IAEA 60 Years
Atoms for Peace and Development

Status of TENDL

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Contents

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

Vertical nuclear data evaluation

- Improve nuclear data evaluation of a particular projectile - target (- reaction) combination:
  - Sometimes driven by a sponsor
  - Sometimes driven by a new measurement
  - Sometimes driven by feedback from suboptimal integral validation
  - Hackatons needed because of evaluator diversity and manual file updating
  - Frankenstein files
    - We should never throw away data which work well (although we may not remember why they work well), often in the RR
    - If safe, add missing categories: emission spectra (TENDL —> ENDF/B-VIII.1), gamma data, covariances, data above 20 MeV, etc.
  - Major ‘continental’ NDL’s, ENDF/B-VIII.1, JEFF-3.3, JENDL-5.0, CENDL-3.2, based on this.
  - Leads to currently the best nuclear data libraries for fission applications
  - IAEA-INDEN wish list for evaluations a good example
  - Almost no evaluators left

Horizontal nuclear data evaluation

- Ensure a reproducible nuclear data flow with all experimental, theoretical and evaluated data directly available. Requires:
  - a parsed, interpreted, outlier-cleaned and normalised EXFOR database
  - evaluated experimental databases with rich metadata:
    - Thermal cross sections, resonance integrals
    - Full resonance databases
    - Maxwellian cross sections (MACS), average radiative widths etc.
  - Automated non-model evaluation software for low energies
  - Full control over existing nuclear data libraries for optimisation, ML, plotting etc.
  - Time spent by evaluator on retrieval of all the above should be minimal
- Can go (far) beyond ENDF
- TALYS code system and TENDL is based on this
- Ideal situation: A Horizontal nuclear data approach in which Vertical knowledge is inserted. This is happening already for JEFF: Improved RR parameters (mostly from CEA-Cadarache) —> TARES —> autotalys —> TENDL —> JEFF

Building blocks of TENDL

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- Complete automated Resonance Parameter system including covariance data:
  - TARES-1.61 (Dimitri Rochman)
  - Regularly updated with latest recommendations (CEA-Cad, etc.) for best resonance parameters
- EXFOR database
  - Entire database normalized to the latest standard and monitor reactions (Viktor Zerkin)
  - Based on XC5 database (Viktor Zerkin) and EXFOR_JSON/directory structured database (Shin Okumura)
  - 11 500 experimental cross section sets validated, 2050 data sets declared outlier: 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, in JEFF-4 are not from TENDL:
  - H, He, Li, Be, B, C, N, O, F:
    - No reproducible system exists for light nuclides
  - Al, Si, Cl, Cr, Mn, Fe, Cu, Rh, Gd, Hf, Ta, W, Au, Pb:
    - TALYS failure for structural nuclides (Cr, Fe, Cu etc.) up to a few MeV, need Gaussian Processes for model defects. TENDL approach can not yet outperform the manual evaluation of nuclides with strong sensitivity to crit-safety or some other applications. INDEN evaluations are better.
    - For JEFF-4.1: Aim to replace Cl, Rh, Gd, Au, Hf, Ta by TENDL
  - Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm:
    - Consistent approach for actinides not yet ready
    - For JEFF-4.1: Minor actinides when new BSKG3 fission barrier level densities are available
- TENDL goes from low-, to mid- to high-hanging fruit
- In total, current JEFF-4 pre-release tests looking good (in part thanks to TENDL)

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

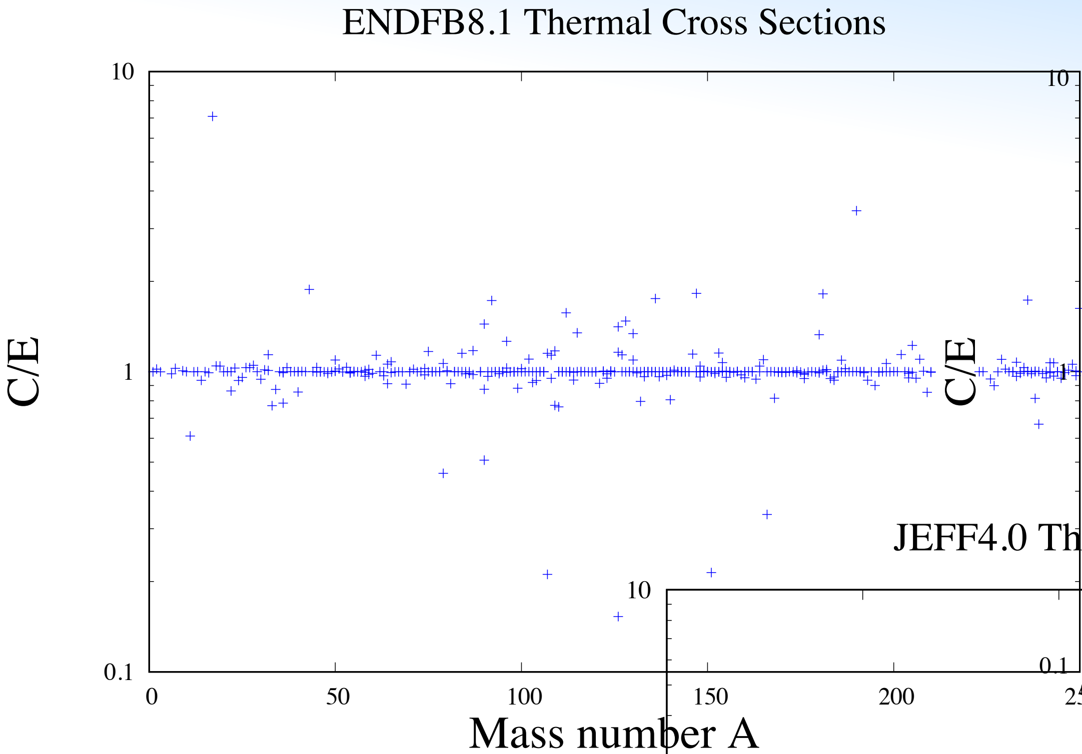
$$\begin{aligned} r_i &= 1-(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1){\rm erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} < \sigma^i_{\rm exp}, \\ &= 1+(\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}}-1){\rm erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} > \sigma^i_{\rm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

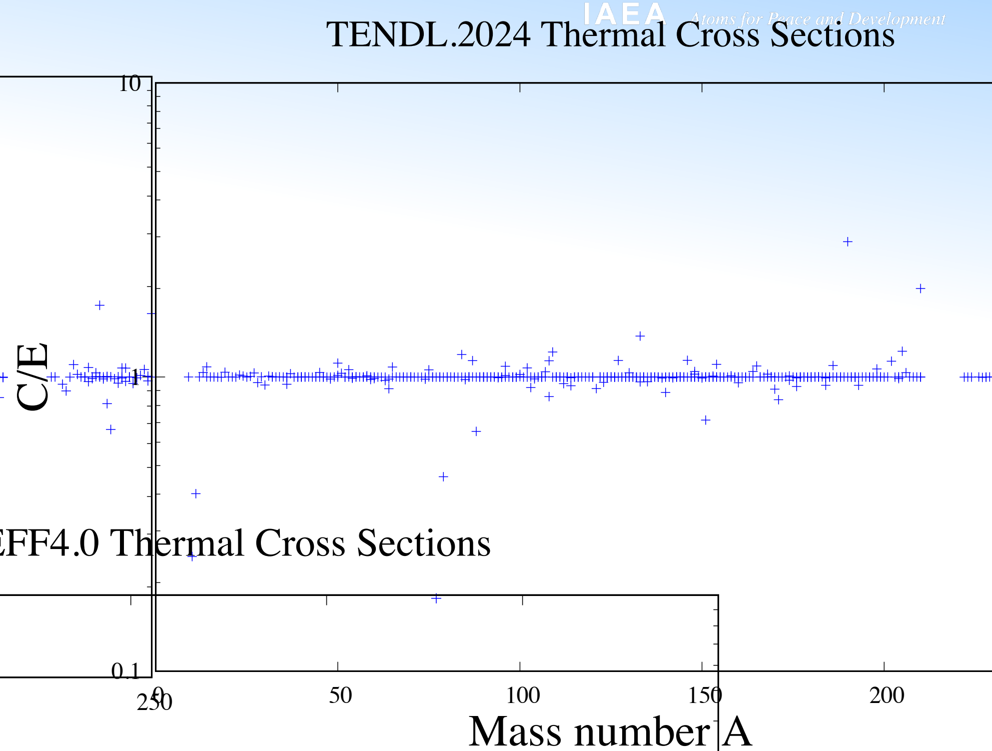
C/E value including uncertainties

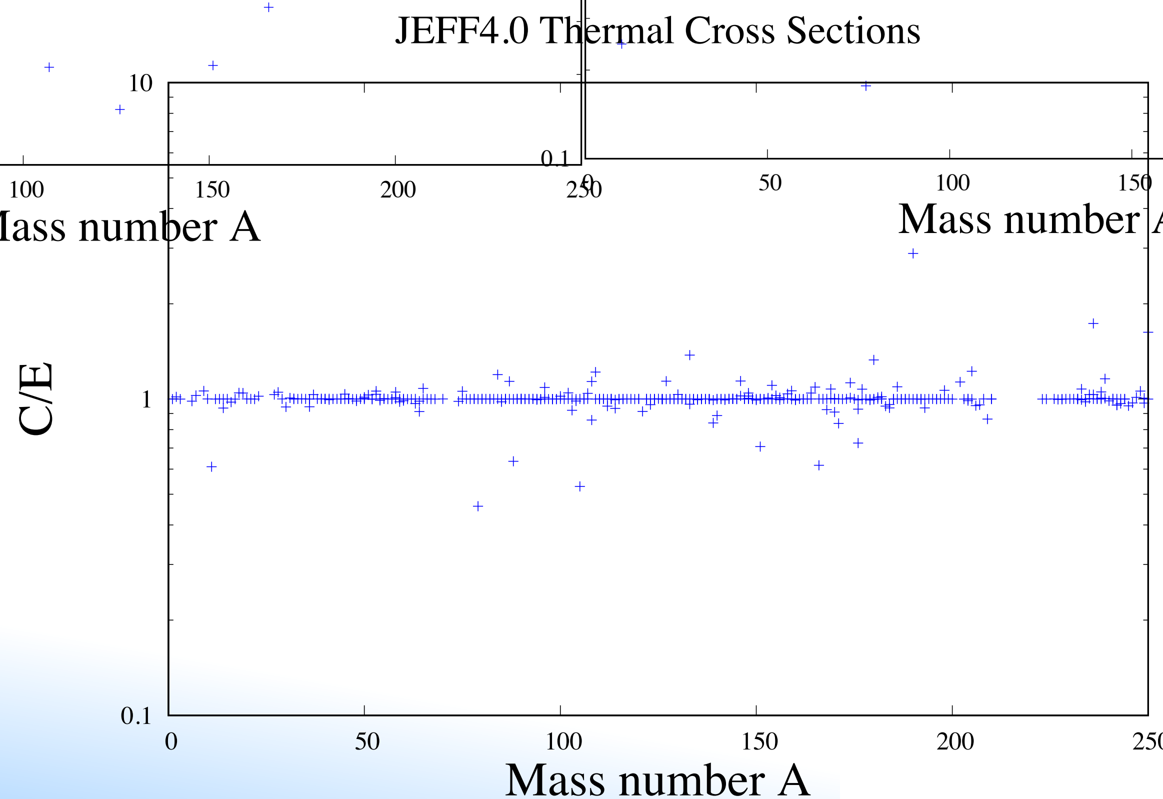
$$x = \frac{\sigma^i_{\rm th} - \sigma^i_{\rm exp}}{\delta\sigma^i_{\rm exp}}$$

Compare all world NDL's to a cleaned-up EXFOR. Continue until TENDL is equally good or better

NDL's versus Atlas-2016 thermal capture cross sections

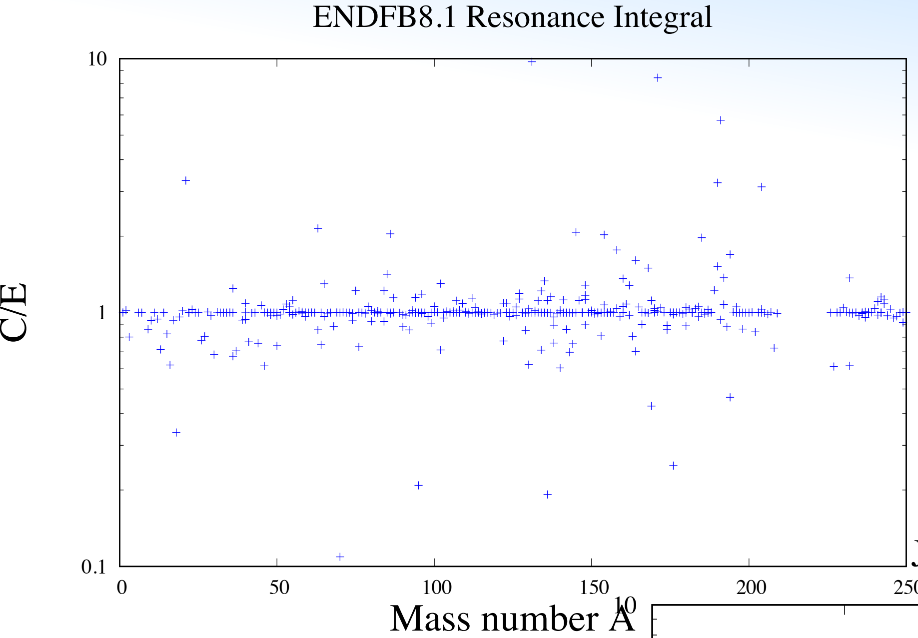


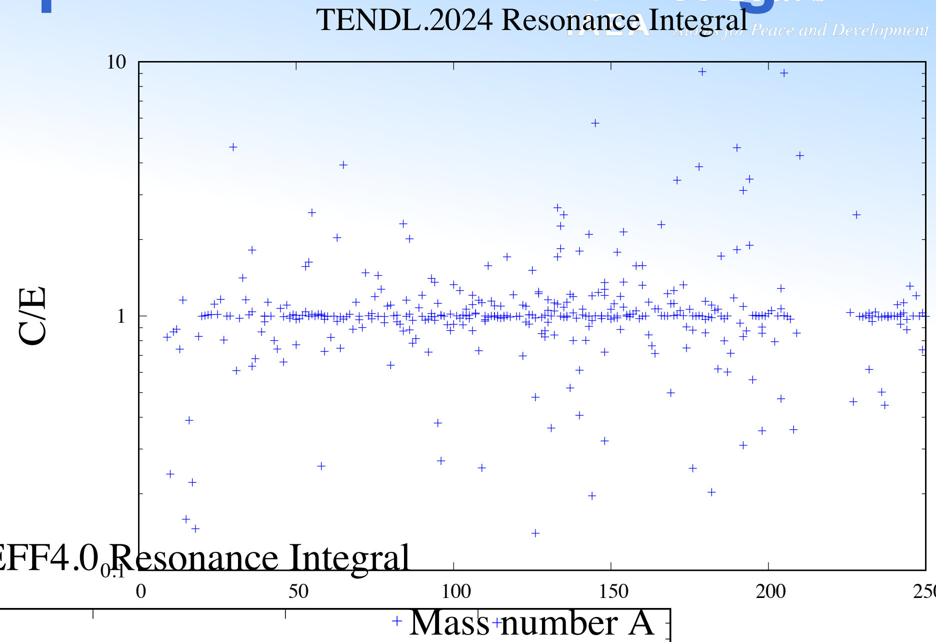


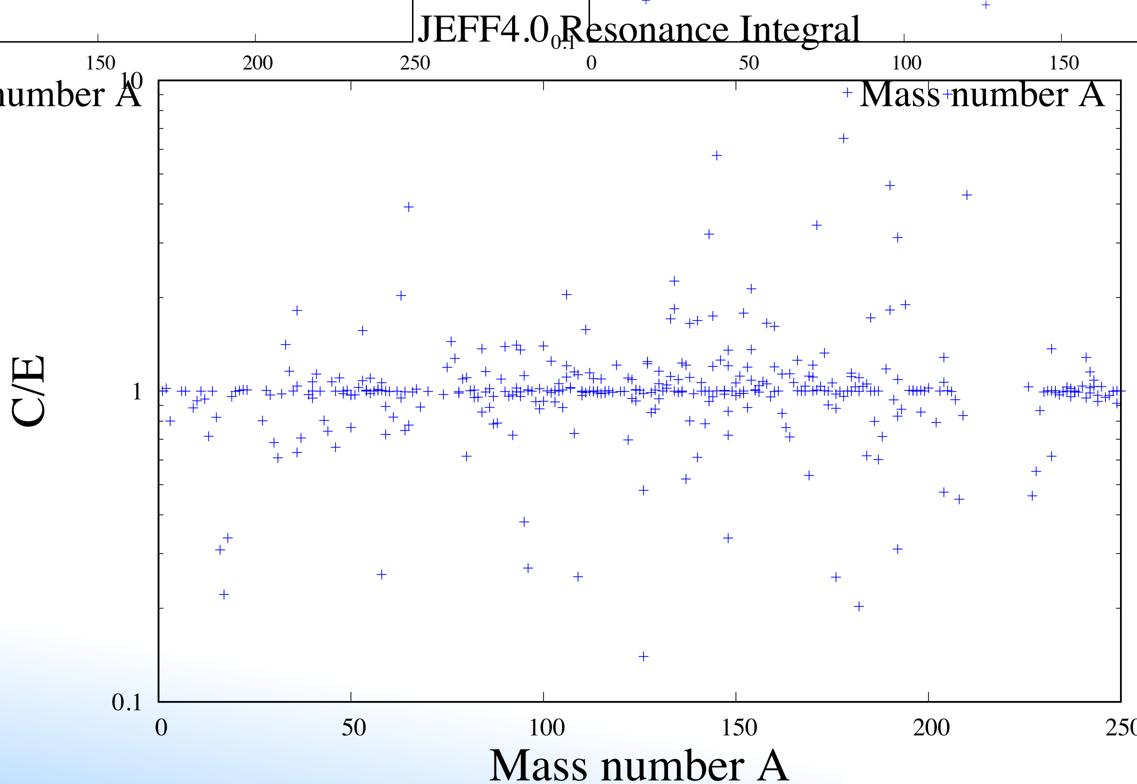


	Frms
CENDL-3.2:	1.034
JENDL-5.0:	1.020
ENDF/B8.1:	1.021
TENDL-2024:	1.011
JEFF-3.3:	1.024
JEFF-4.0:	1.015

NDL's versus Atlas-2016 capture resonance integrals

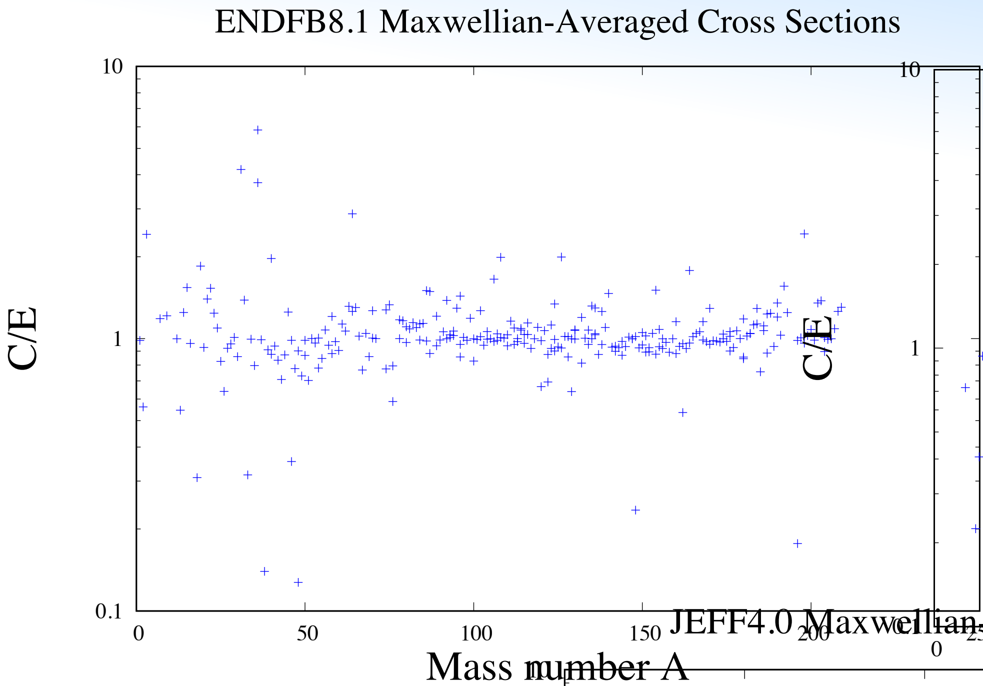


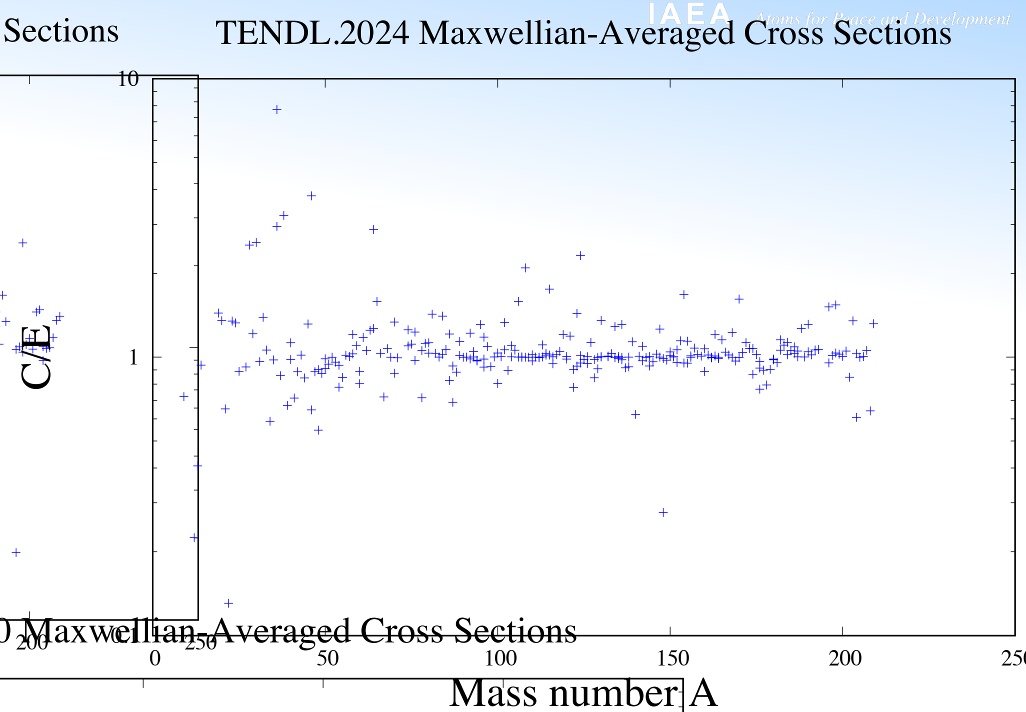


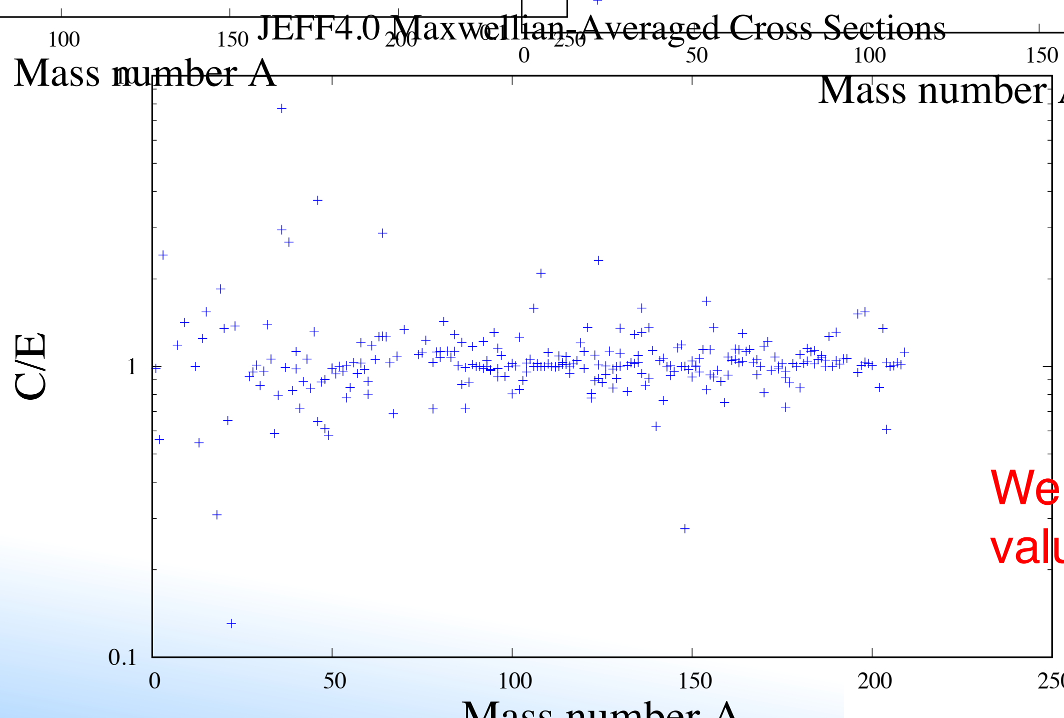


	Frms
CENDL-3.2:	1.034
JENDL-5.0:	1.038
ENDF/B8.1:	1.030
TENDL-2024:	1.045
JEFF-3.3:	1.038
JEFF-4.0:	1.043

NDL's versus Astral/Kadonis MACS at 30 keV







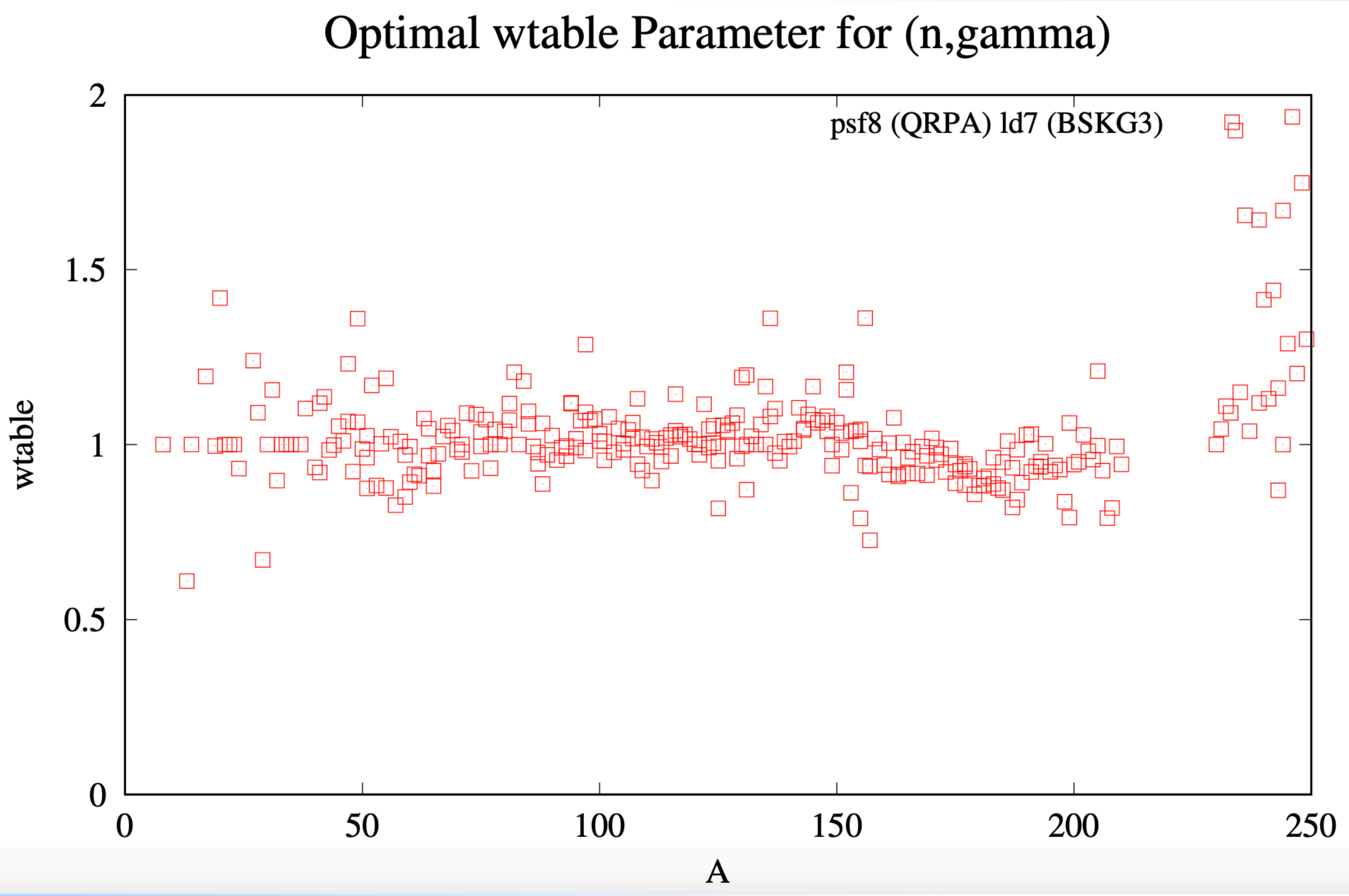
	Frms
CENDL-3.2:	1.069
JENDL-5.0:	1.064
ENDF/B8.1:	1.064
TENDL-2024:	1.052
JEFF-3.3:	1.076
JEFF-4.0:	1.062

We don't believe 9 values in Kadonis

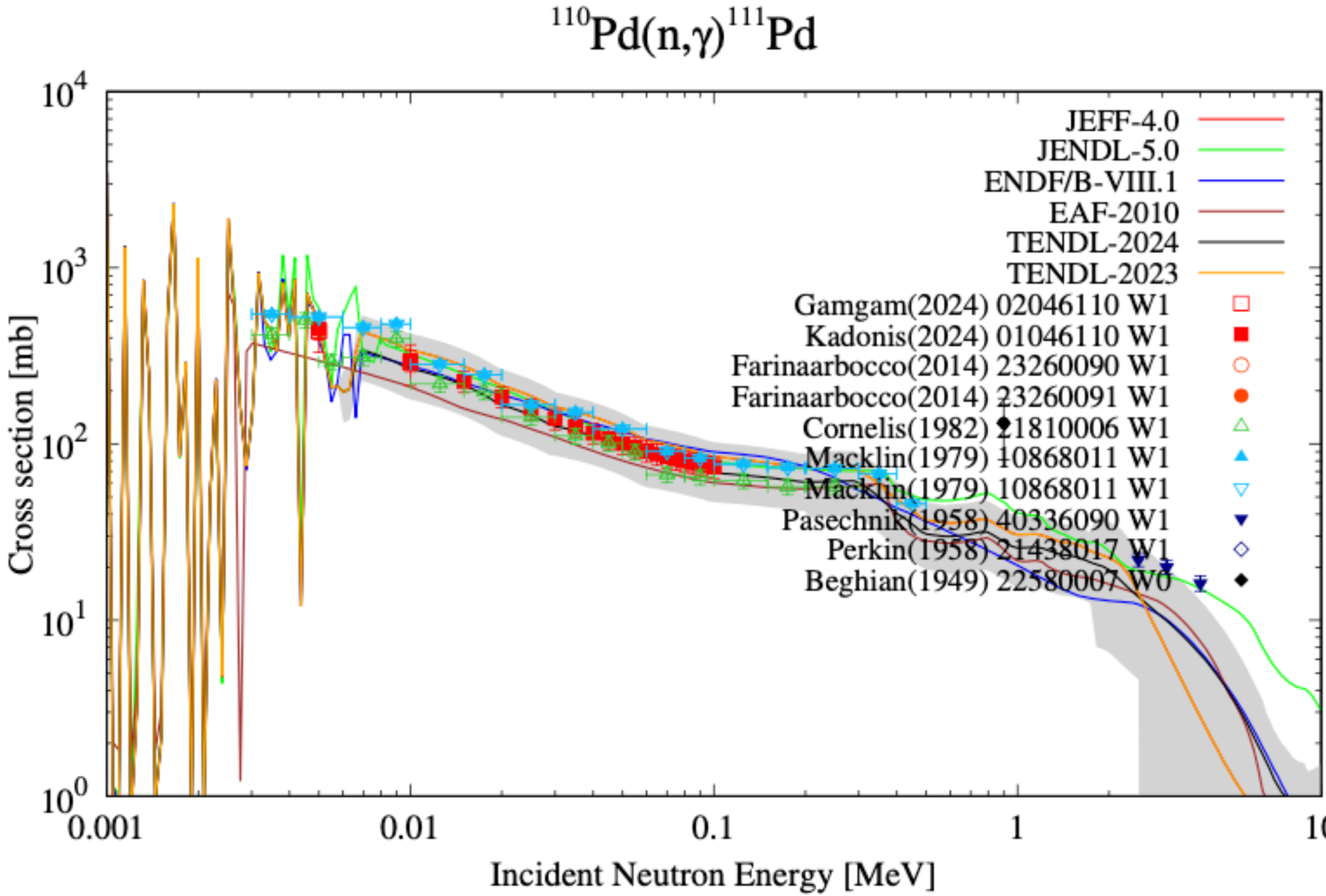
Parameter optimisation in fast range

- Use TASMAN for parameter optimisation
  - Multi-dimensional parameter landscape not too wild
  - 20 TALYS runs per parameter
  - Optimisation per level density model (i.e. LD parameters unchanged)
- (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

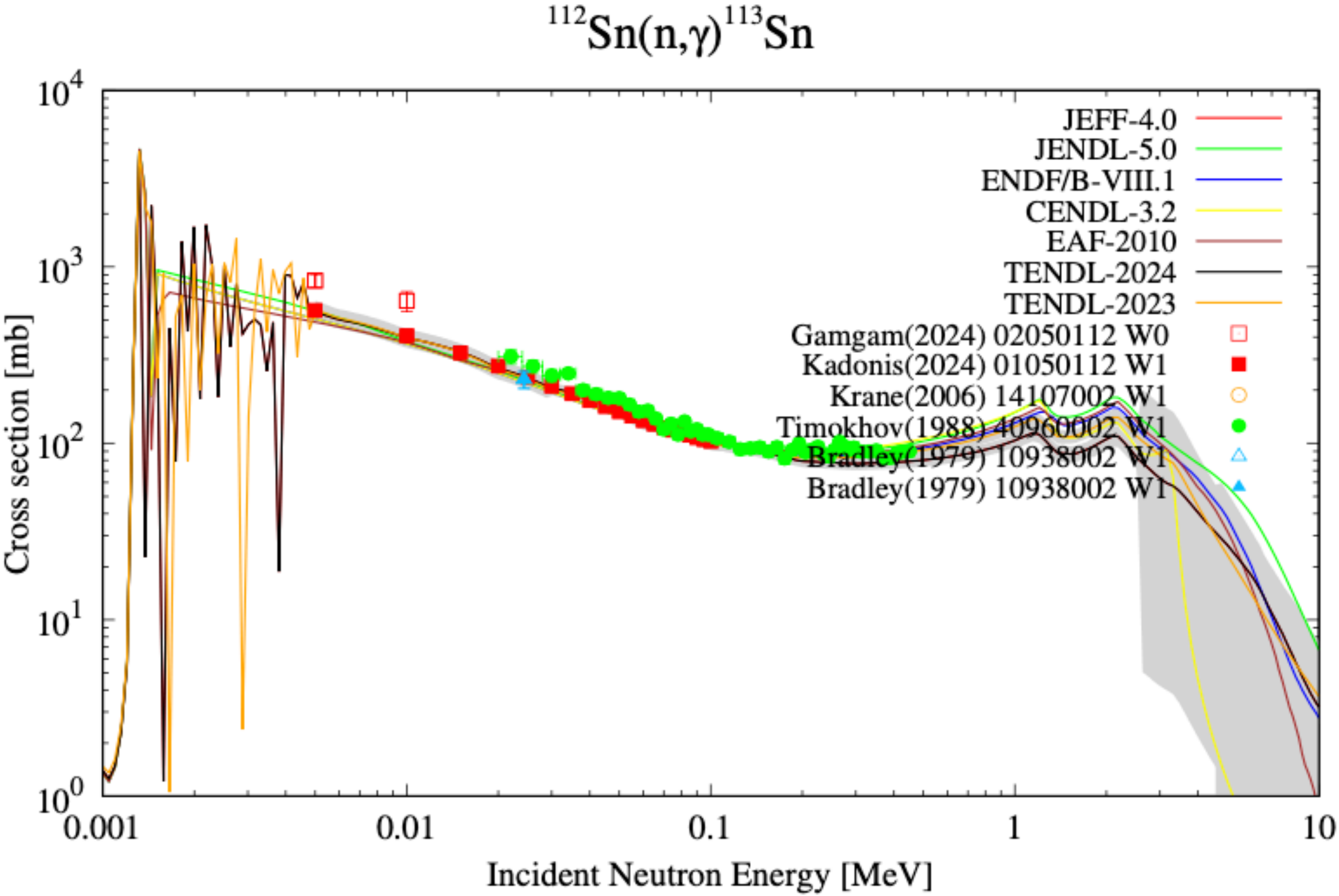
Current optimal combination of level density and photon strength function

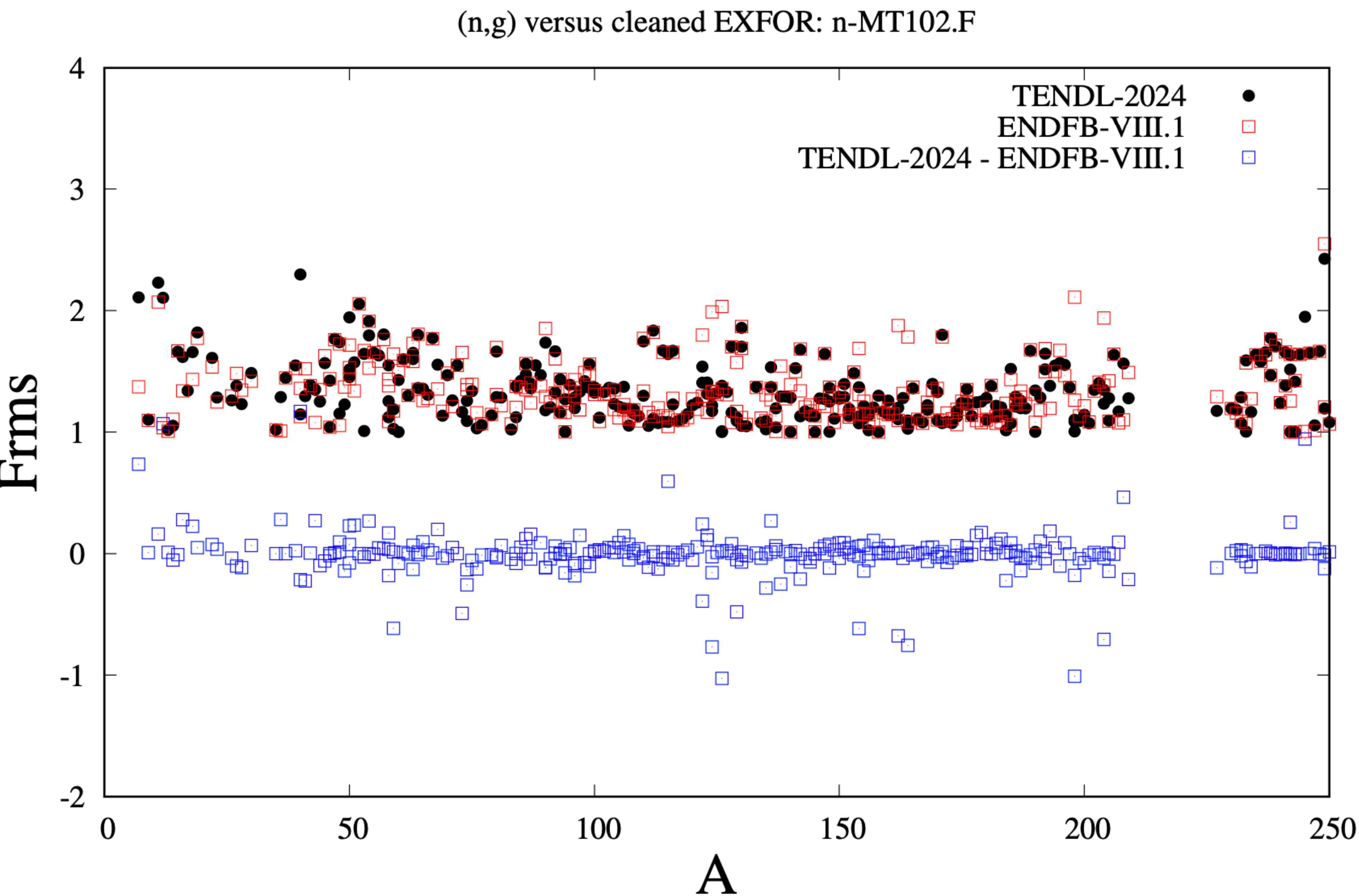


Usually: (n,γ) cross sections, MACS and Γγ are consistent

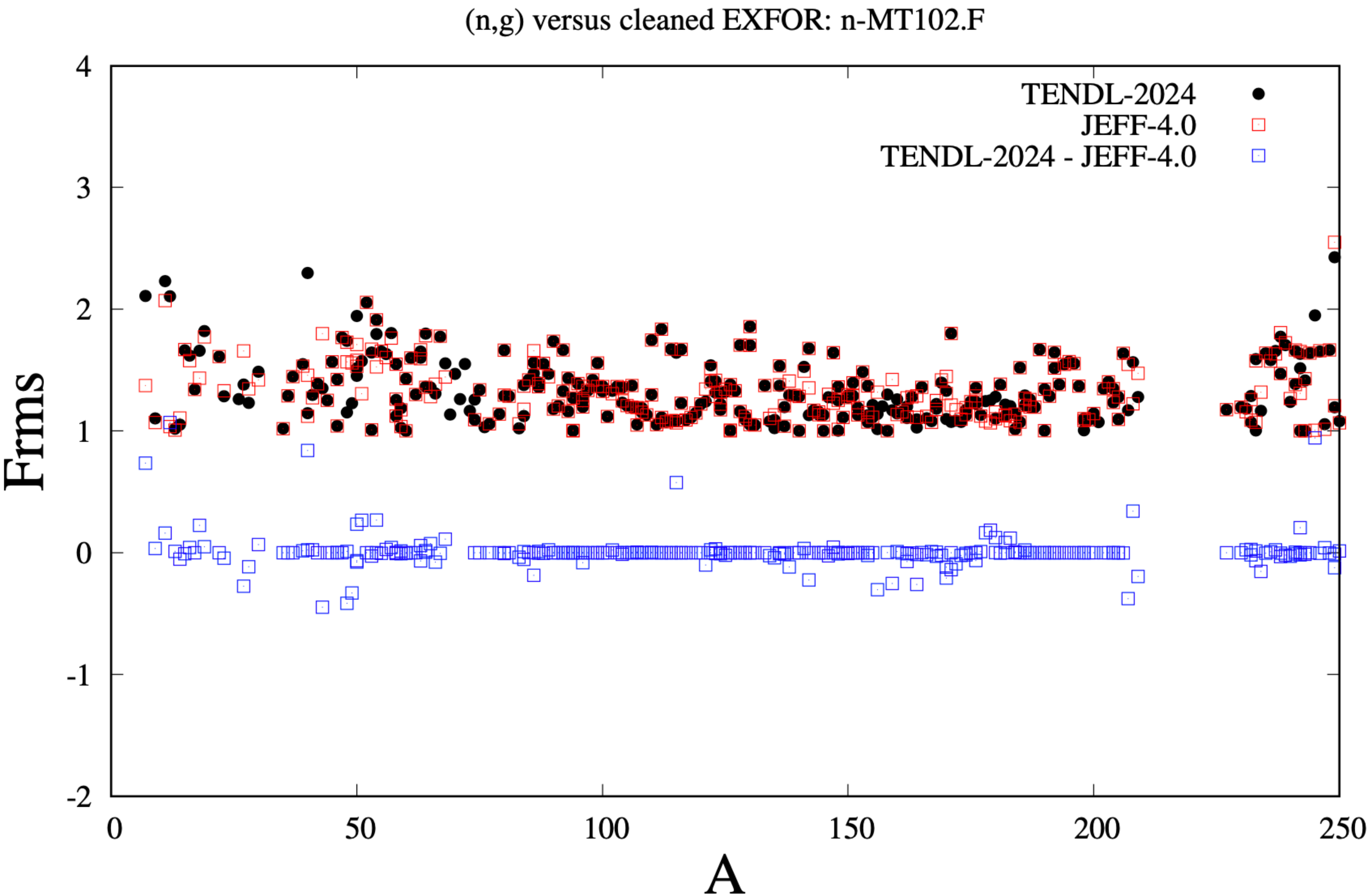


Average radiative width Γγ considered outlier



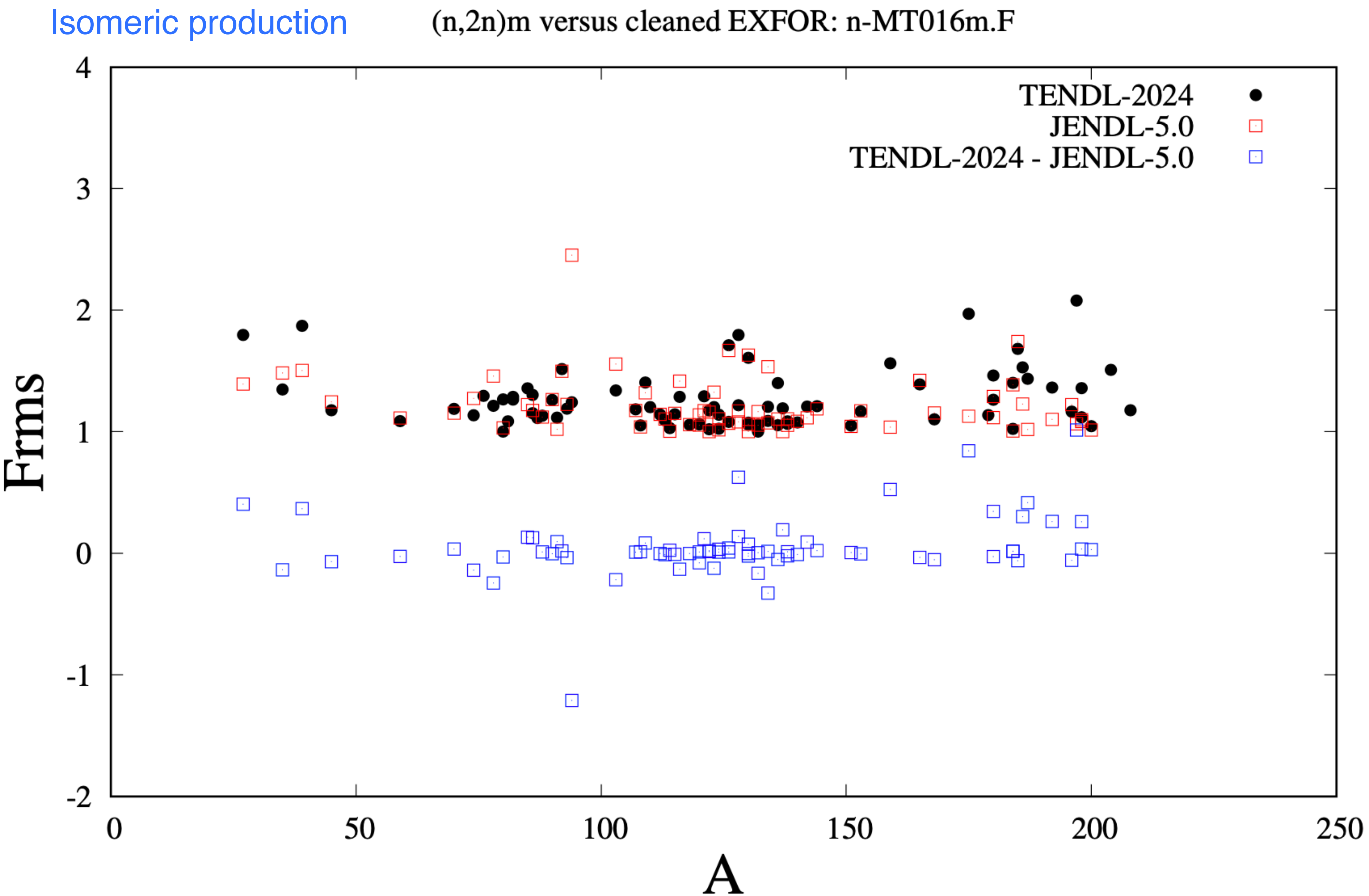


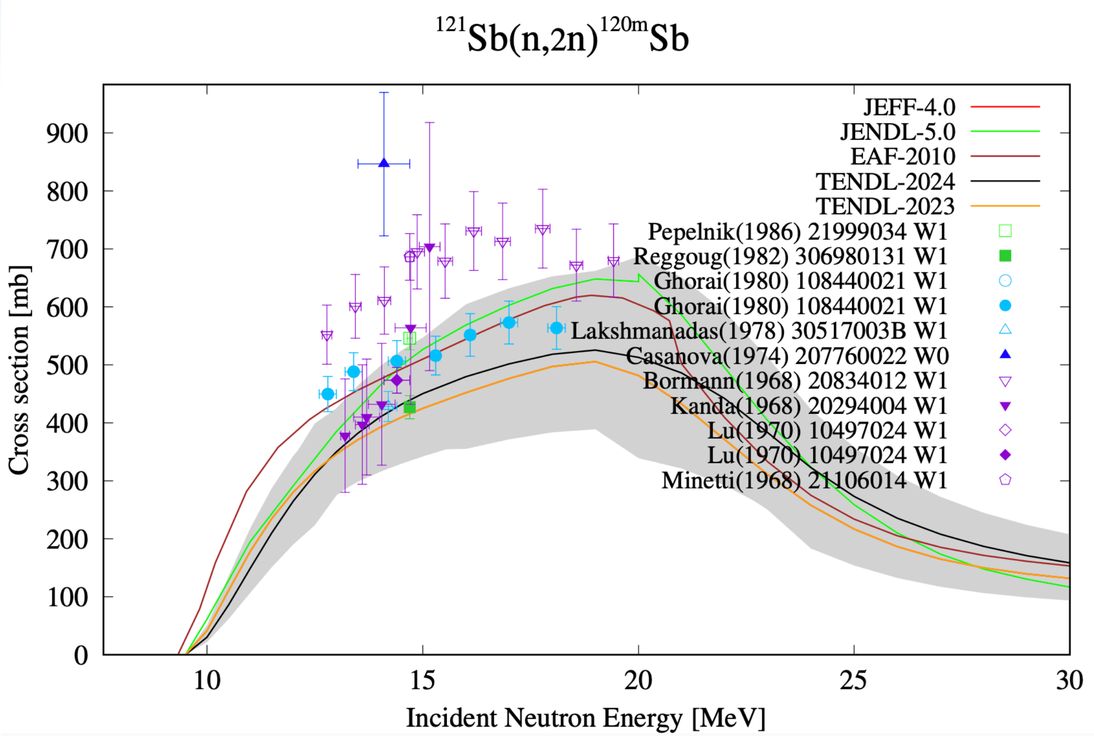
(n,g) versus cleaned EXFOR: n-MT102.F
TENDL-2024
ENDFB-VIII.1
TENDL-2024 - ENDFB-VIII.1
Frms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250



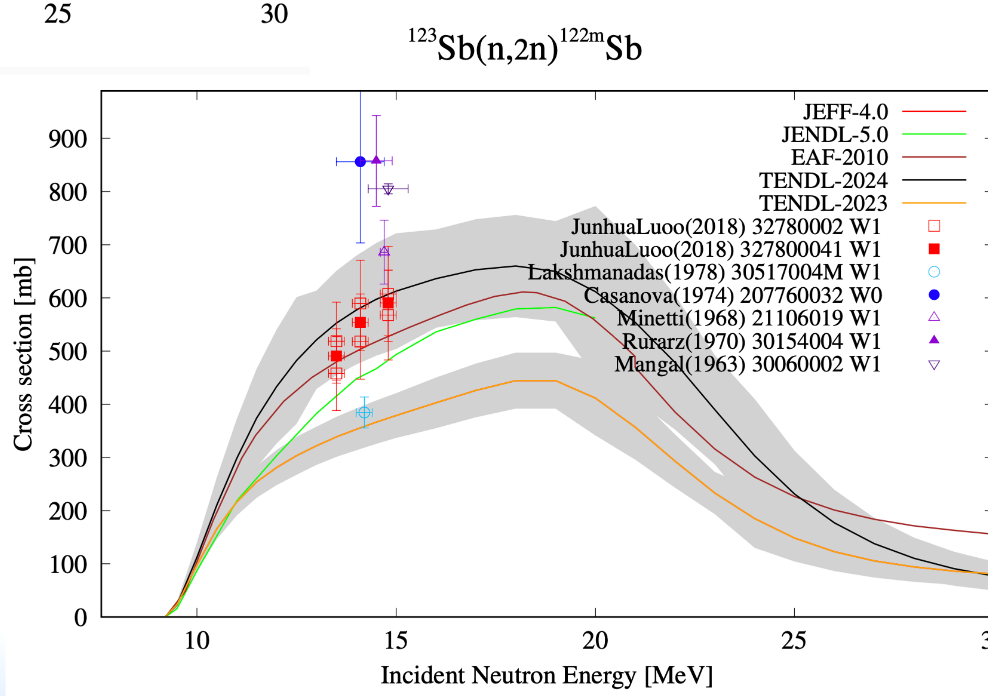
(n,g) versus cleaned EXFOR: n-MT102.F
TENDL-2024
JEFF-4.0
TENDL-2024 - JEFF-4.0
Frms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250

Isomeric production

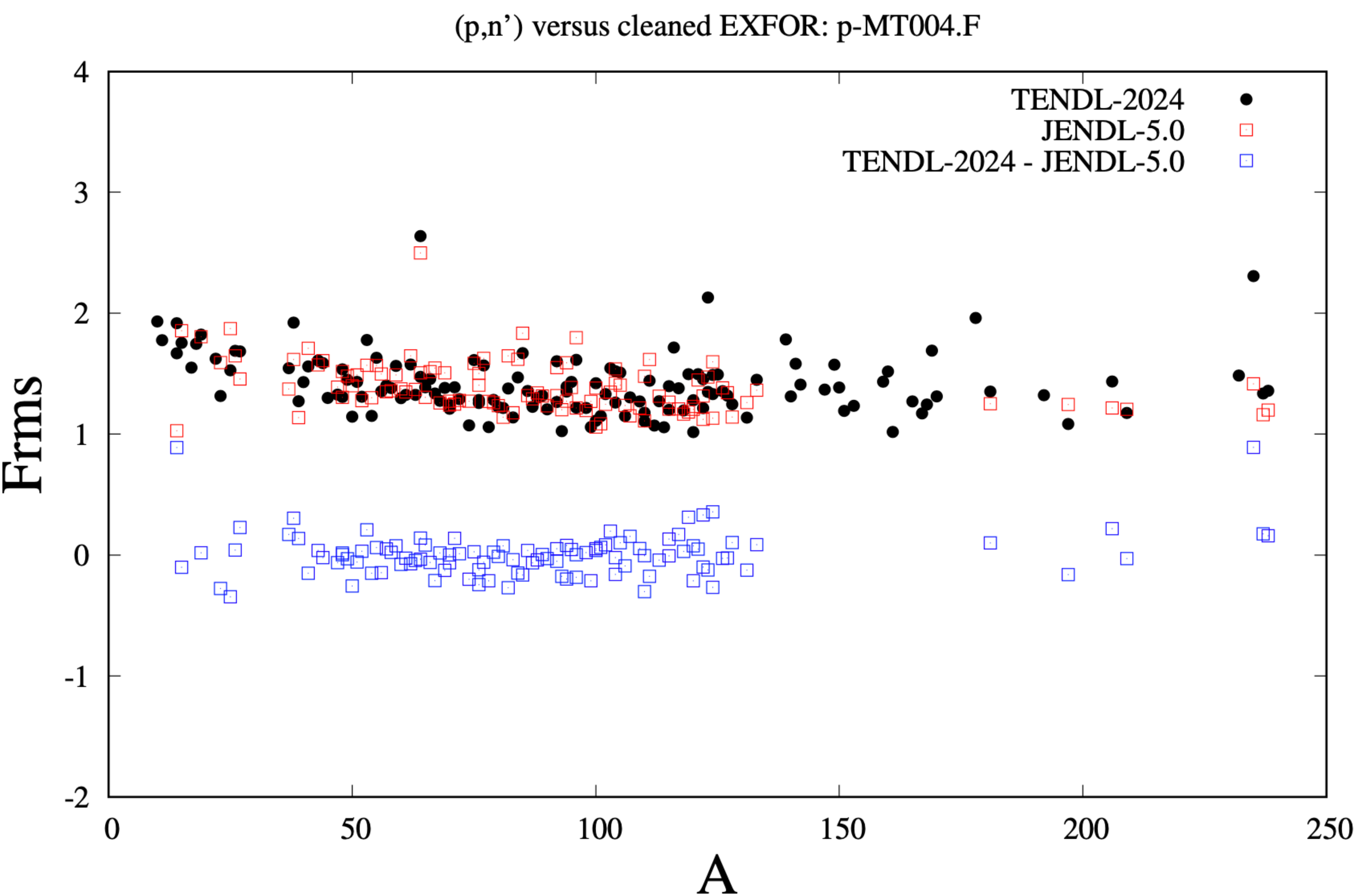




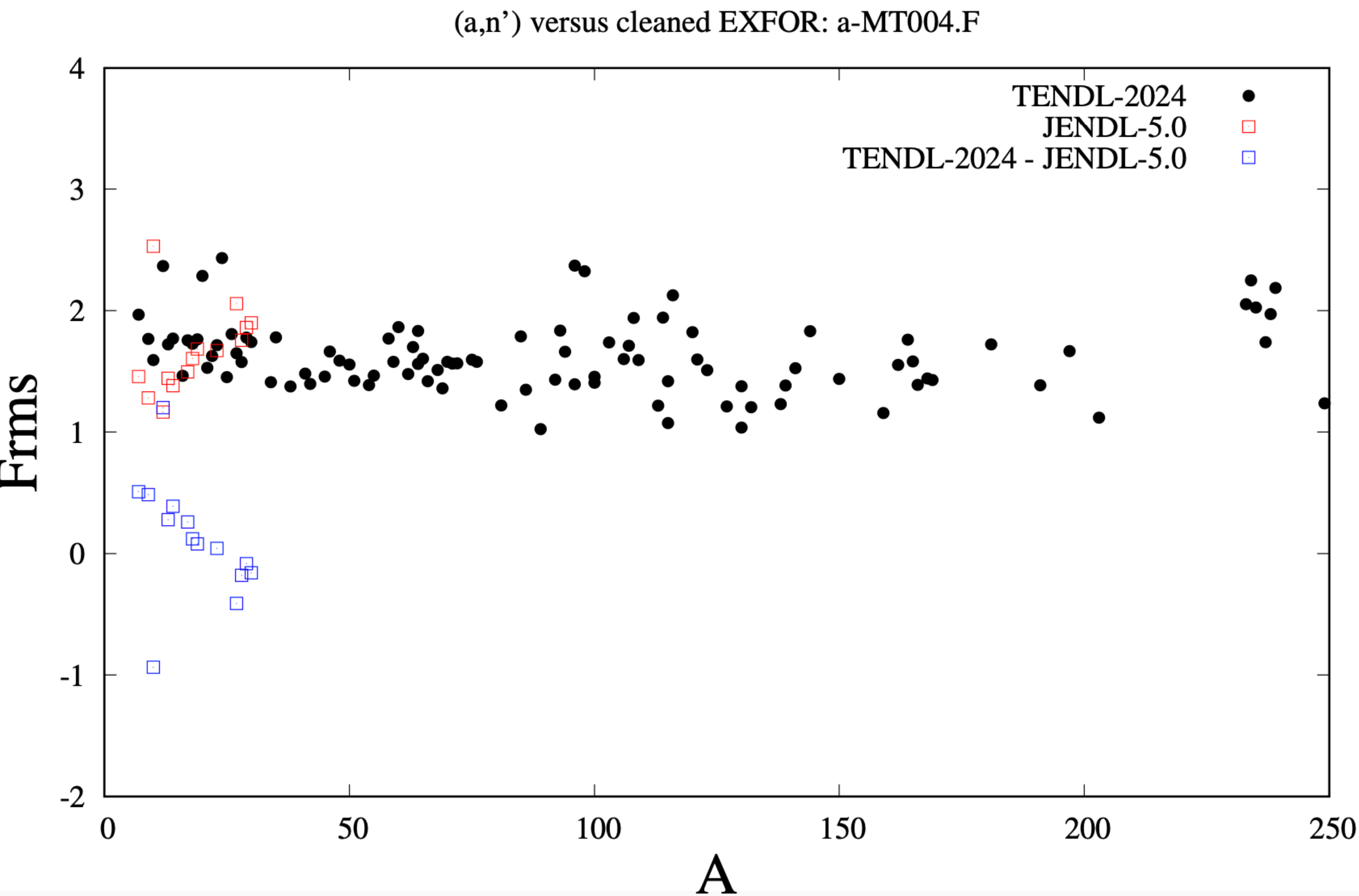
JENDL better



TENDL better

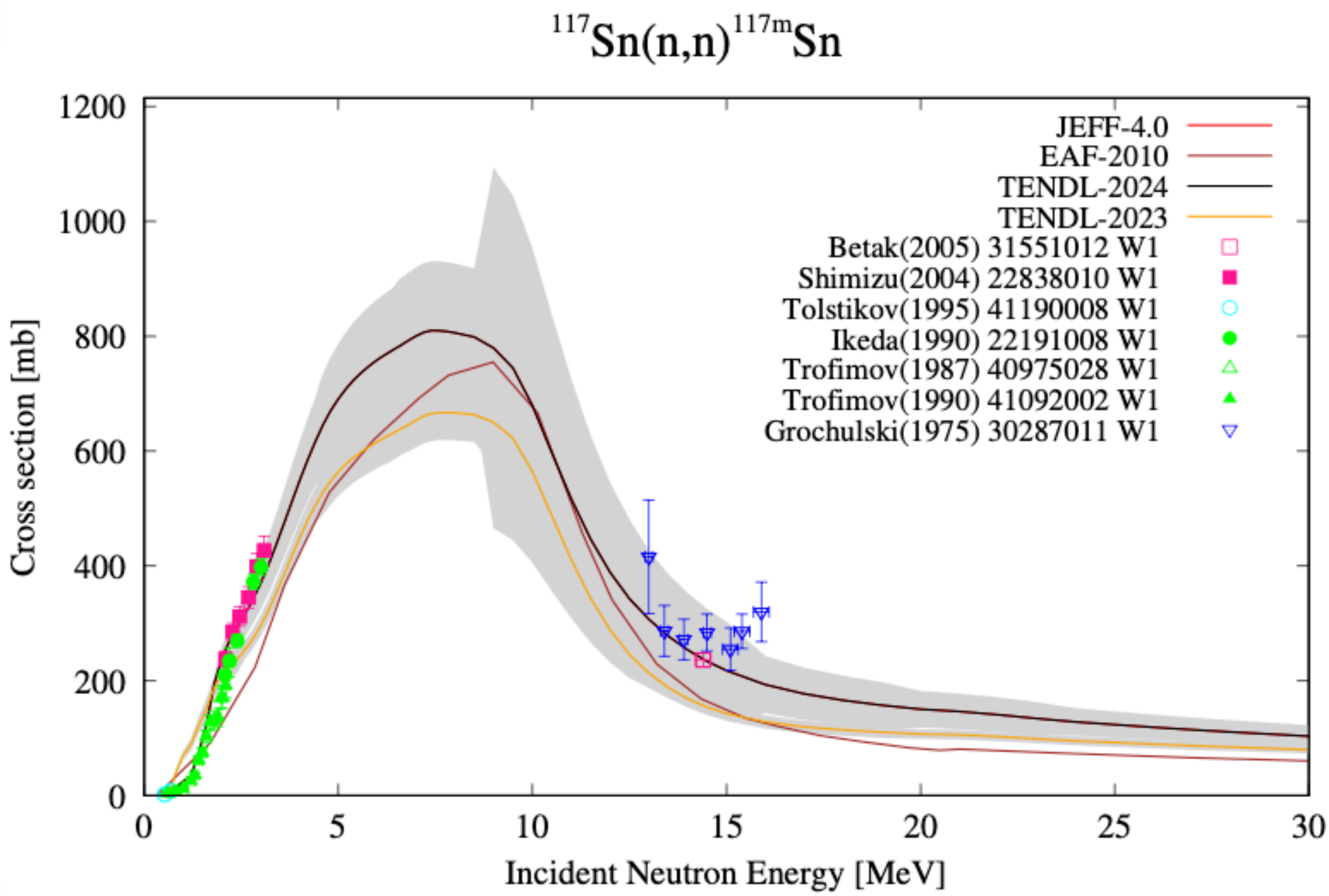


(p,n') versus cleaned EXFOR: p-MT004.F
TENDL-2024
JENDL-5.0
TENDL-2024 - JENDL-5.0
Frms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250


(a,n') versus cleaned EXFOR: a-MT004.F
TENDL-2024
JENDL-5.0
TENDL-2024 - JENDL-5.0
Frms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250

TALYS and all satellite software now use YANDF (Yet Another Nuclear Data Format)

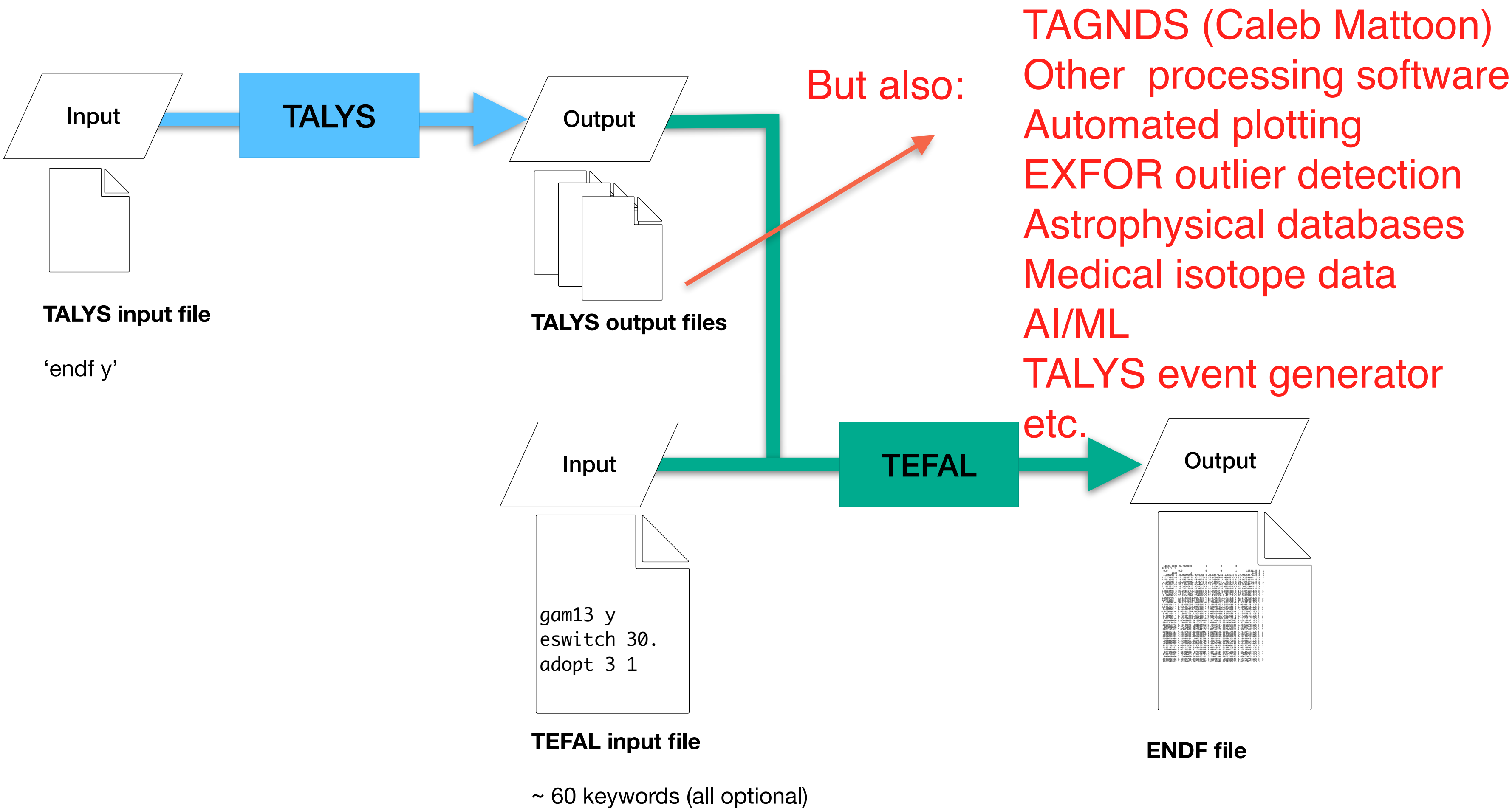
```
# header:
#   title: Th232(n,g)Th233 cross section
#   source: TALYS-2.1
#   user: Arjan Koning
#   date: 2025-05-27
#   format: YANDF-0.3
# target:
#   Z: 90
#   A: 232
#   nuclide: Th232
# reaction:
#   type: (n,g)
#   Q-value [MeV]:  4.786385E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 3
#   ENDF_MT: 102
# residual:
#   Z: 90
#   A: 233
#   nuclide: Th233
# quantity:
#   type: cross section
#   datablock:
#     columns: 4
#     entries: 31
##       E              xs           gamma_xs     xs/res.prod.xs
##     [MeV]           [mb]           [mb]            []
   1.000000E-11   3.691955E+05   1.553648E+06   1.000000E+00
   2.530000E-08   7.340001E+03   3.088819E+04   1.000000E+00
   2.000000E-07   2.610606E+03   1.098595E+04   1.000000E+00
   1.000000E-06   1.393251E+05   5.863077E+05   1.000000E+00
   1.000000E-05   3.832905E+04   1.612982E+05   1.000000E+00
```



Malec, Trkov: important dosimetry reaction

TALYS applications

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

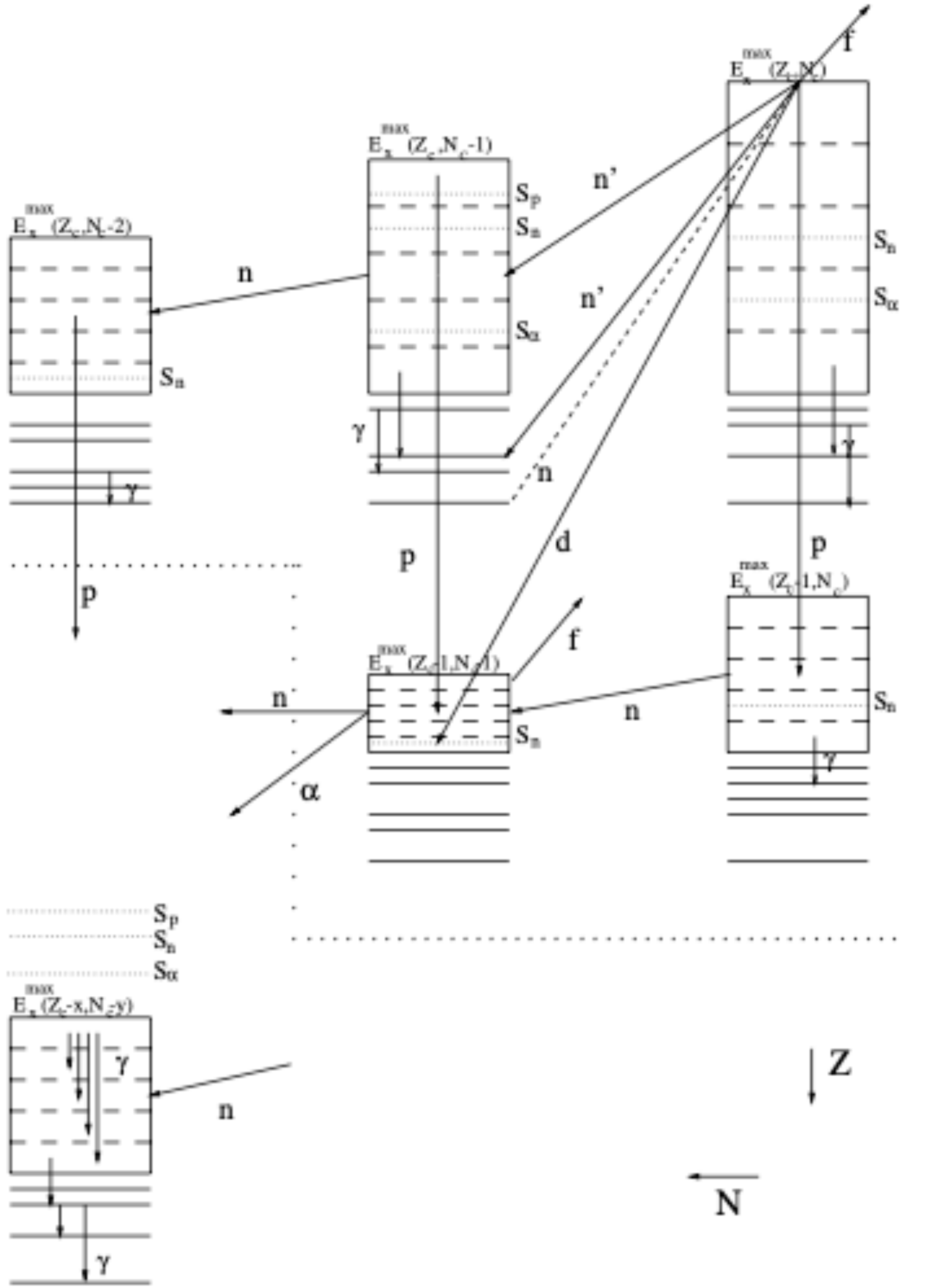


This is the TENDL library in ENDF format

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 (Krticka)
  - Give all resonance parameter databases in human/modern readable format: Atlases, all NDL's (again: TARES code)
- Finalising EXFOR outlier identification
- 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
- Publish all TALYS sensitivity profiles and covariance matrices in YANDF. Possibly extend to cross-isotope correlations. Connect further to LLNL Deep learning approach (Wendt et al) with VAE.
- 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 and codes like GEANT4, PHITS etc.

TALYS event generator



Store probabilities instead of cross sections, spectra etc. In YANDF format

Skip ENDF altogether

One (large) probability table per event: projectile at one incident energy on a nuclide

Verify that it gives ‘normal’ TALYS results after MC sampling

CGMF-like (LANL) but now for entire reaction

Normalize low energy data with existing ENDF libraries

Retain all possible correlations

Feed directly into the MC codes that are ready for this

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Thank you!

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)