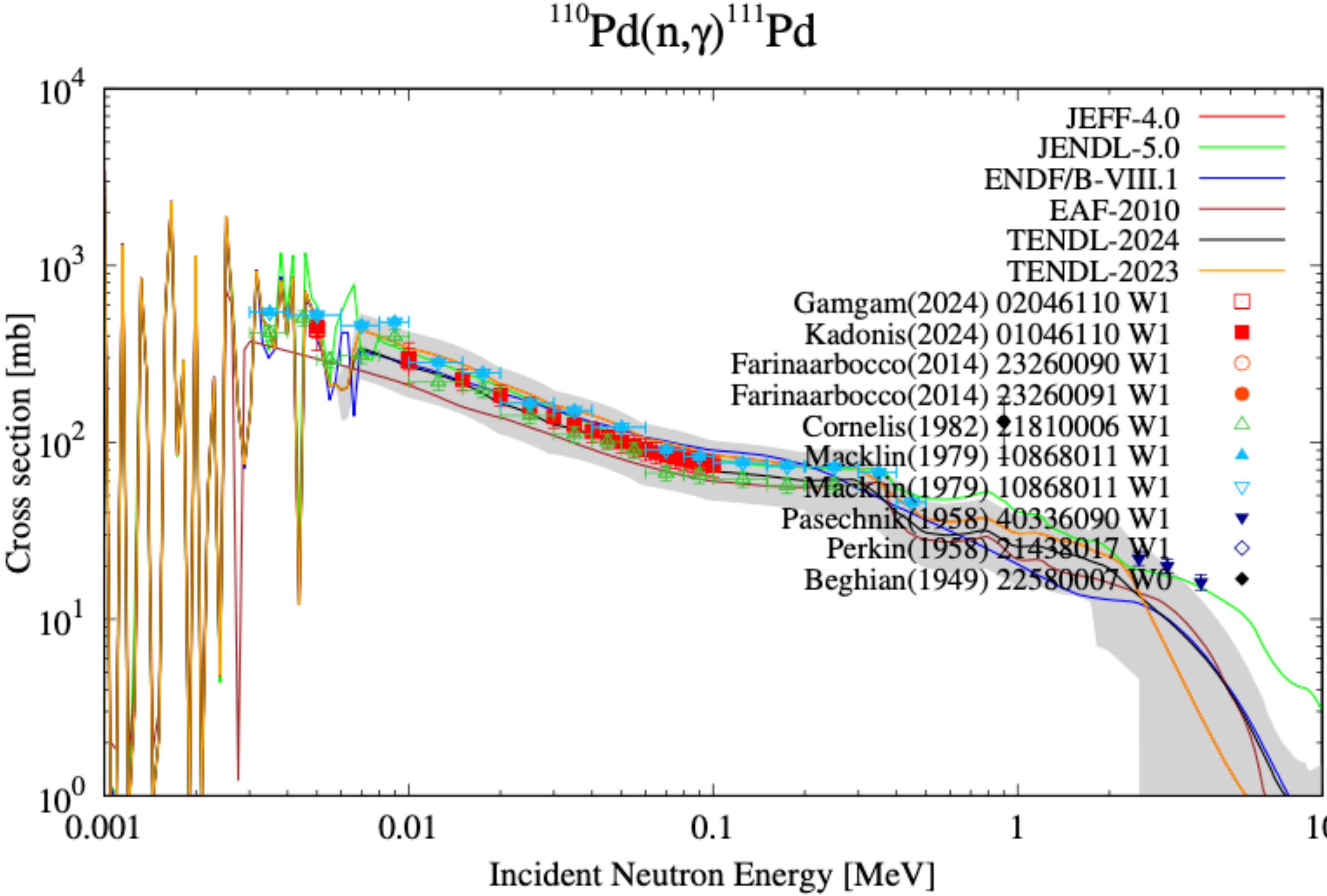


In general: uncertainties require some attention (this one seems to wide)

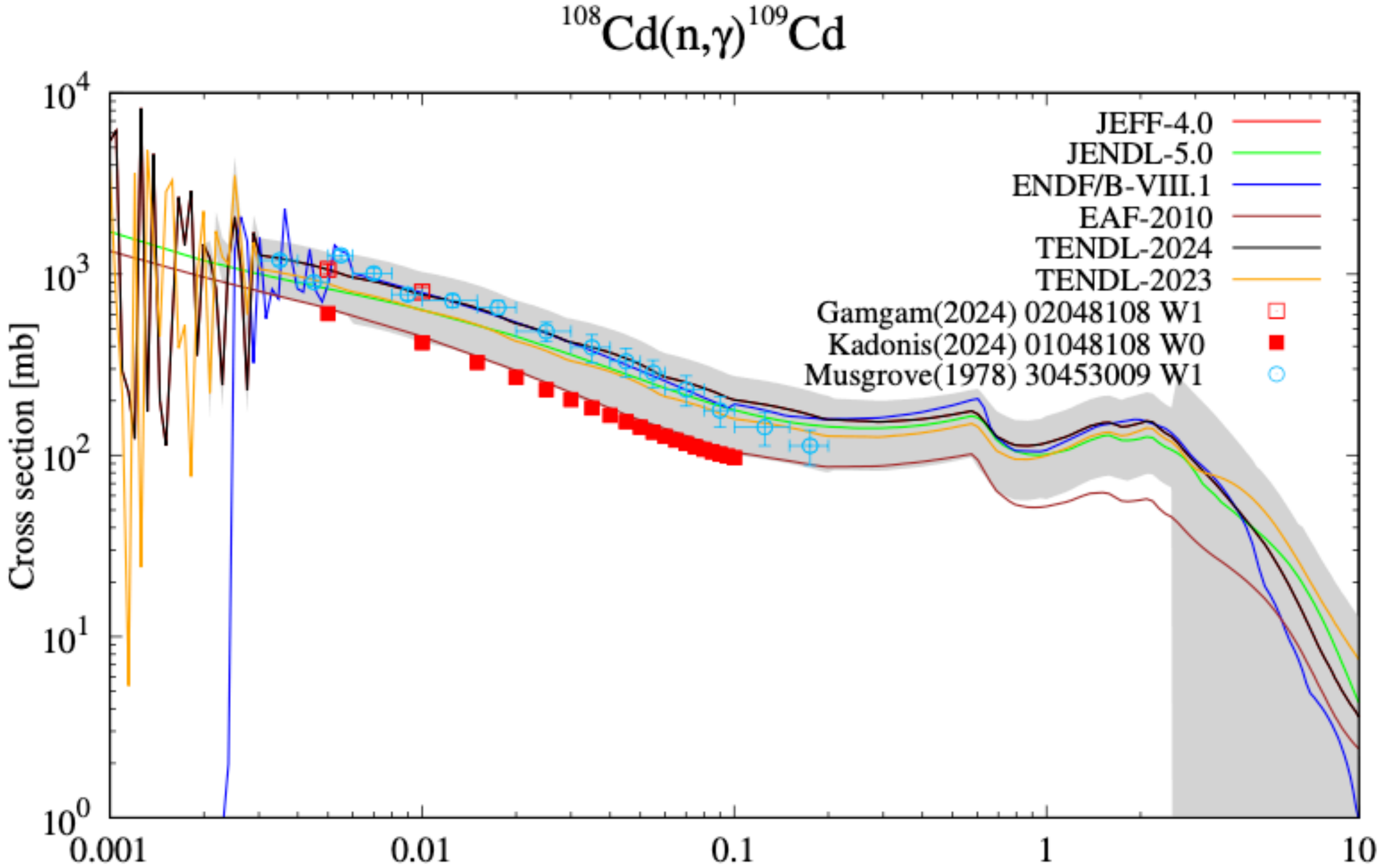
Average radiative width Γγ considered outlier



Usually: (n,γ) cross sections, MACS and Γγ are consistent



MACS (Kadonis) considered outlier



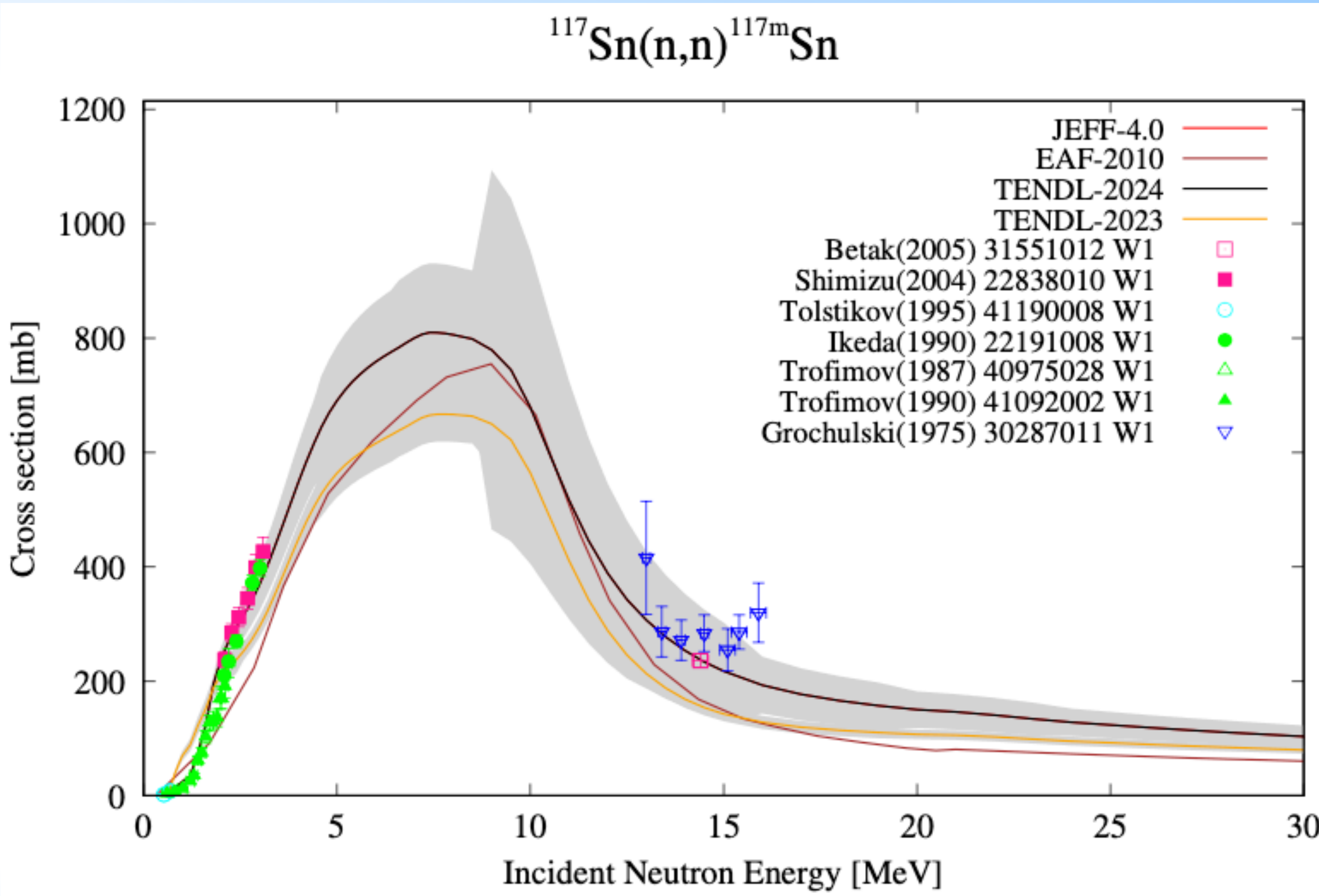
Outliers for TENDL (n,γ) evaluation

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

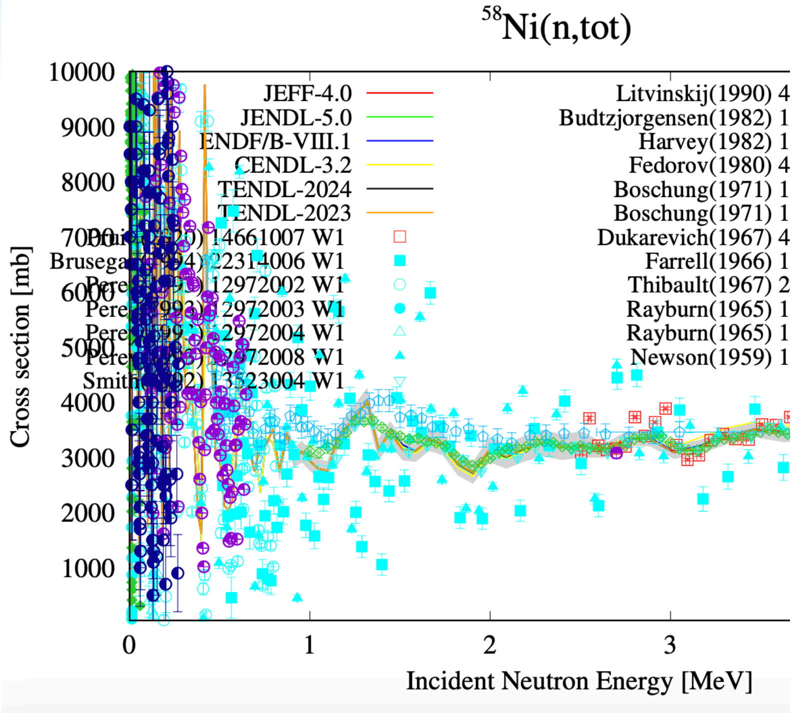
36 isotopes with Γγ considered as outlier:
Ca-40,42,44,……Hg-198

My notebook of remaining cases to solve

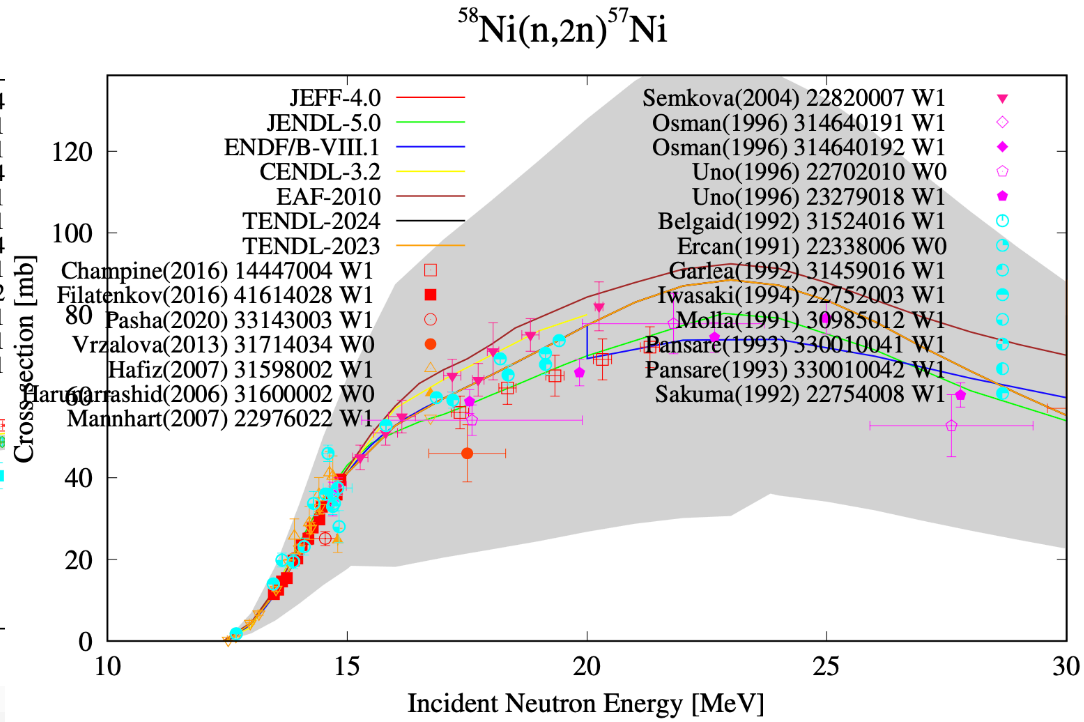
```
Gd157 0.3 - 1 MeV too low, discrete levels seem OK
Hf177 very weird peak at 2 MeV
Hf178 weird peak at 2 MeV
Hf180 0.5 - 1 MeV too high
In115 - totally too high , suppress fit for g, m, n
Lu175 around 1 MeV too low?
Mo95 0.1 - 1 MeV too low  solved after removing discrete levels for target
Mo97 0.2 - 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
```



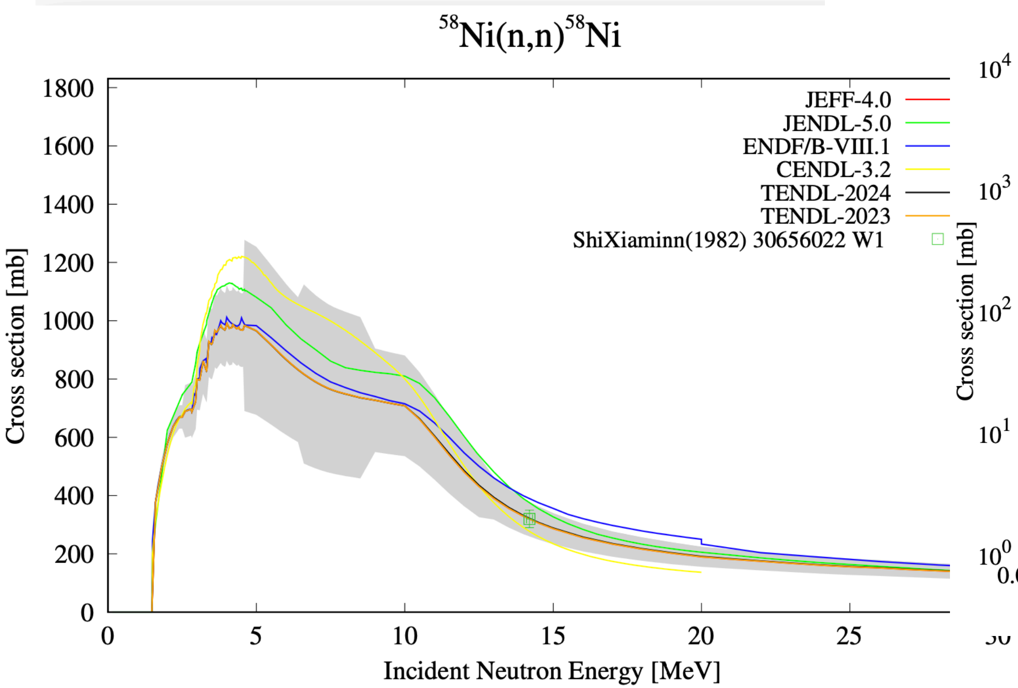
Malec, Trkov: important dosimetry reaction



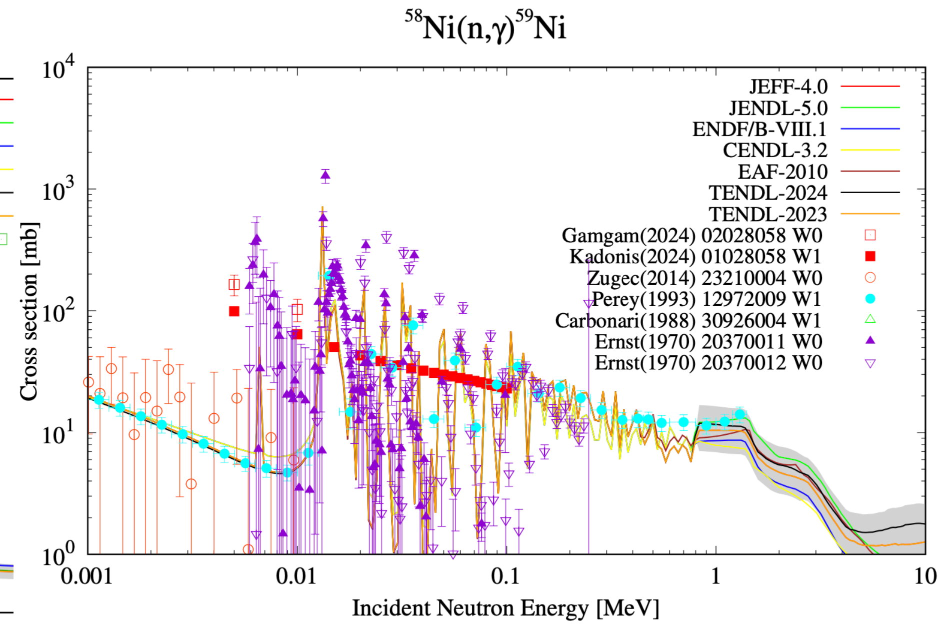
^{58}Ni(n,tot)
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
TENDL-2024
TENDL-2023
14661007 W1
22314006 W1
12972002 W1
2972003 W1
2972004 W1
2972008 W1
13523004 W1
Litvinskij(1990) 4
Budtzjorgensen(1982) 1
Harvey(1982) 1
Fedorov(1980) 4
Boschung(1971) 1
Boschung(1971) 1
Dukarevich(1967) 4
Farrell(1966) 1
Thibault(1967) 2
Rayburn(1965) 1
Rayburn(1965) 1
Newson(1959) 1



^{58}Ni(n,2n)^{57}Ni
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
EAF-2010
TENDL-2024
TENDL-2023
Champine(2016) 14447004 W1
Filatenkov(2016) 41614028 W1
Pasha(2020) 33143003 W1
Vrzalova(2013) 31714034 W0
Hafiz(2007) 31598002 W1
Harunarrashid(2006) 31600002 W0
Mannhart(2007) 22976022 W1
Semkova(2004) 22820007 W1
Osman(1996) 314640191 W1
Osman(1996) 314640192 W1
Uno(1996) 22702010 W0
Uno(1996) 23279018 W1
Belgaid(1992) 31524016 W1
Ercan(1991) 22338006 W0
Garlea(1992) 31459016 W1
Iwasaki(1994) 22752003 W1
Molla(1991) 30985012 W1
Pansare(1993) 33010041 W1
Pansare(1993) 33010042 W1
Sakuma(1992) 22754008 W1



^{58}Ni(n,n)^{58}Ni
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
TENDL-2024
TENDL-2023
ShiXiaminn(1982) 30656022 W1



^{58}Ni(n,γ)^{59}Ni
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
EAF-2010
TENDL-2024
TENDL-2023
Gamgam(2024) 02028058 W0
Kadonis(2024) 01028058 W1
Zugec(2014) 23210004 W0
Perey(1993) 12972009 W1
Carbonari(1988) 30926004 W1
Ernst(1970) 20370011 W0
Ernst(1970) 20370012 W0

Frms values per nuclide, reaction channel and NDL

```
# Average Frms values per MT number for neutron  + Ni 58
#         MT Iso        ENDFB8.1                     JEFF4.0
#                   Frms     #points #sets         Frms     #points #sets
(n,tot)   1 -1     1.42       63182     19         1.47       62657     19
(n,el)    2 -1     1.10          16      8         1.11          16      8
(n,inl)   4 -1     1.21           1      1         1.00           1      1
(n,2n)   16 -1     1.19         324     76         1.19         324     76
(n,3n)   17 -1     2.28           2      1         1.72           2      1
(n,np)   28 -1     1.13         171     34         1.15         178     35
(n,n1)   51 -1     1.48         113     11         1.46         111     11
(n,g)   102 -1     1.44          28      2         1.26          27      2
(n,p)   103 -1     1.21         735     90         1.21         737     90
(n,p)g  103  0     0.00           0      0         1.62          10      4
(n,p)m  103  1     0.00           0      0         1.15          80     16
(n,a)   107 -1     1.31          60      8         1.37          60      8
```

Only makes sense when EXFOR outliers are removed
Available for all nuclides, reaction channels and NDL's
Statistics available in all kinds of different forms (summed over nuclides, channels etc.)
Such statistics could go, in some form, into the JEFF paper

What next

- Establish new evaluated databases of thermal cross sections, RI, MACS, Γ_γ, D0, etc.
  - Data mining of all existing compilations and EXFOR
  - New level density CRP (Krticka)
  - Give all resonance parameter databases in human/modern readable format: Atlases, all NDL's (again: TARES)
- Finalising EXFOR outlier collection
- Finding new home for TENDL production (?) (i.e. computer power)
  - Possibly make new TENDL before September 2025
- Translate negative feedback for JEFF-4 (leading to manual corrections of TENDL files for JEFF-4) into next automated TENDL scheme
- TALYS event generator
  - Skipping ENDF and cross sections altogether, true nuclear reaction simulator with all correlations included
  - Fully populated by probability tables
  - Direct input to next generation transport codes
- Contribute to JEFF and TENDL papers

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Thank you!