IAEA

60 Years

Atoms for Peace and Development

TALYS and TENDL for the future of FENDL

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Contents

- TENDL approach
- Some examples
- Summary

TENDL: TALYS Evaluated Nuclear Data Library

- General purpose nuclear reaction data library
- Simultaneous focus on
  - Reproducibility ✓
  - Completeness ✓
  - Quality (ongoing, never enough)
- Heavily based on the TALYS nuclear model code
- Extent:
  - Neutrons, photons, protons, deuterons, tritons, Helium-3, alpha-particles
  - 2853 nuclides (all stable or with half-life > 1 sec.)
  - 0-200 MeV
  - All cross sections and secondary distributions (particle and gamma spectra)
  - UQ with covariance matrices or random distributions
  - A variety of data formats
- TENDL ranges from global TALYS calculations to detailed isotopic evaluations
- TENDL-2025 to be released in December 2025

Building blocks of TENDL: horizontal nuclear data evaluation

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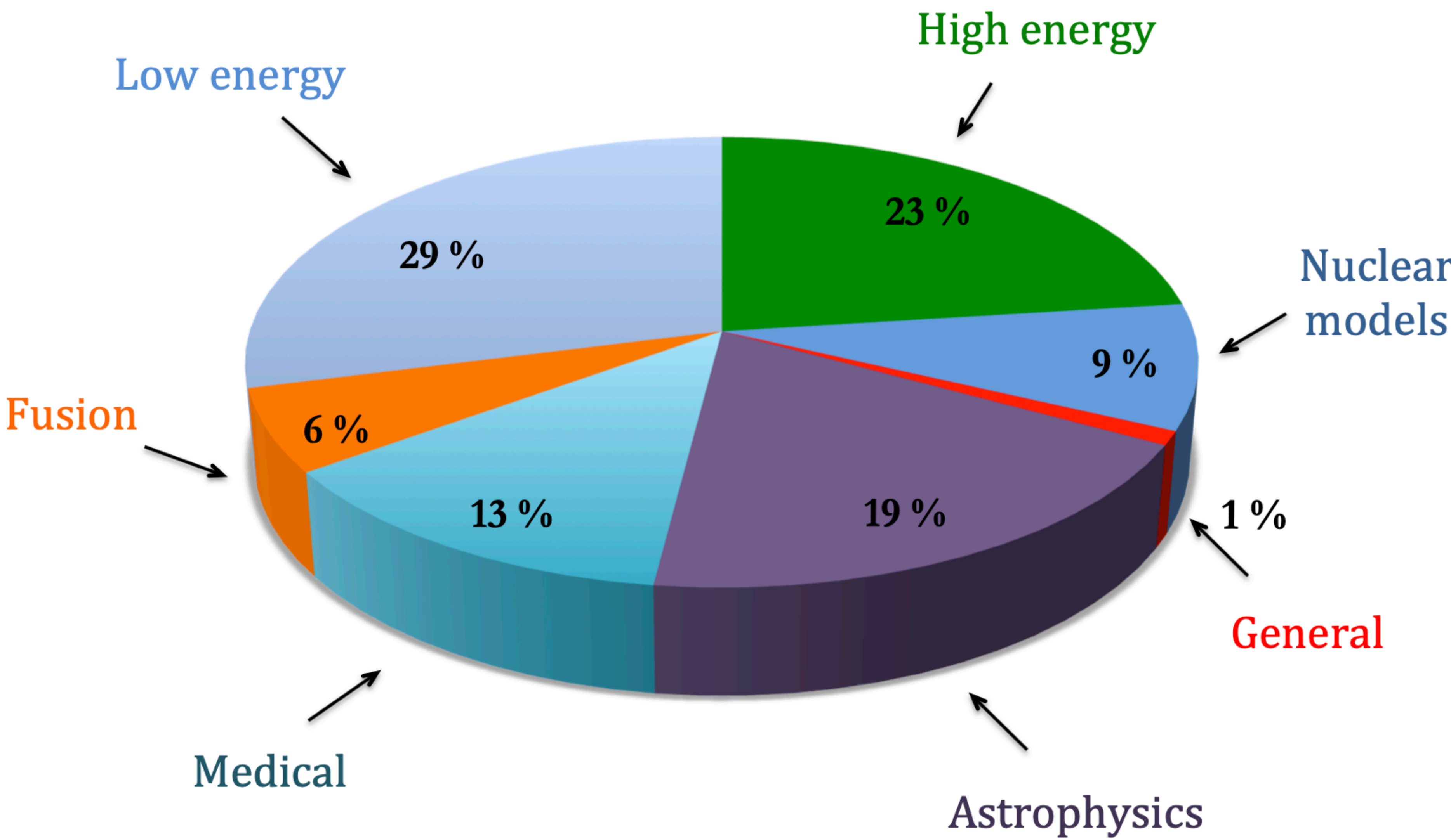
- Complete automated Resonance Parameter system including covariance data:
  - TARES-1.6 (Dimitri Rochman)
  - Regularly updated with latest recommendations for best resonance parameters
  - Tested for format and basic physics errors and declared correct (AK)
- EXFOR database
  - Entire database renormalized to the latest standard and monitor reactions
  - Based on Viktor Zerkin's XC5 database and Shin Okumura's EXFOR_JSON database
  - 11 500 experimental cross section sets validated, 2050 data sets declared outlier (needed for automatic optimisation): Essential for automated TALYS model parameter 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")
    - "Best" nuclear model parameters for reactions up to 30 MeV
- 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 -best -ntalys 100 -sdefault -s20 -s60 -acf -eaf -mt

- ……which produces the TENDL file for n + Sn117, up to 200 MeV, including all secondary distributions and covariance data, i.e. from MF1 - MF40. All adjustment to experimental data is in underlying databases.

Example: Upcoming JEFF-4.0 neutron library

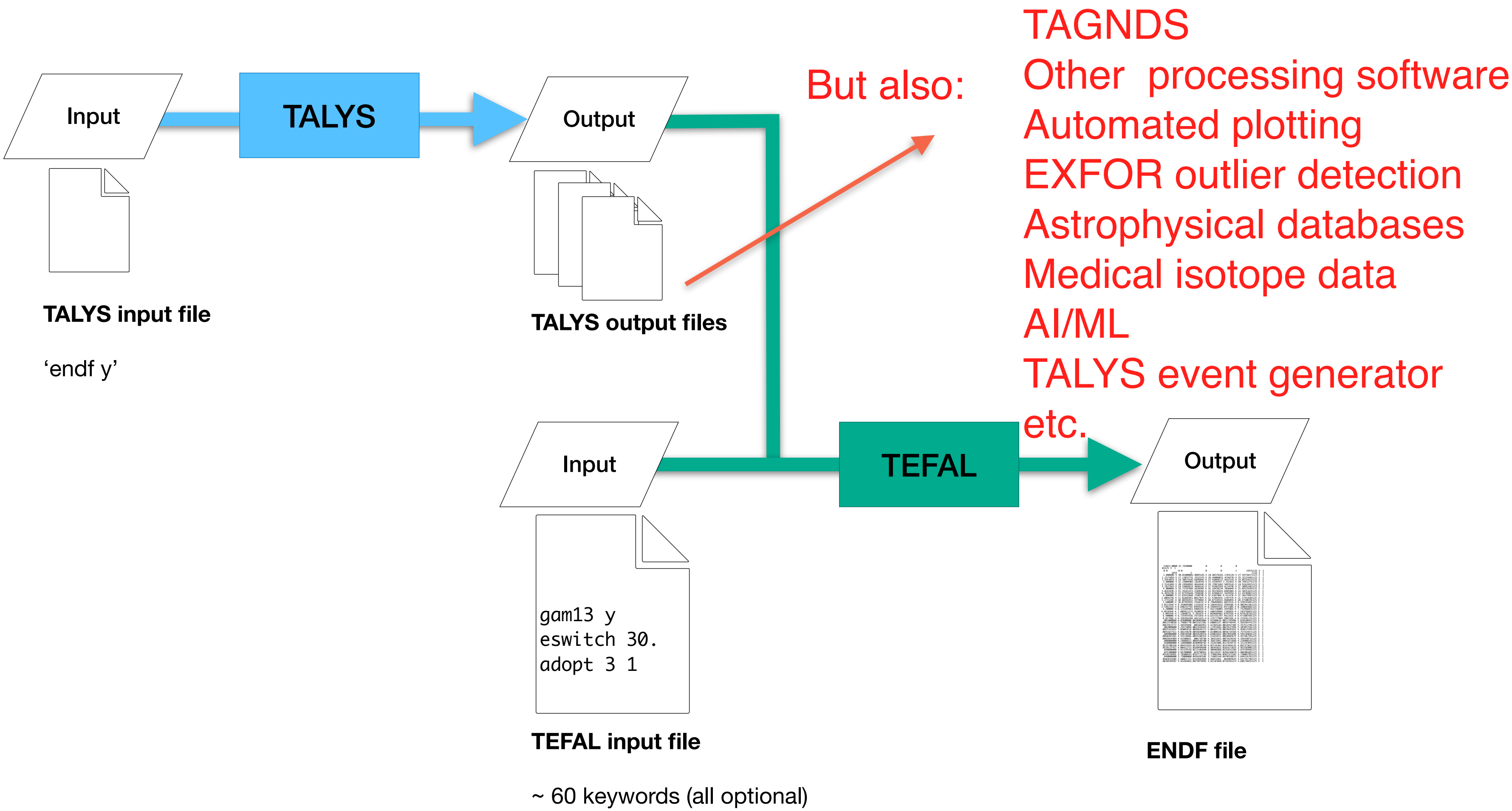
- Consist for 80% of isotopes from the TENDL-2025 beta version, which at least guarantees true general purpose application (MF1-40)
- 106 nuclides, or 34 materials, not from TENDL: H, He, Li, Be, B, C, N, O, F, Al, Si, Cl, Cr, Mn, Fe, Cu, Rh, Sn, Gd, Hf, Ta, W, Au, Pb, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm
- Non-TENDL isotopes for the right reasons:
  - No reproducible system (anywhere) for light nuclides
  - TALYS 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 or some other applications. INDEN evaluations are better.
  - Consistent approach for actinides not yet ready
- In total, current JEFF-4 pre-release tests looking good (in part thanks to TENDL)

Global use of TALYS (~ 7000 papers)



TALYS applications

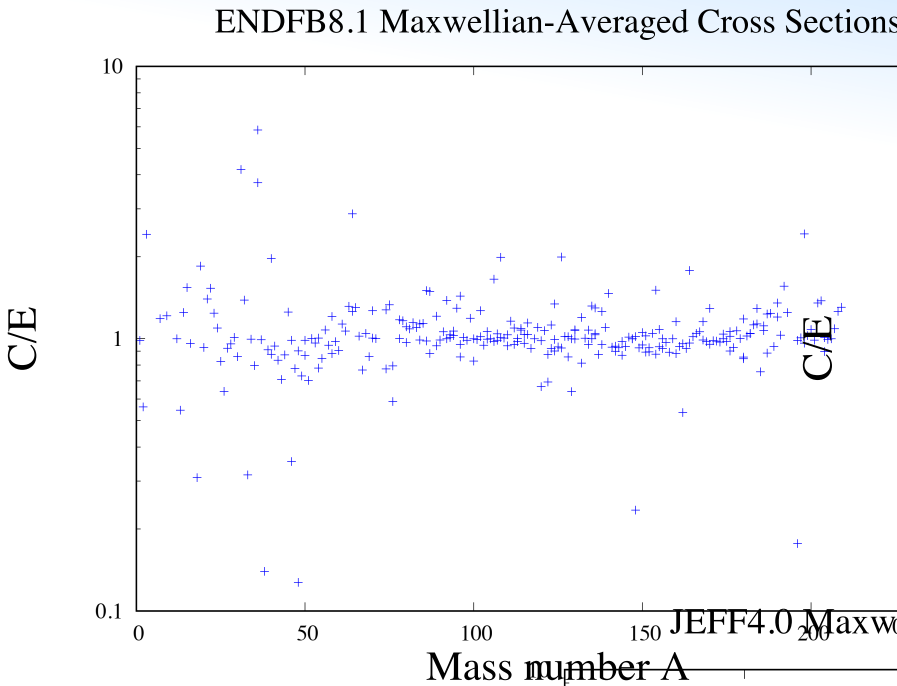
- TEFAL processes the output of TALYS, and data from other sources, into an ENDF-6 data library

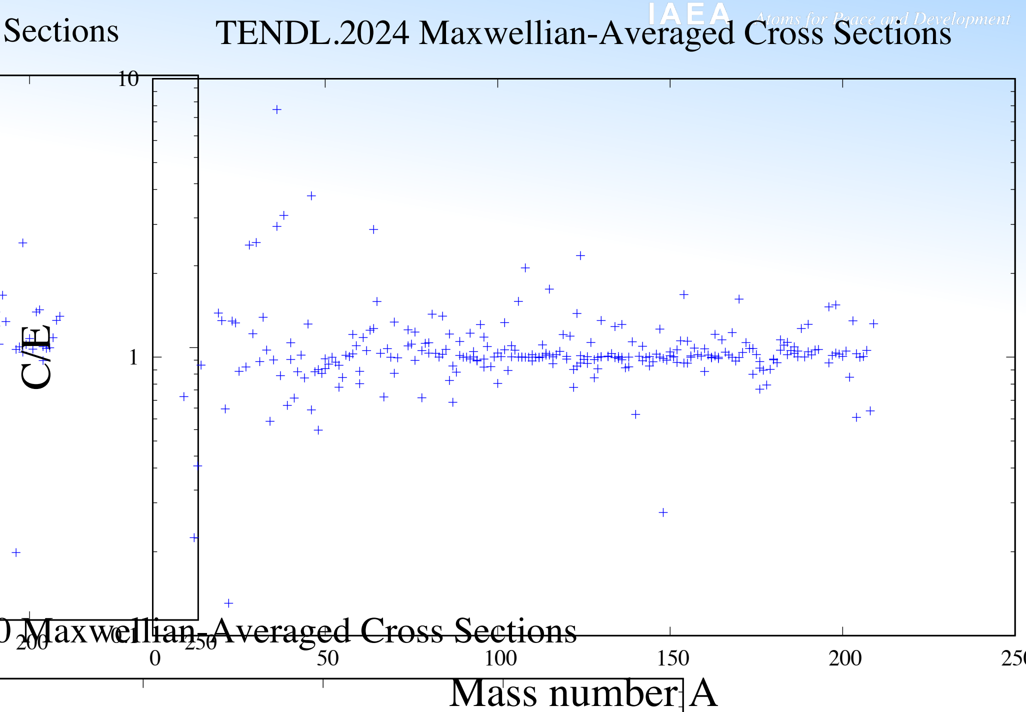


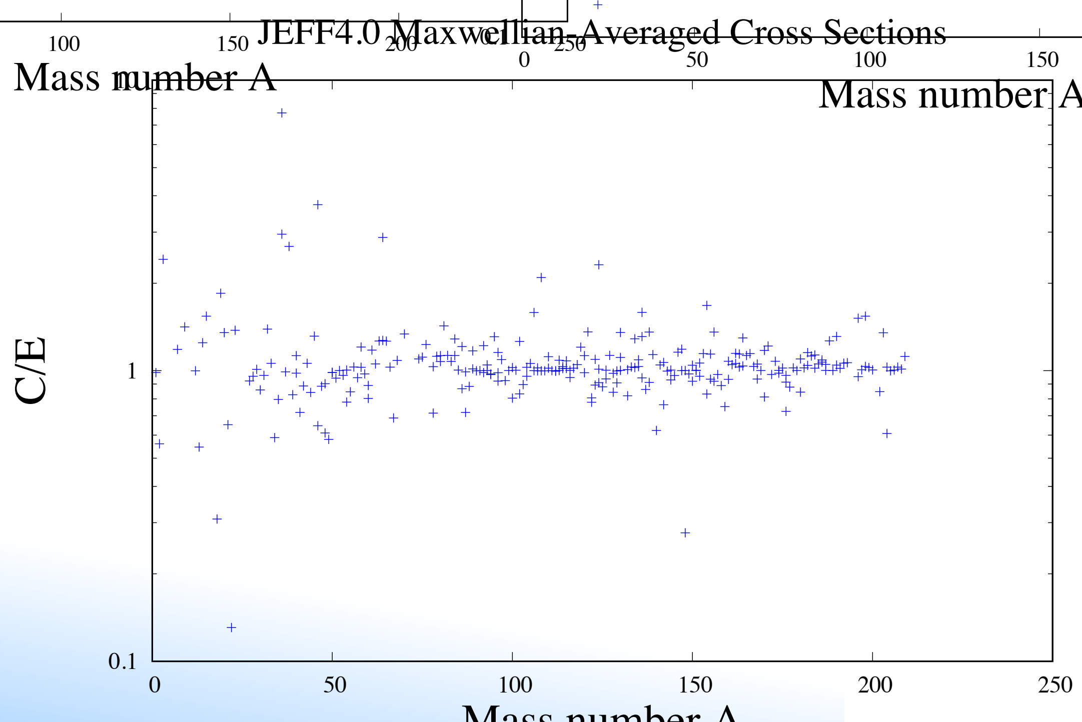
Some recent and upcoming TENDL versions

- 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: (n,α) generally too high above 14 MeV due to bug in implementation of knock-out mechanism, solved
- TENDL-2025 (in development): 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 30 MeV for cross sections, including isomers
  - In the range from F - Bi: ~ 80 individual reaction channels still unsatisfactory due to model defects. The rest is competitive with or better than the other NDL's.
- Recommendation, also for FENDL: wait for TENDL-2025
  - For possible adoption of missing isotopes in "transport" library (FENDL-3.2c++)
  - Activation library
  - Having TENDL in standard validation schemes (JADE, FISPACT, etc.) would be beneficial for development…thank you!!!

NDL’s (n,γ) versus Astral/Kadonis exp. MACS at 30 keV





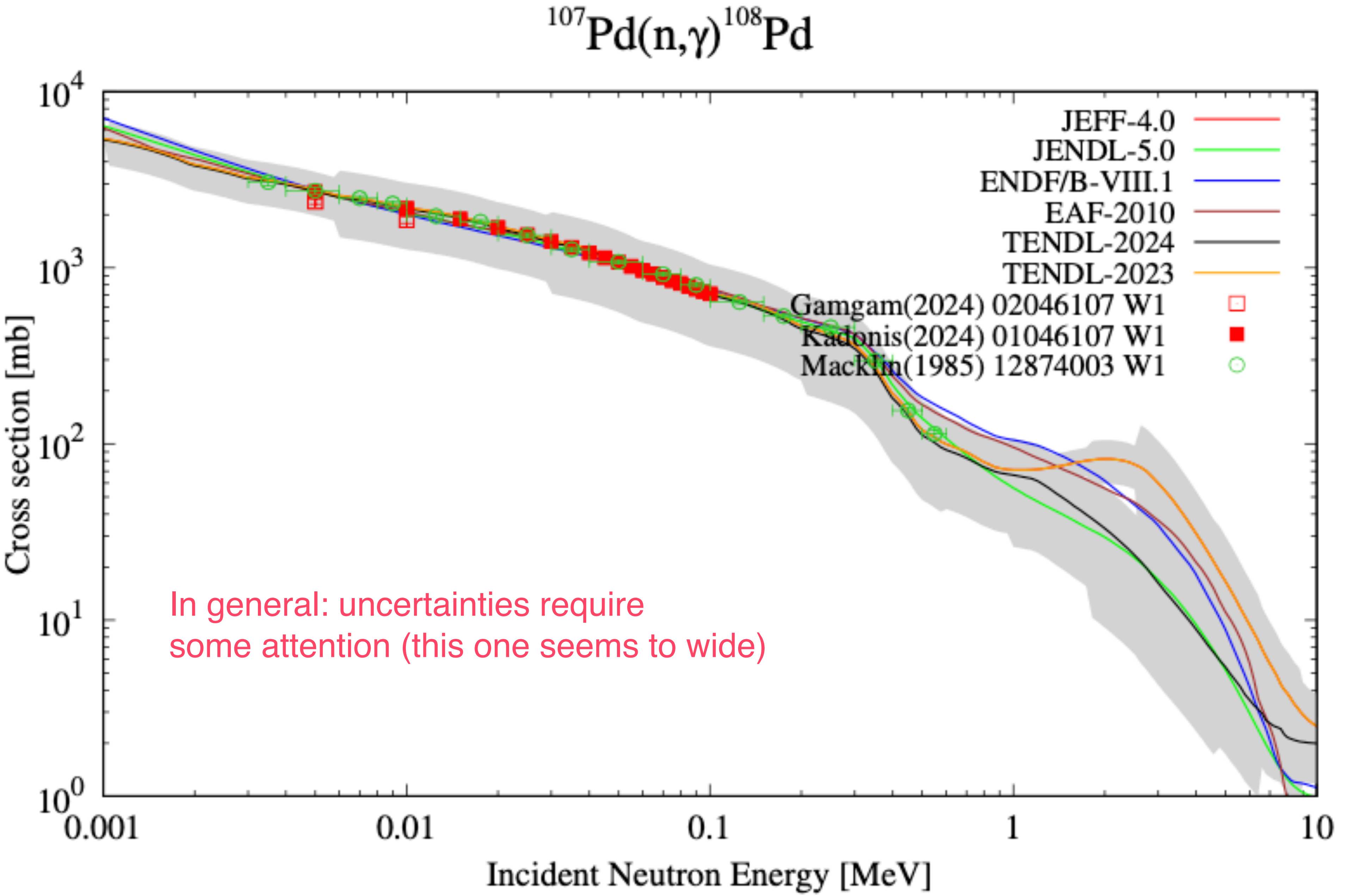


	Frms
CENDL-3.2:	1.069
JENDL-5.0:	1.064
ENDF/B8.1:	1.064
TENDL-2025:	1.052
JEFF-3.3:	1.076
JEFF-4.0:	1.062

Parameter optimisation in fast range

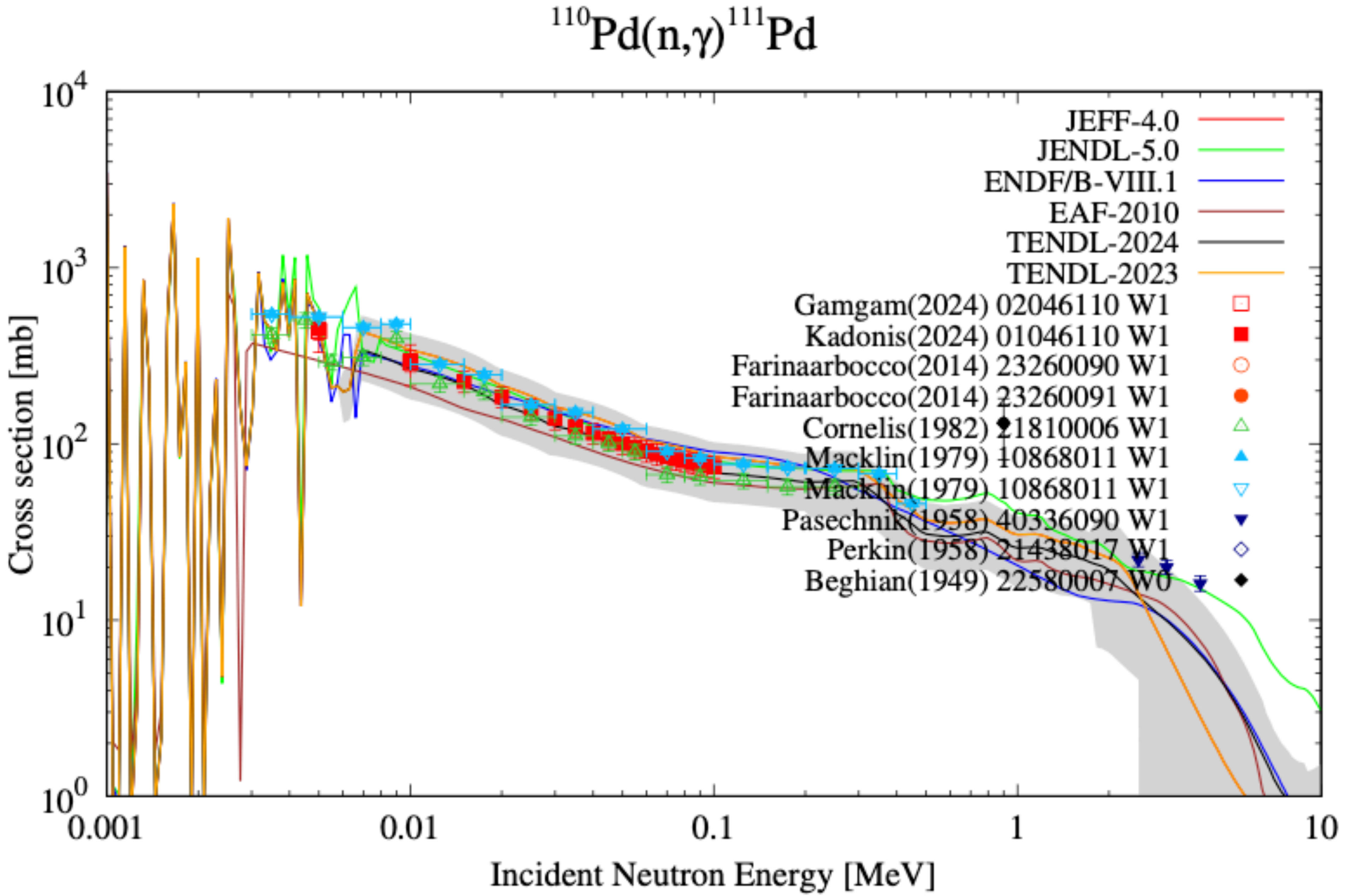
- Use TASMAN for parameter optimisation
  - Multi-dimensional parameter landscape not too wild
  - 20 TALYS runs per parameter
- (n,γ):
  - Photon strength function: wtable(0,0) of compound nucleus
- (n,n'), (n,2n), (n,p) and (n,np):
  - Optical model: rvadjust p
  - Pre-equilibrium: gadjust(0,0), gadjust(1,0), 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

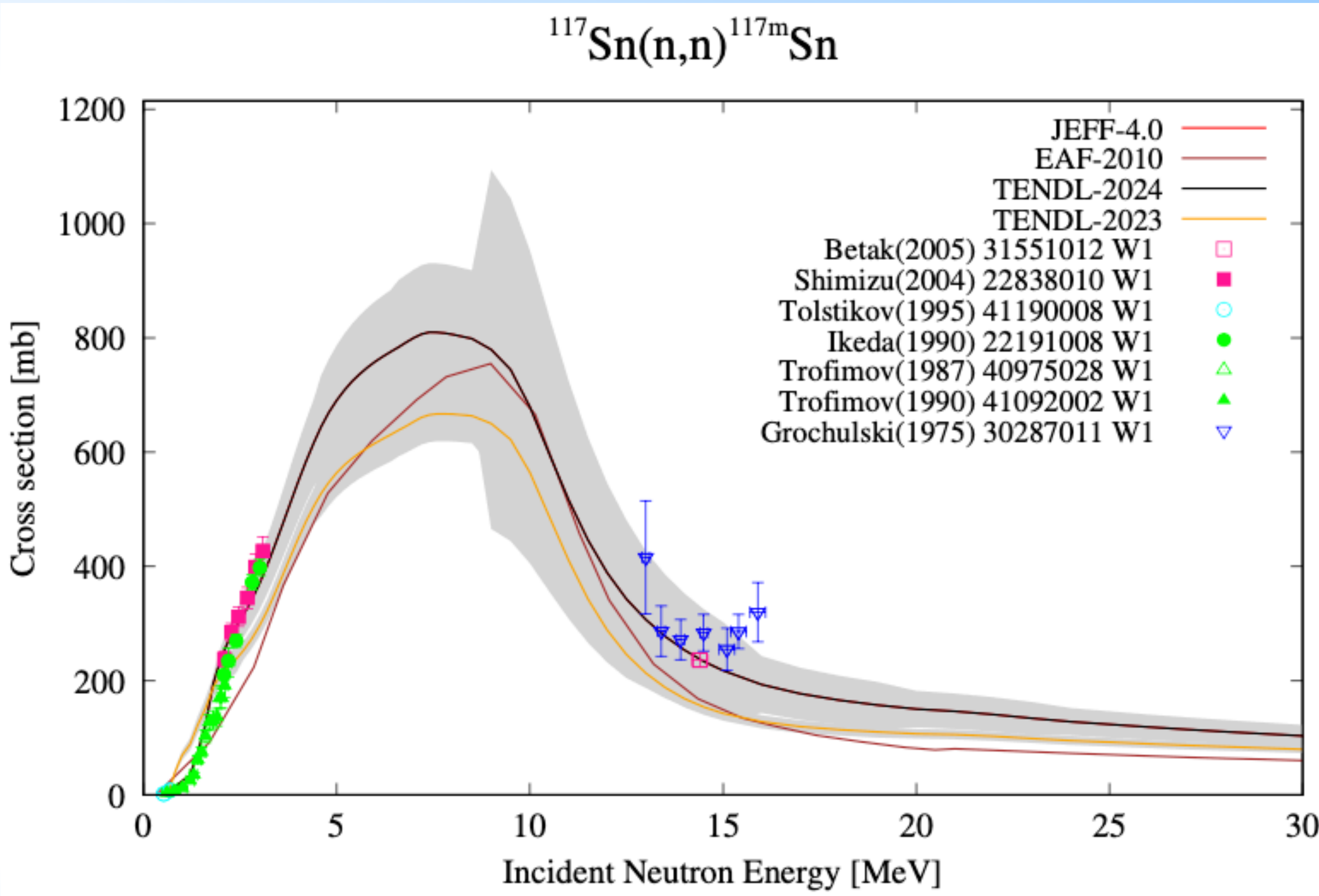
Typical case



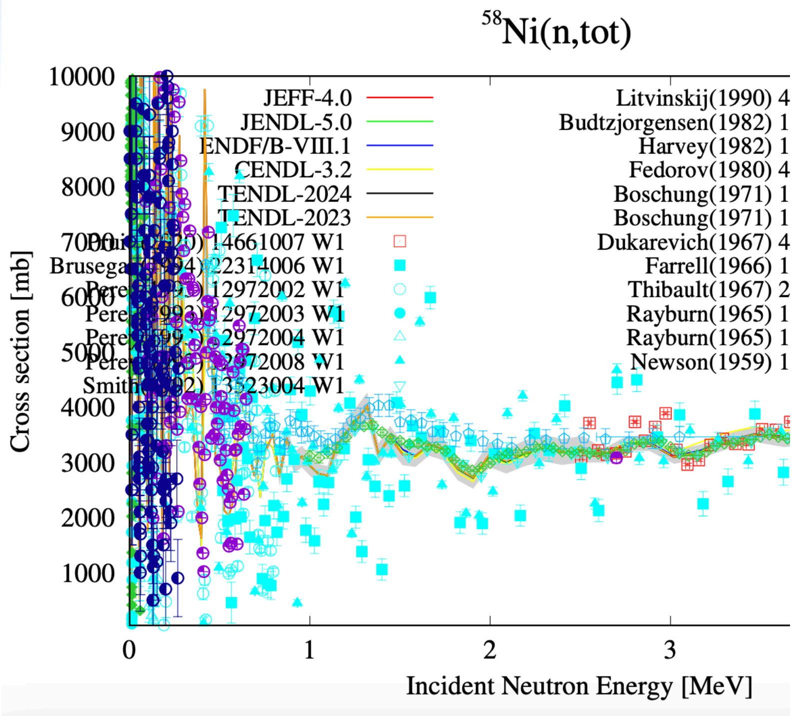
In general: uncertainties require some attention (this one seems to wide)

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

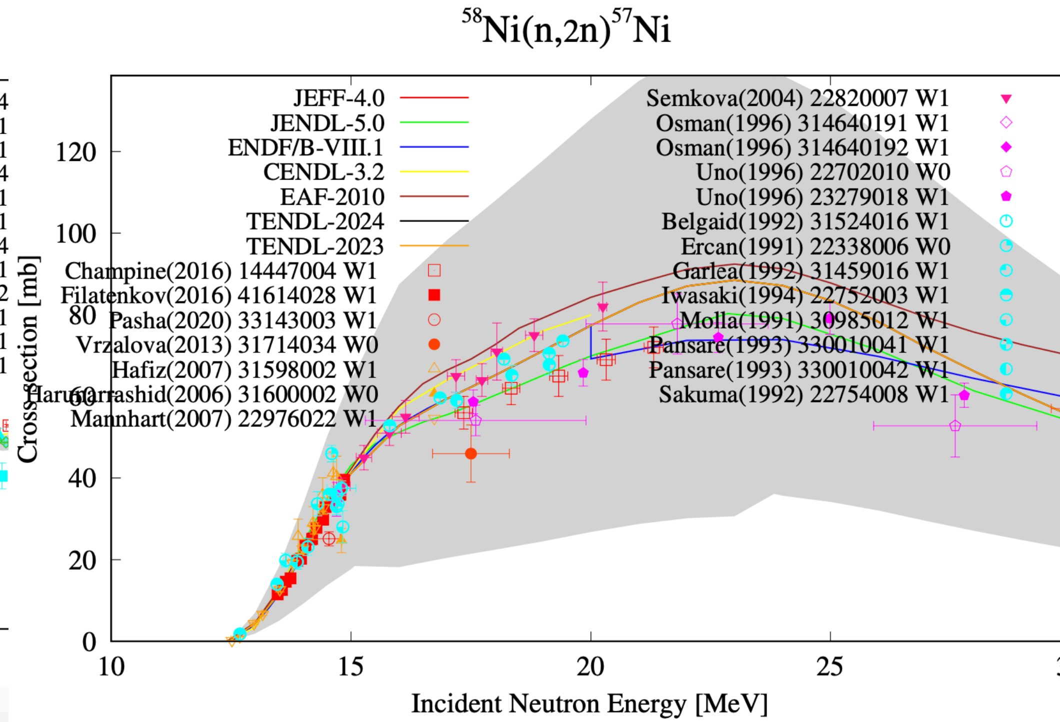




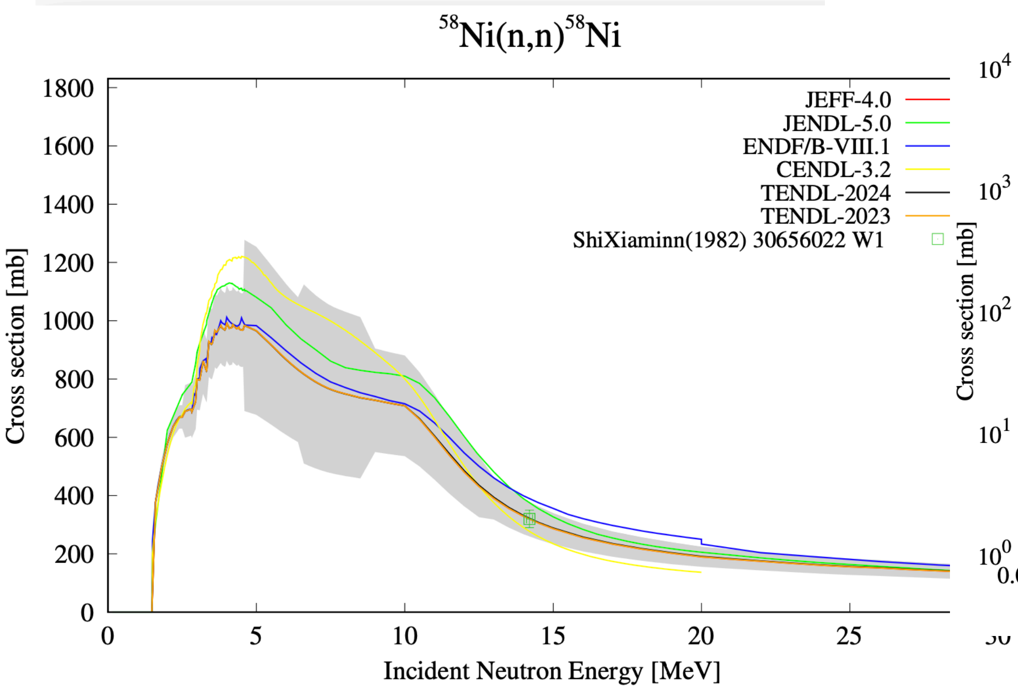
Malec, Trkov: important dosimetry reaction



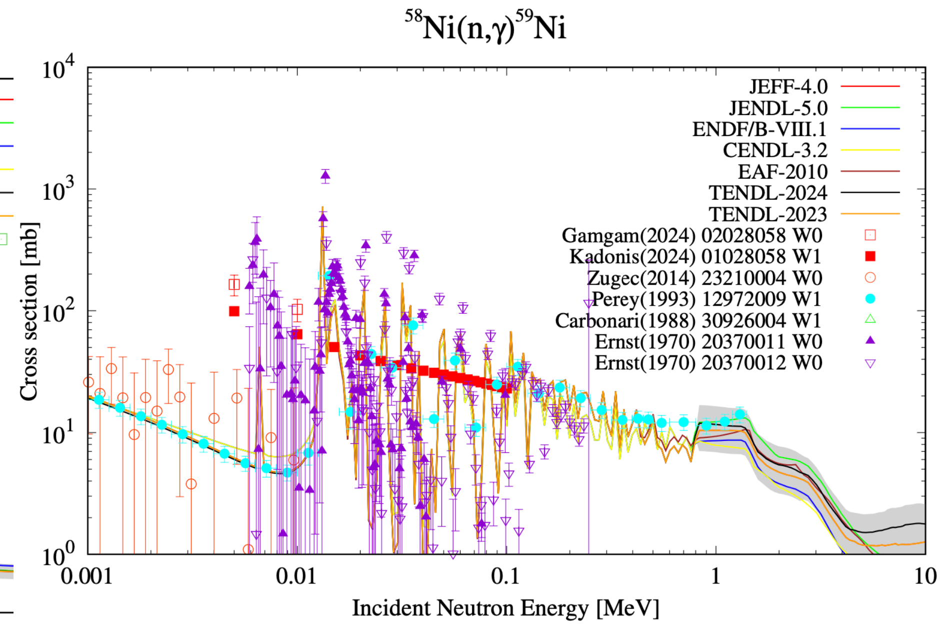
58Ni(n,tot)
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
TENDL-2024
TENDL-2023
Litvinskij(1990) 4
Budtzjorgensen(1982) 1
Harvey(1982) 1
Fedorov(1980) 4
Boschung(1971) 1
Boschung(1971) 1
Dukarevich(1967) 4
Farrell(1966) 1
Thibault(1967) 2
Rayburn(1965) 1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



58Ni(n,2n)57Ni
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



58Ni(n,n)58Ni
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



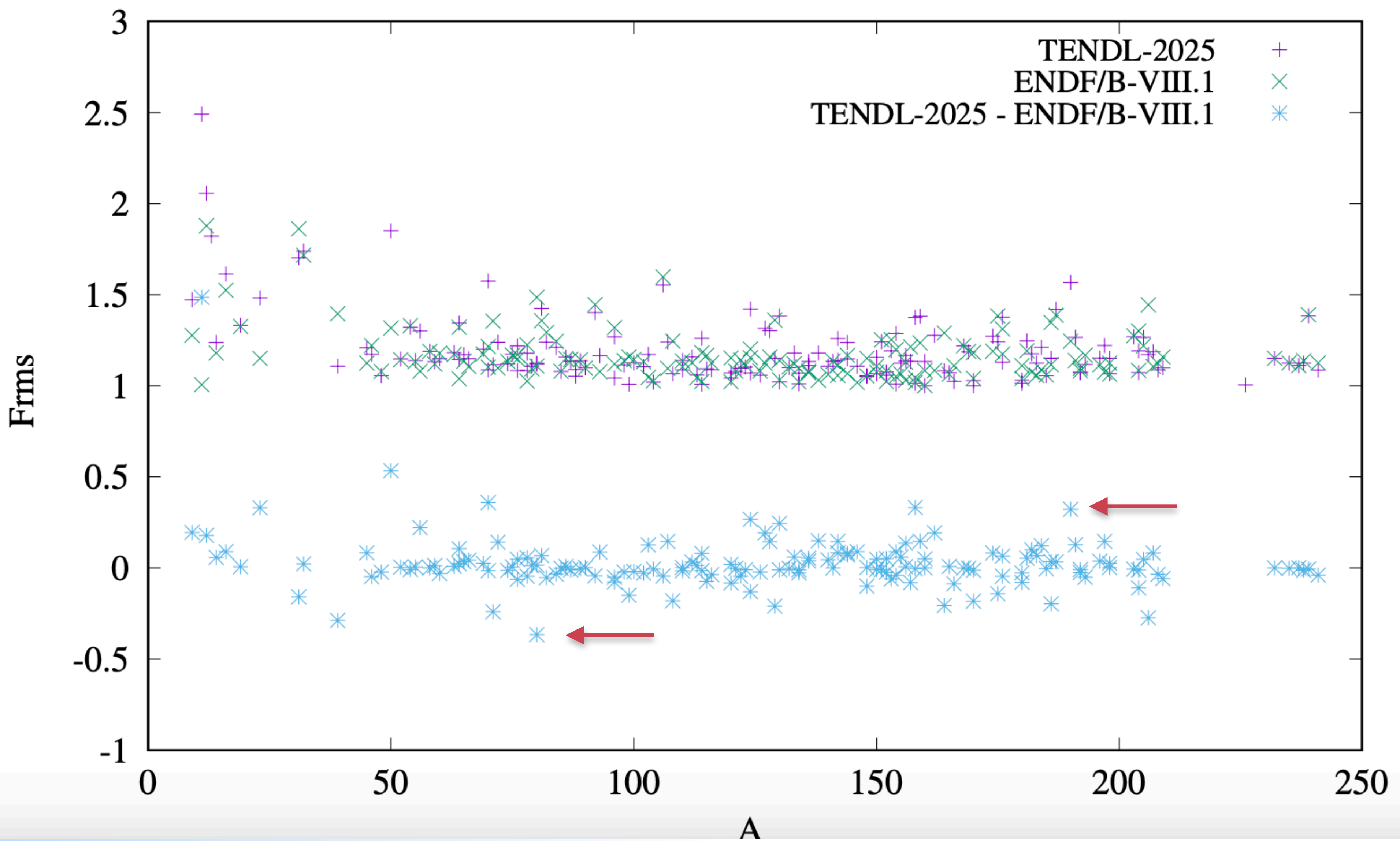
58Ni(n,γ)59Ni
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
CENDL-3.2
EAF-2010
TENDL-2024
TENDL-2023
Gamgam(2024) 02028058 W0
Kadonis(2024) 01028058 W1
Zugec(2014) 23210004 W0
Perey(1993) 12972009 W1
Carbonari(1988) 30926004 W1
Ernst(1970) 20370011 W0
Ernst(1970) 20370012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

EXFORtables: Frms values per nuclide, reaction channel and NDL

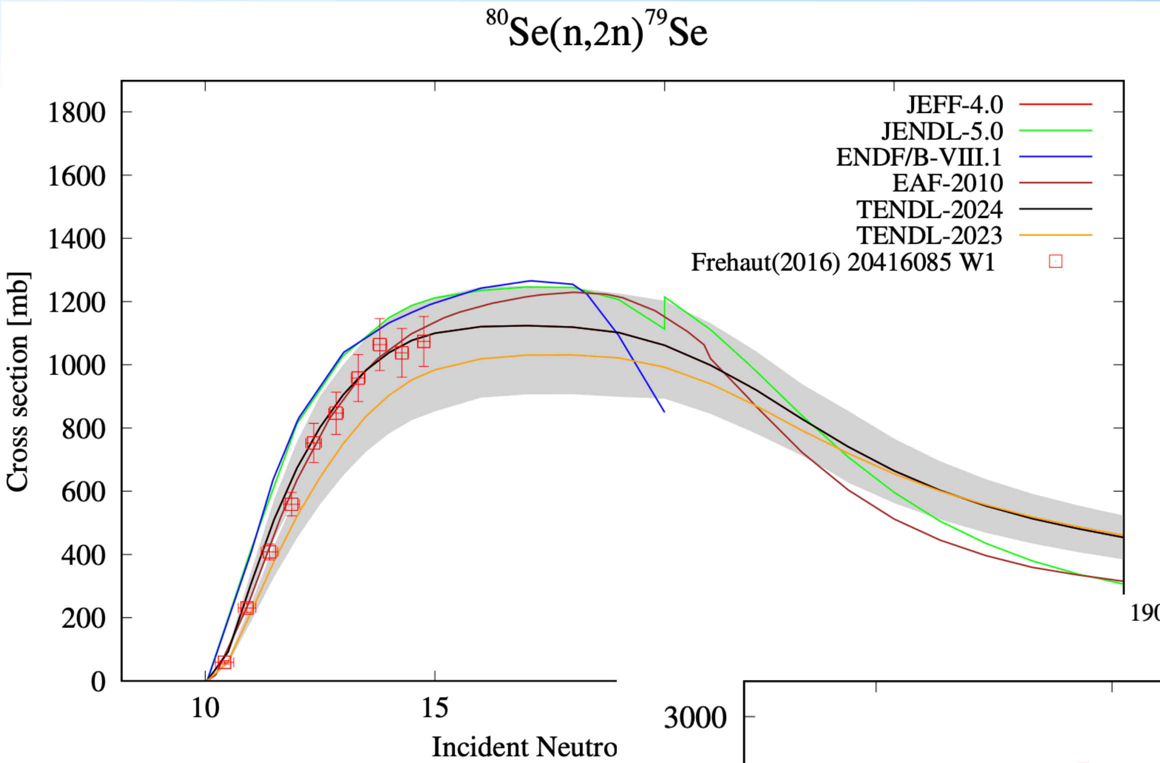

```
# Average Frms values per MT number for neutron  + Ni 58
#         MT Iso        ENDFB8.1                       JEFF4.0
#                Frms     #points #sets         Frms     #points #sets
(n,tot)   1 -1   1.42       63182    19         1.47       62657    19
(n,el)    2 -1   1.10          16     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
```

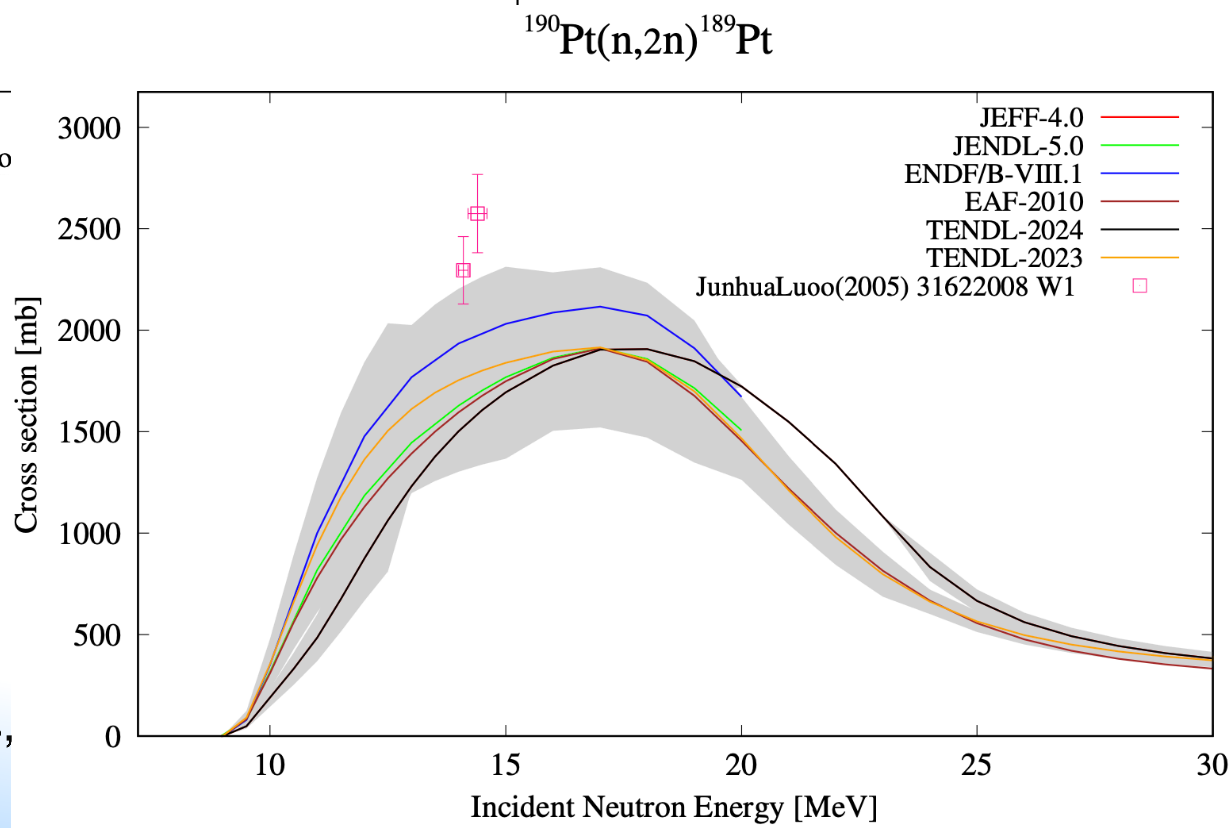
Only makes sense when EXFOR outliers are removed
Available for all nuclides, reaction channels and NDL’s
Statistics available in all kinds of different forms (summed over nuclides, channels etc.)

(n,2n): Frms for all nuclides



Good enough for the moment





Work to be done on weights, other channels etc.

YANDF (Yet Another Nuclear Data Format)

- Zen of Python: Explicit is better than implicit
- Key - value approach: allow ‘easy’ parsing into JSON, YAML, GNDS/XML etc.
- Not as non-descriptive as ENDF
- Not as heavy as GNDS
- Not as extensive and abbreviated as EXFOR
- More metadata than in the previous TALYS output files
- Human-readable
- Same schema for TALYS, EXFOR and ENDF
- From the point of view of a nuclear physicist, not from EXFOR or ENDF
- Would make ALL nuclear reaction data programmatically available at the same time: good for TENDL, other large data projects, AI/ML

TALYS output file: rp039090.L02


```
# header:
#   title: Nb93(n,x)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,x)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 6
#   ENDF_MT: 5
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   mass [amu]:  8.990714E+01
#   level:
#     number: 2
#     energy [MeV]:  6.820100E-01
#     spin:  7.000000E+00
#     parity: 1
#     isomer: 1
#     half-life [sec]:  1.148000E+04
# datablock:
#   quantity: cross section
#   columns: 3
#   entries: 25
##       E              xs        Isomeric ratio
##     [MeV]           [mb]             []
   2.000000E-01   0.000000E+00   0.000000E+00
   4.000000E-01   0.000000E+00   0.000000E+00
   6.000000E-01   0.000000E+00   0.000000E+00
   8.000000E-01   0.000000E+00   0.000000E+00
   1.000000E+00   0.000000E+00   0.000000E+00
   1.200000E+00   0.000000E+00   0.000000E+00
   1.400000E+00   8.135896E-05   0.000000E+00
   1.600000E+00   1.296808E-04   1.266436E-01
   1.800000E+00   2.699952E-04   1.644318E-01
   2.000000E+00   5.832345E-04   2.057970E-01
```

'#' for direct use in various software, e.g. Gnuplot

Without '#': YAMLesque 2 space indentation per level

Parsing to JSON should be easy

Only 5 main attributes for nuclear reactions

TALYS: 2 more main attributes: 'parameters' and 'observables'

EXFOR: All specific metadata may follow after the datablock

TALYS

```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-16
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 10
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     number: 2
#     energy [MeV]:  6.820100E-01
#     spin:  7.000000E+00
#     parity: 1
#     isomer: 1
#     half-life [sec]:  1.148000E+04
# datablock:
#   quantity: cross section
#   columns: 3
#   entries: 25
##       E              xs          Isomer
##     [MeV]           [mb]
   2.000000E-01  5.000000E-08  5.000
   4.000000E-01  5.000000E-08  5.000
   6.000000E-01  0.000000E+00  0.000
   8.000000E-01  0.000000E+00  0.000
   1.000000E+00  0.000000E+00  0.000
   1.200000E+00  0.000000E+00  0.000
```

JENDL5.0

```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: ENDF
#   user: Arjan Koning
#   date: 2024-01-02
#   format: YANDF-0.1
# endf:
#   library: jendl5.0
#   author: A.Ichihara
#   year: 2018
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   Q-value [MeV]:  4.246250E+00
#   E-threshold [MeV]:  1.000000
#   ENDF_MF: 10
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     isomer: 1
# datablock:
#   quantity: cross section
#   columns: 2
#   entries: 802
##       E              xs
##     [MeV]           [mb]
   1.000000E-11  4.231872E-04
   1.032229E-11  4.165287E-04
   1.065491E-11  4.099758E-04
   1.099830E-11  4.035247E-04
   1.135271E-11  3.971754E-04
   1.171859E-11  3.909265E-04
```

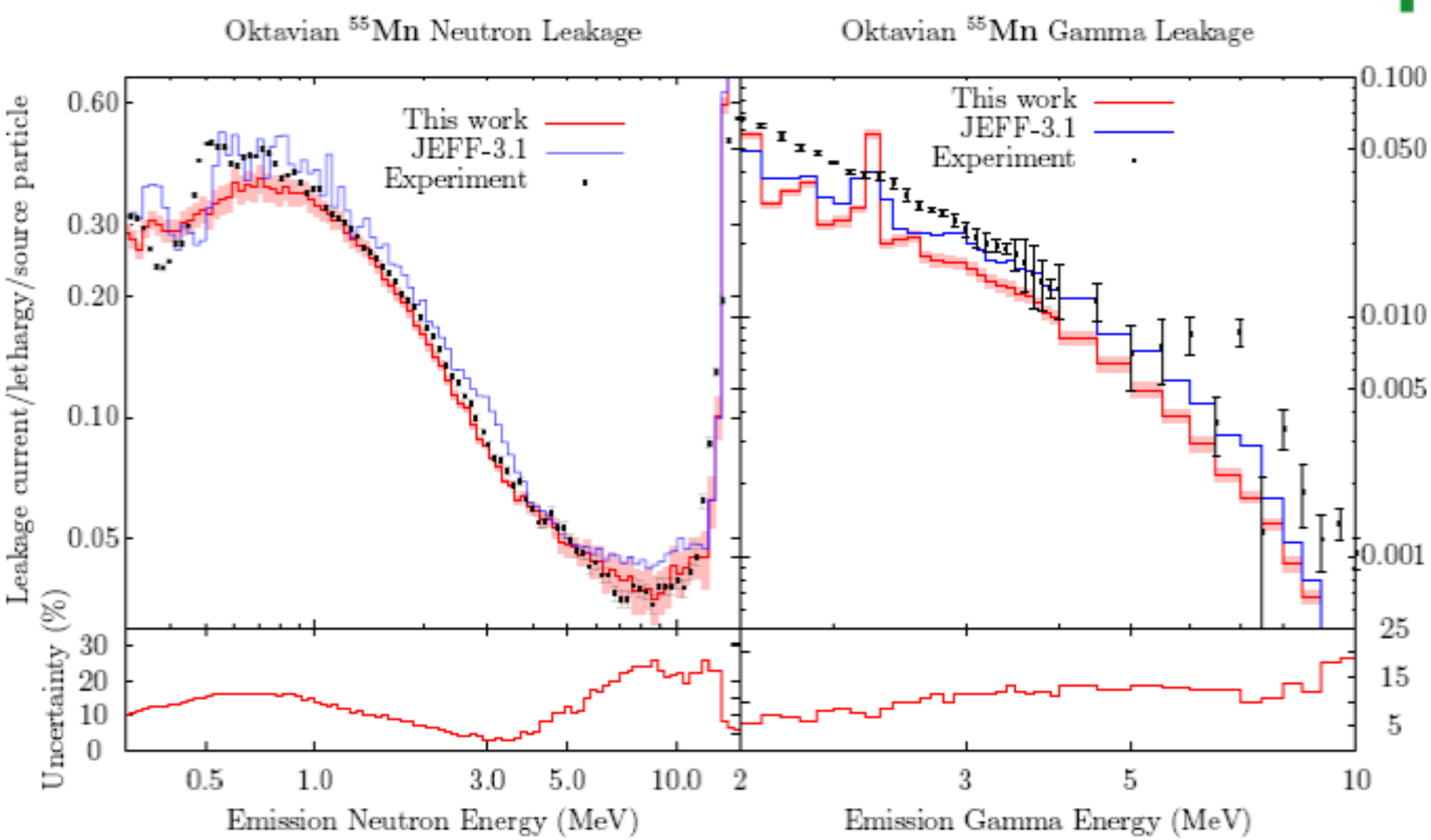
EXFOR
(One file per data set)

```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: EXFOR
#   user: Arjan Koning
#   date: 2023-12-30
#   format: YANDF-0.1
# exfor:
#   author: Fessler
#   year: 2000
#   subentry: 22414020
#   X4 reaction: 41-NB-93(N,A)39-Y-90-M,,SIG
#   X4 source: IAEA-NDS C5 file, database version 2023-08-08
#   X4 link: https://nds.iaea.org/EXFOR/22414020
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   ENDF_MF: 3
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     number: 0
#     energy [MeV]:  0.000000E+00
#     spin:  0.000000E+00
#     parity: 0
# datablock:
#   quantity: cross section
#   columns: 5
#   entries: 5
##       E              dE             xs            dxs          Normali
##     [MeV]          [MeV]          [mb]          [mb]            []
   1.603300E+01  6.200000E-02  5.220000E+00  3.100000E-01  1.00000
   1.698100E+01  4.000000E-02  4.960000E+00  3.100000E-01  1.00000
   1.772300E+01  3.200000E-02  5.220000E+00  3.100000E-01  1.00000
```

2010 FENDL meeting, IAEA: Total Monte Carlo with MCNP

0:15:52

Application for Mn Oktavian benchmark



Why did this data file work so well?
Can integral data be translated back to differential data (with uncertainties) to which we can fit TALYS?

What next

- Establish new evaluated databases of thermal cross sections, RI, MACS, Γγ, D0, etc.
  - Data mining of all existing compilations and EXFOR
  - New level density CRP
  - Give all resonance parameter databases in human/modern readable format: Atlases, all NDL's (TARES code)
- Finalising EXFOR outlier collection
- Translate negative feedback for JEFF-4, FENDL etc into next automated TENDL scheme
- TENDL-2025 in development:
  - Clean up remaining ENDF-6 format glitches
  - Apply automated optimisation to improve agreement with differential data
    - Applied for neutrons up to 30 MeV with ~10 parameters
    - Improved description of isomeric data
    - Further improvement of all photon and charged particle induced libraries (untouched since 2021)
  - Do more completeness tests and integral tests **before** release
- After 2025:
  - more efficient integral validation
  - More focus on angular distributions and (double-differential) emission spectra
- 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

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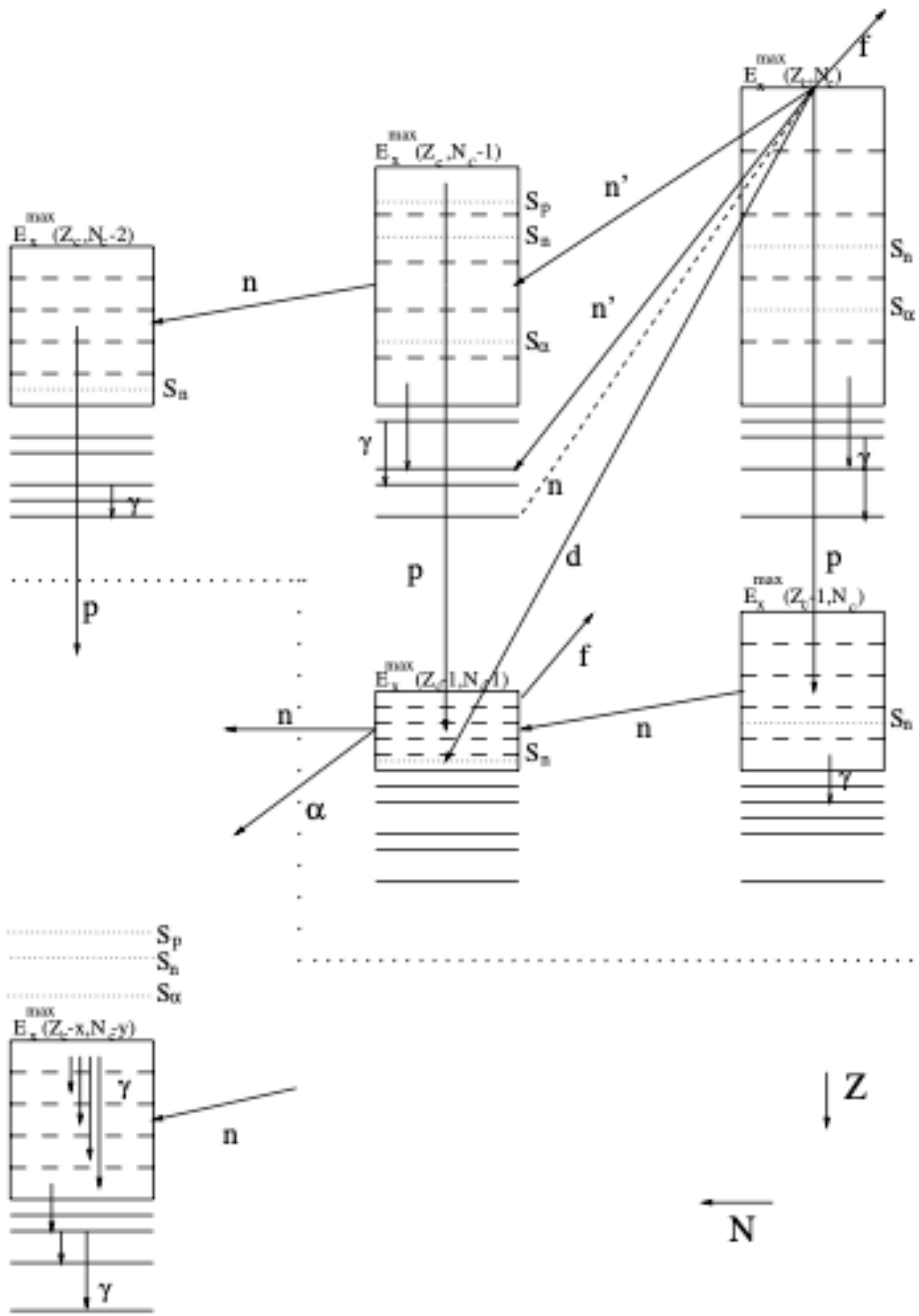
Thank you!


$E_x^{max}(Z_c,N_c)$
$E_x^{max}(Z_c,N_c-1)$
$E_x^{max}(Z_c,N_c-2)$
$E_x^{max}(Z_c-1,N_c)$
$E_x^{max}(Z_c-1,N_c-1)$
$E_x^{max}(Z_c-x,N_c-y)$
S_p
S_n
S_α
n
n'
p
d
f
γ
α
Z
N