IAEA 60 Years
Atoms for Peace and Development

The TENDL library: Progress, success and lessons learned

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ND-2022, July 24-29 2022, Sacramento, USA (virtual)

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  - Fast neutron range: new photon strength functions from IAEA CRP
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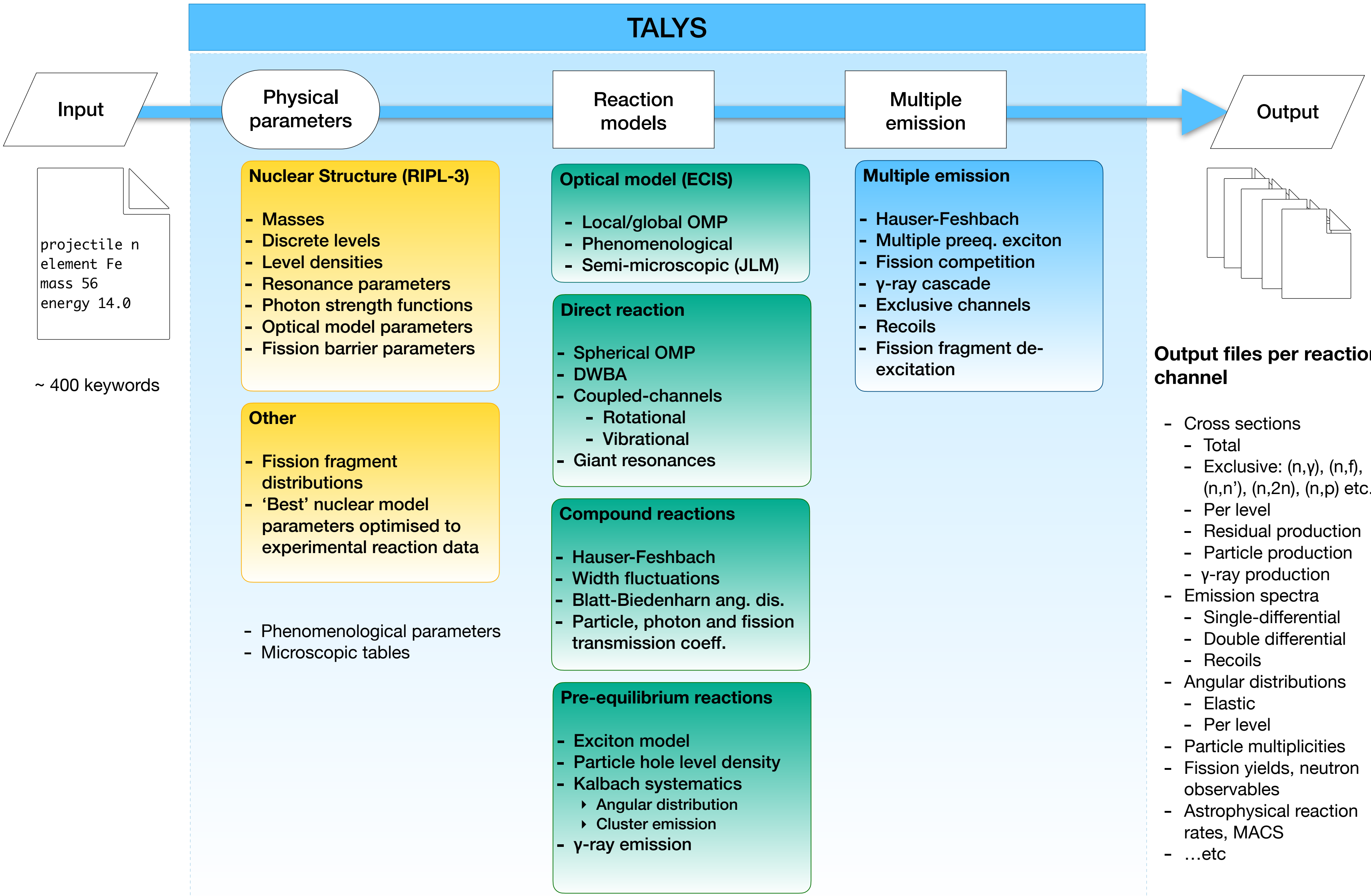
TALYS-1.96/TALYS-2.0

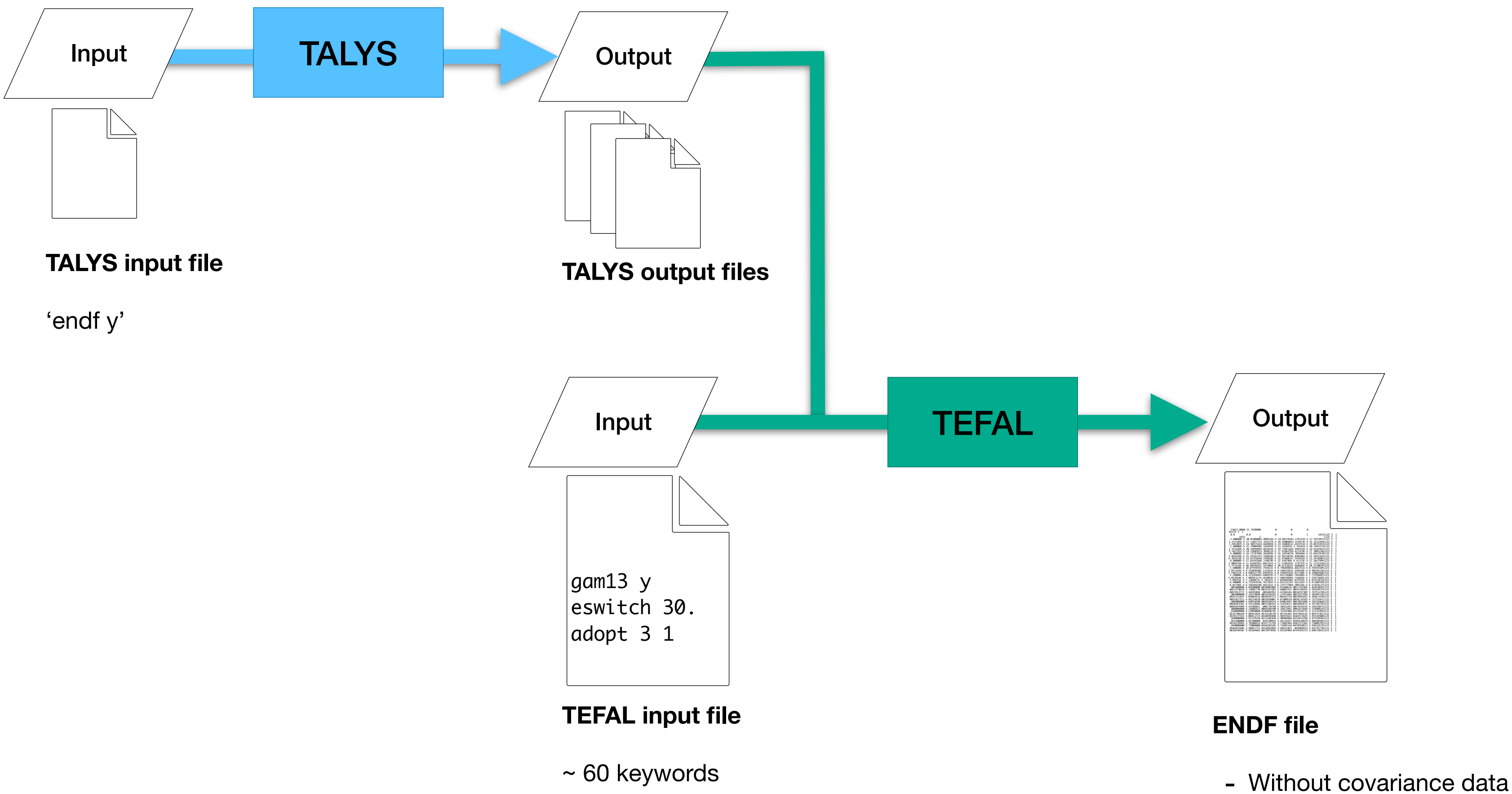
- Some important new features since TALYS-1.95 (Dec 2019)
  - Explicit evaporation of fission fragments via Hauser-Feshbach: FY, nubar, nu(A), PFNS, etc.
  - Latest photon strength function models from IAEA CRP: SMLO, QRPA, M1 PSF with low energy upbend (Stephane Goriely)
  - Ability to use RIPL optical models for actinides
  - Improved deuteron break-up model by M. Avrigeanu
  - Good global description of subactinide and charged-particle induced fission cross sections
  - Phenomenological descriptions of nubar (Wahl) and PFNS (Iwamoto)
- TALYS-1.96 was released 30 December 2021, TALYS-2.0 not yet



TALYS
Input
Physical parameters
Reaction models
Multiple emission
Output
projectile n
element Fe
mass 56
energy 14.0
~ 400 keywords
Nuclear Structure (RIPL-3)
- Masses
- Discrete levels
- Level densities
- Resonance parameters
- Photon strength functions
- Optical model parameters
- Fission barrier parameters
Other
- Fission fragment distributions
- 'Best' nuclear model parameters optimised to experimental reaction data
- Phenomenological parameters
- Microscopic tables
Optical model (ECIS)
- Local/global OMP
- Phenomenological
- Semi-microscopic (JLM)
Direct reaction
- Spherical OMP
- DWBA
- Coupled-channels
- Rotational
- Vibrational
- Giant resonances
Compound reactions
- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.
Pre-equilibrium reactions
- Exciton model
- Particle hole level density
- Kalbach systematics
Angular distribution
Cluster emission
- γ-ray emission
Multiple emission
- Hauser-Feshbach
- Multiple preeq. exciton
- Fission competition
- γ-ray cascade
- Exclusive channels
- Recoils
- Fission fragment de-excitation
Output files per reaction channel
- Cross sections
- Total
- Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
- Per level
- Residual production
- Particle production
- γ-ray production
- Emission spectra
- Single-differential
- Double differential
- Recoils
- Angular distributions
- Elastic
- Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …etc

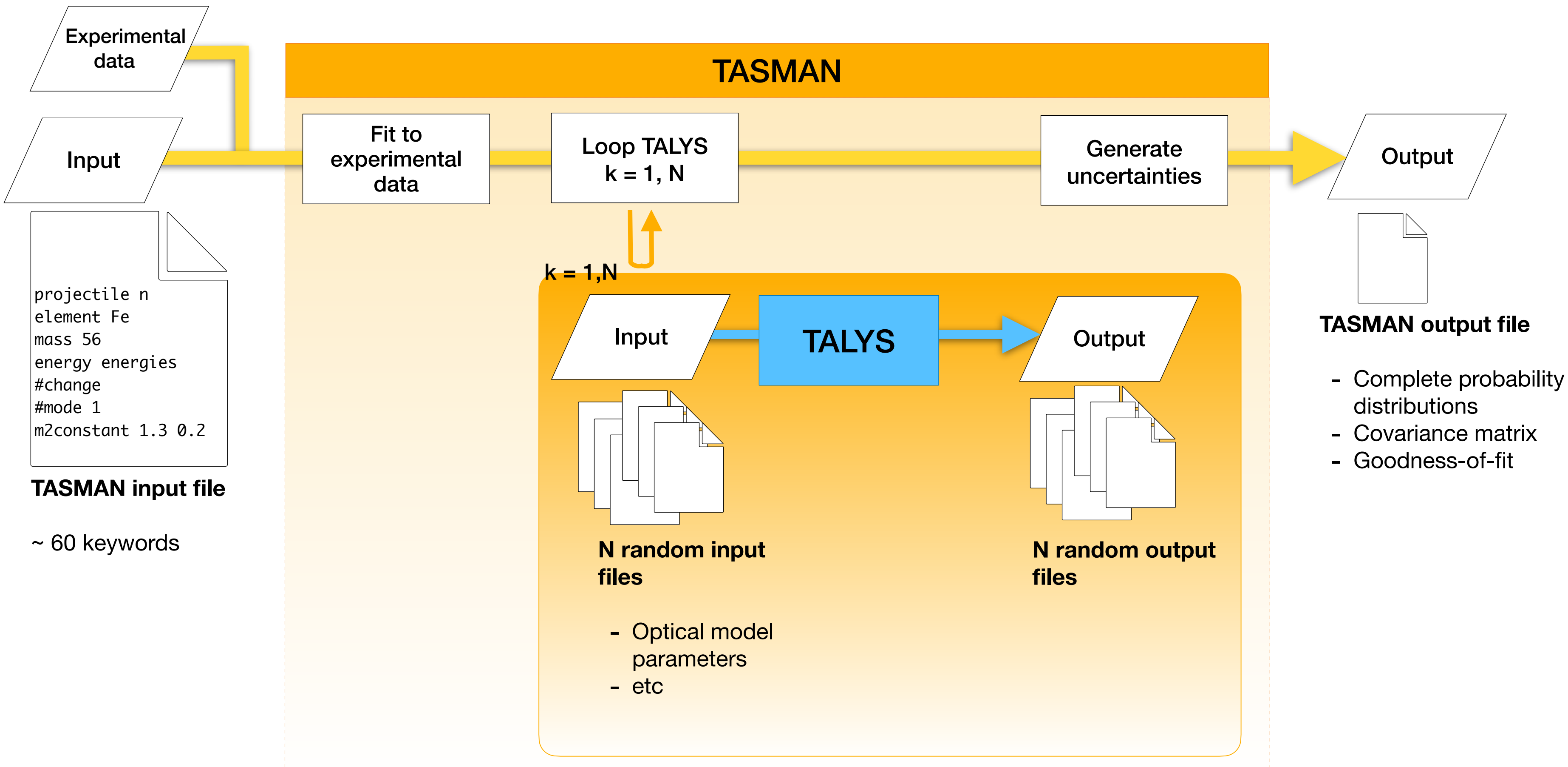
TEFAL + TALYS

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



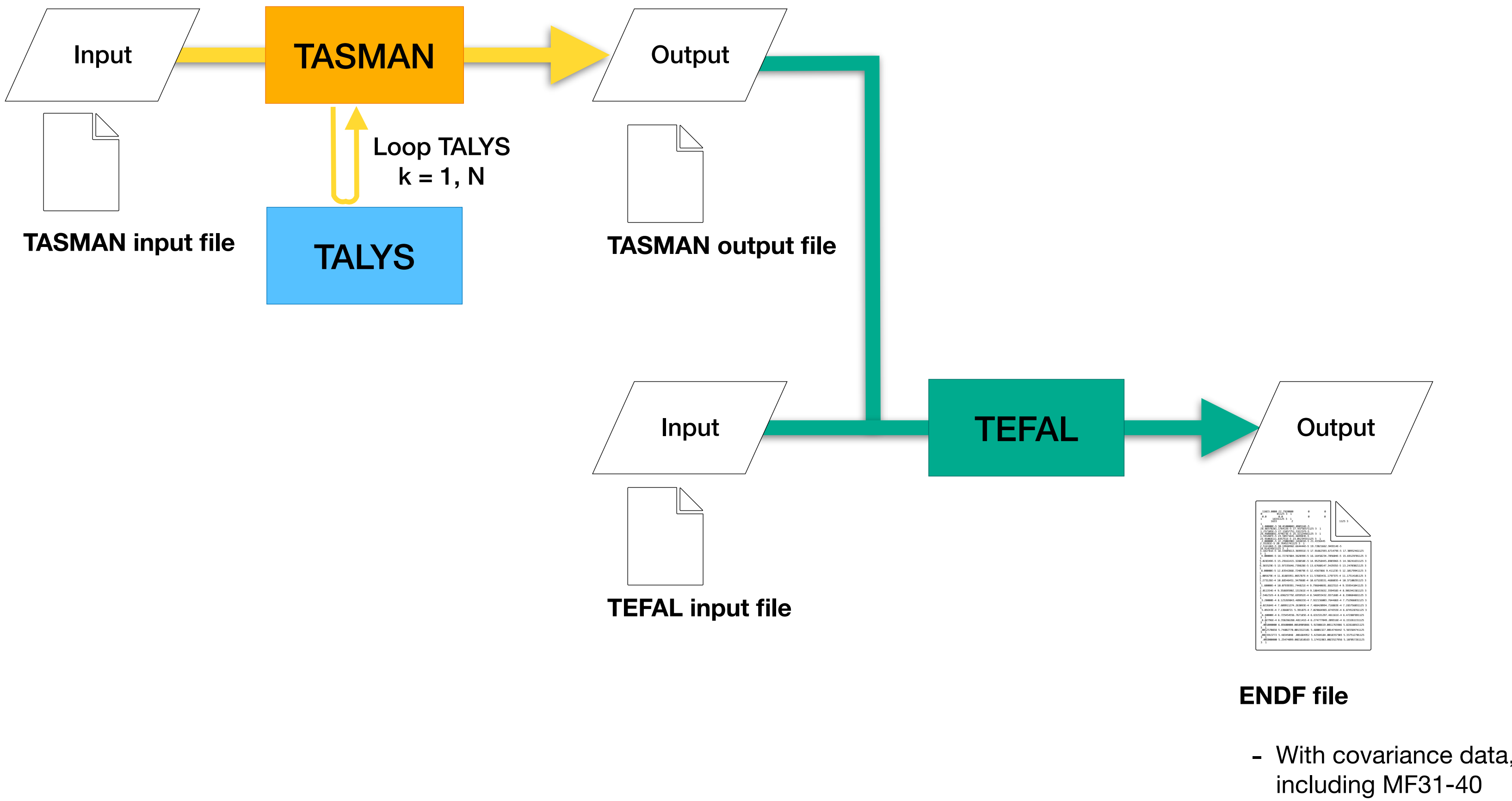
TASMAN + TALYS

- TASMAN produces uncertainty distributions based on random input/output files of TALYS
- TASMAN automatically fits TALYS to experimental reaction data



TASMAN + TALYS + TEFAL 1: Covariance data

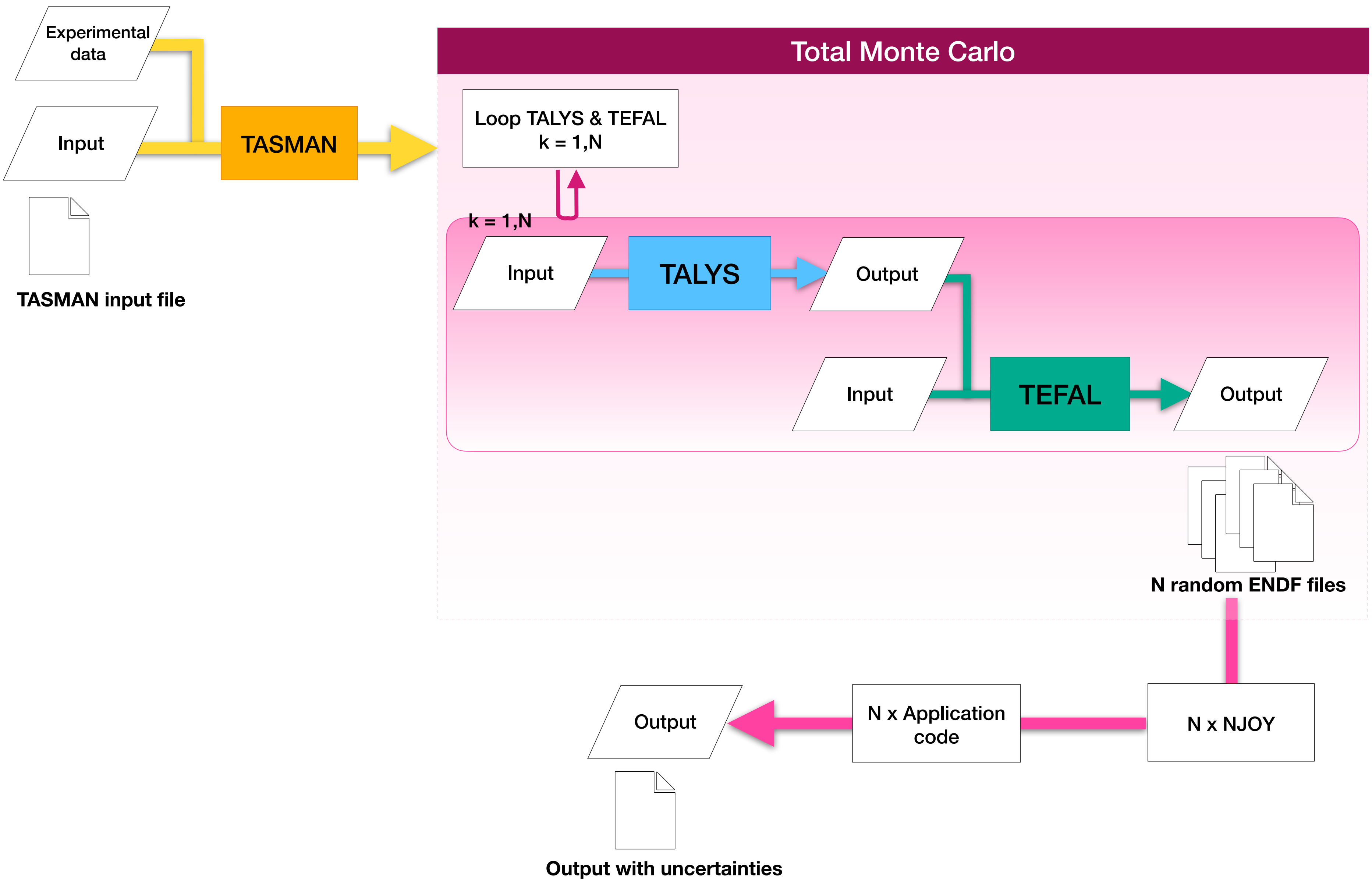
- TASMAN generates random input N times and runs TALYS



Loop the above over all nuclides = TENDL

TASMAN + TALYS + TEFAL 2: Total Monte Carlo

- TASMAN generates random input N times and runs TALYS and TEFAL for each ‘k’



TENDL: TALYS Evaluated Nuclear Data Library

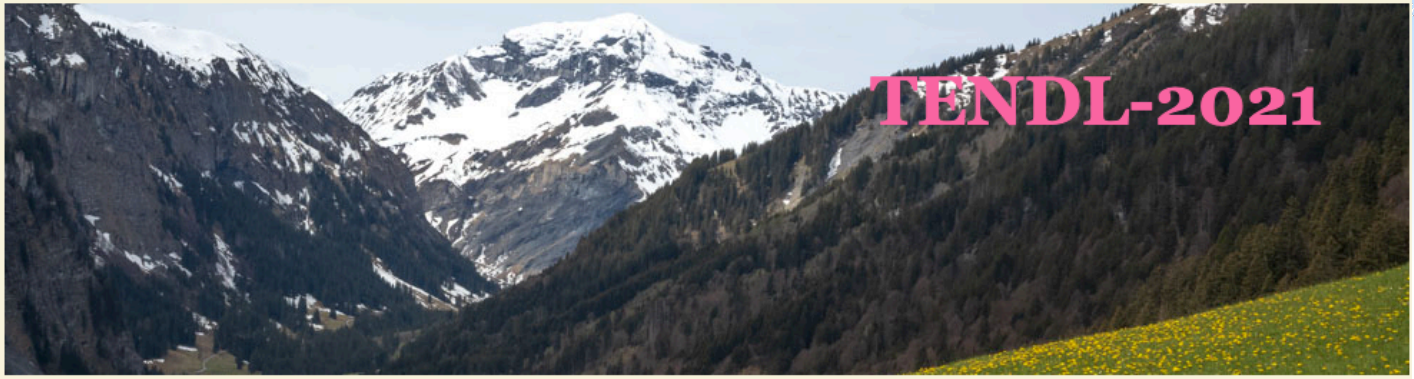
- General purpose nuclear reaction data library
- Simultaneous focus on
  - Reproducibility ✓
  - Completeness ✓
  - Quality (ongoing, never enough)
- TENDL ranges from detailed experiment-based evaluations to global TALYS calculations
- Extent:
  - Neutrons, photons, protons, deuterons, tritons, Helium-3, alpha-particles
  - TSL, astrophysical reaction rates (new), FY
  - 2813 nuclides (all stable or with half-life > 1 sec.)
  - 0-200 MeV
  - All cross sections and secondary distributions (particle and gamma spectra)
  - UQ with covariances or statistical distributions (Total Monte Carlo, “random files”)
  - A variety of data formats: ENDF, PENDF, ACE, GNDS, HDF5, ASCII

- TENDL-2021 was released in December 2021
- https://tendl.web.psi.ch/tendl_2021/tendl2021.html

TALYS-based evaluated nuclear data library

Years

or Peace and Development



"We believe that our great goal can be achieved with systematism and reproducibility. We are so outside the box, that the box is a point"

How to reference

Sub-library files

1. Neutron
2. Proton
3. Deuteron (updated)
4. Triton
5. He3
6. Alpha
7. Gamma
8. Fission yields
9. Thermal scattering
10. For astrophysics

Application libraries & tar files (ENDF, GND, ACE, PENDF...)

V&V

1. FISPACT-II reports
2. FISPACT-II validation

Total Monte Carlo files

3. Random ENDF-6 files from other libraries
4. Random ACE files based on ENDF/B-VII.1
5. Random ACE files based on TENDL
6. Random ENDF files based on TENDL

TENDL-2021: (release date: December 30, 2021)

Last update: February 23, 2022

TENDL is a nuclear data library which provides the output of the **TALYS** nuclear model code system for direct use in both basic physics and applications. The 11th version is **TENDL-2021**, which is based on both default and adjusted **TALYS** calculations and data from other sources (previous releases can be found here: 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2017 and 2019).

Up to 2014, TENDL was produced at NRG Petten. Since 2015, TENDL is mainly developped at PSI and the IAEA (Nuclear Data Section). Still, many people contribute to TENDL with the testing and processing of the files.

TENDL contains evaluations for seven types of incident particles, for all isotopes living longer than 1 second: Z=1 ^{1}H to Z=115 ^{291}Mc (about 2800 isotopes), up to 200 MeV, with covariances.

TENDL is **not** a default or shadow library. Not a single neutron evaluation is based on default calculations. With the HFR approach, all resonances follow statistical hypothesis. For major isotopes, greater care was used during the evaluation process.

All TENDL-2021 neutron files are original except 24. The 24 following files are taken from JEFF-4.0T0: ^{1,2,3}H, ^{3,4}He, ^{6,7}Li, ^{10,11}B, ^{7,9}Be, ^{12,13}C, ^{14,15}N, ^{16,17,18}O, ^{19}F, ^{232}Th, ^{233,235,238}U and ^{239}Pu.

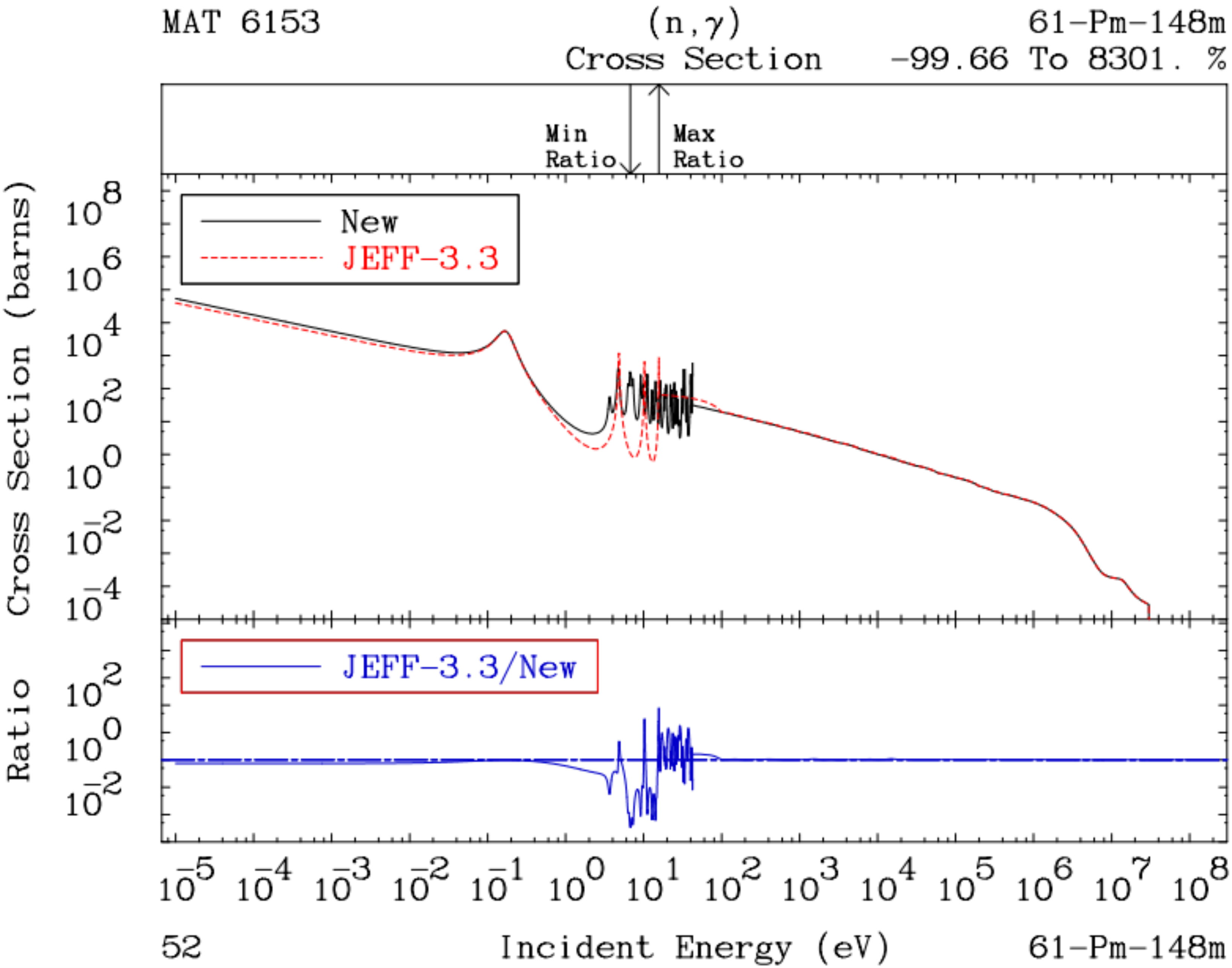
A set of tools, called T6, was used to produce it. T6 stands for TALYS, TEFAL, TASMAN, TARES, TAFIS and TANES. Each code produces a part of the library. Processing tools such as NJOY, CALENDF, PREPRO are also used in T6. These codes, and the processing steps are developed by A.J. Koning, D. Rochman and J.Ch. Sublet. Still, the help and feedback of the whole nuclear data, processing and user community is extremely useful. TENDL would not exist without the constructive remarks from all over the world.

TENDL-2021

- Important differences with TENDL-2019
  - Improved resonance parameters from JEFF community (CEA-Cadarache)
  - Globally improved description of (n, γ) thanks to new photon strength functions (Goriely) and automated fitting to EXFOR data with TASMAN code
  - Photonuclear data library based on new photon strength functions
  - Improved overall description of all charged-particle libraries
    - Improved numerical binning in multiple emission
    - Adjusted global fitting parameter for (alpha,n) reactions
    - Adjusted break-up parameters for deuteron reactions
    - Notable improvement of proton library, especially for (p,n)
    - Good global description of charged-particle induced fission

New evaluations for TENDL-2021 and JEFF-4

- Revised resonance parameters by CEA-Cadarache (Gilles Noguere, David Bernard, Olivier Bouland):
  - $^{107,109}Ag$
  - ^{135}Xe
  - ^{133}Cs
  - ^{148m}Pm
  - $^{151,153,154,155}Eu$
  - $^{173,175,176}Lu$
- All revised parameters inserted in Dimitri Rochman's TARES code
- Fast neutron range evaluation by Arjan Koning and Stephane Goriely
- Combined set of 'best' parameters stored in the T6 system to enable automatic file production
- Same approach used by Titech (Chiba et al) using the TALYS system T6 for LLFP and e.g. ^{36}Cl


MAT 6153
(n,γ)
Cross Section
61-Pm-148m
-99.66 To 8301. %
Min Ratio
Max Ratio
New
JEFF-3.3
JEFF-3.3/New
Cross Section (barns)
Ratio
Incident Energy (eV)
52
61-Pm-148m

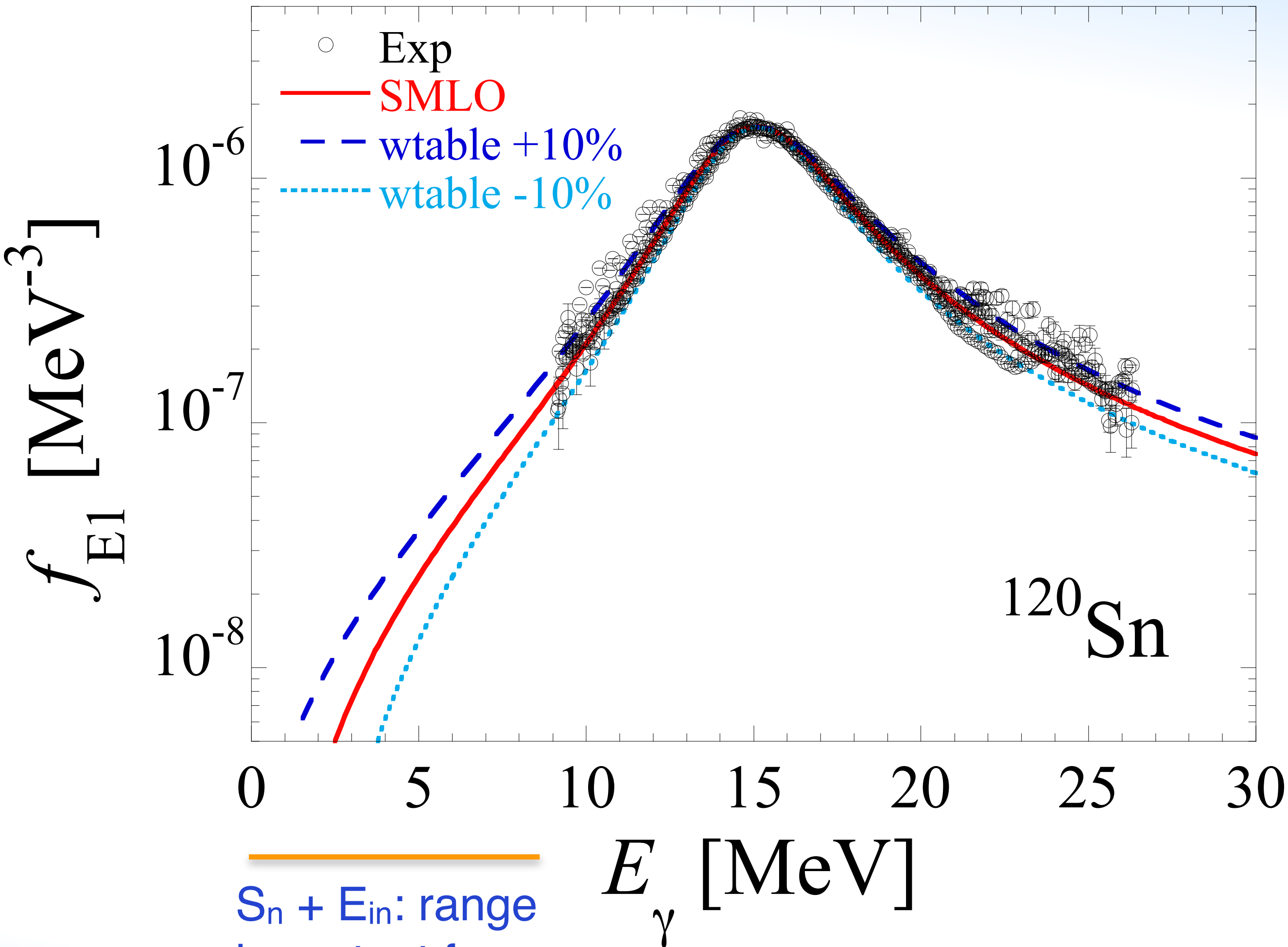
TALYS Application to (n, γ) cross sections

- Adjust width of the E1 SMLO photon strength function (TALYS: ‘wtable’) to match **the best nuclear data library** with
  - Best reproduction of MACS, around 30 keV
  - Best reproduction of experimental (n,γ) cross section from the top of the RR - 100 keV/1 MeV
  - Best nuclear data library **before** TENDL-2021:
    - JENDL-4.0: 97 target isotopes
    - JENDL-AD: 2 target isotopes
    - CENDL-3.2: 2 target isotopes
    - TENDL-2019: 106 target isotopes
    - JEFF-3.3: 8 target isotopes
    - ENDF/B-VIII.0: 61 target isotopes

```
n–Eu153.tasman
#Esearch 0.01 0.1 102
#libinclude 102 endfb8.0
```

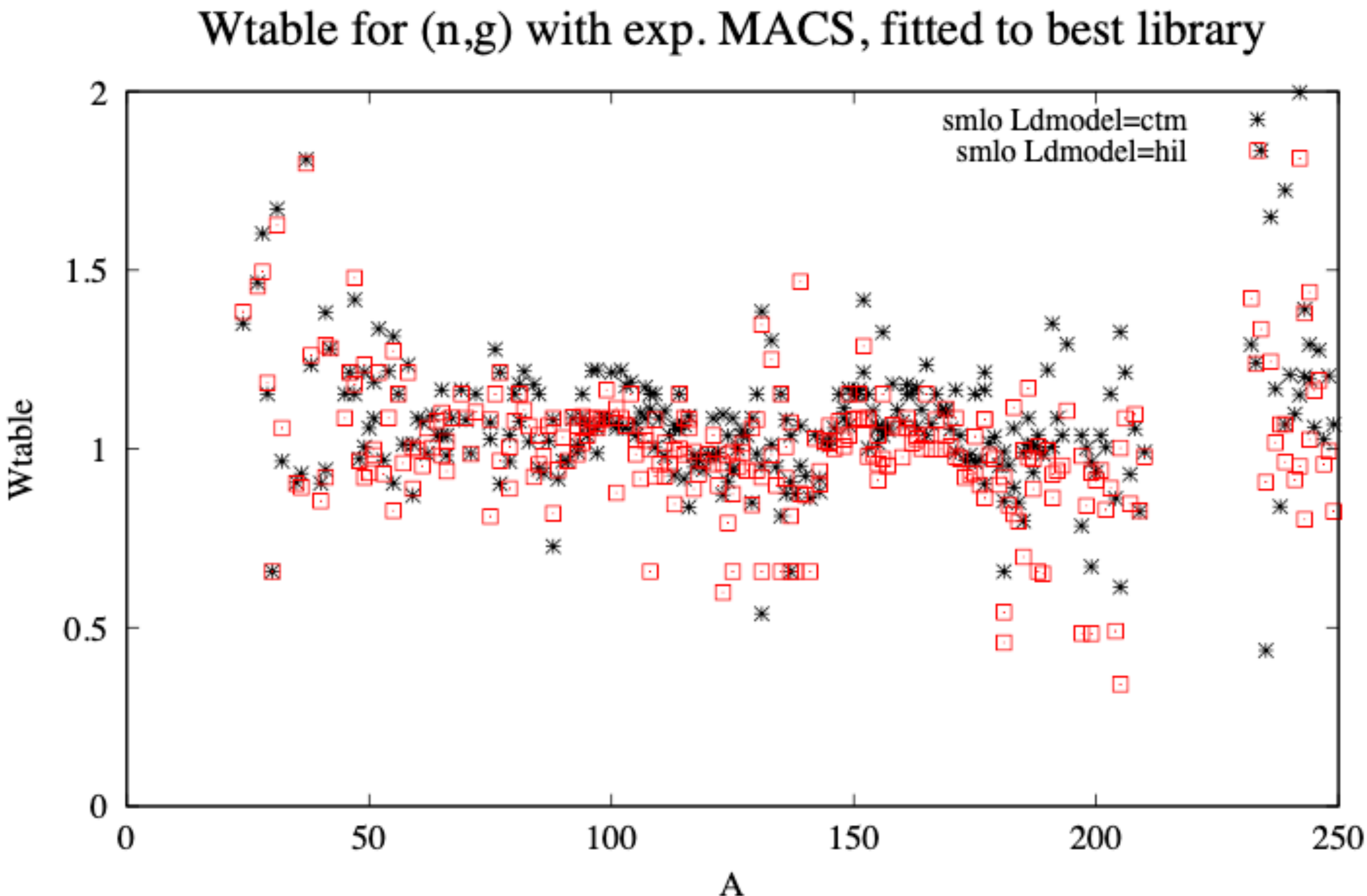
- **Autotalys** automatically optimizes ‘wtable’ to match **above libraries in a restricted energy range**, e.g. autotalys -element Eu -mass 151 -Ltarget 000 -Liso 0 -proj n -bins 40 -search -energyfile /Users/koning/samples/psf/smlo/ctm/energies -best -noautosearch -noparauto -talysfile /Users/koning/samples/psf/smlo/ctm/talys.add -tasmanfile /Users/koning/samples/psf/smlo/ctm/tasman.add

Adjusted width parameter does not affect original photon strength function very much

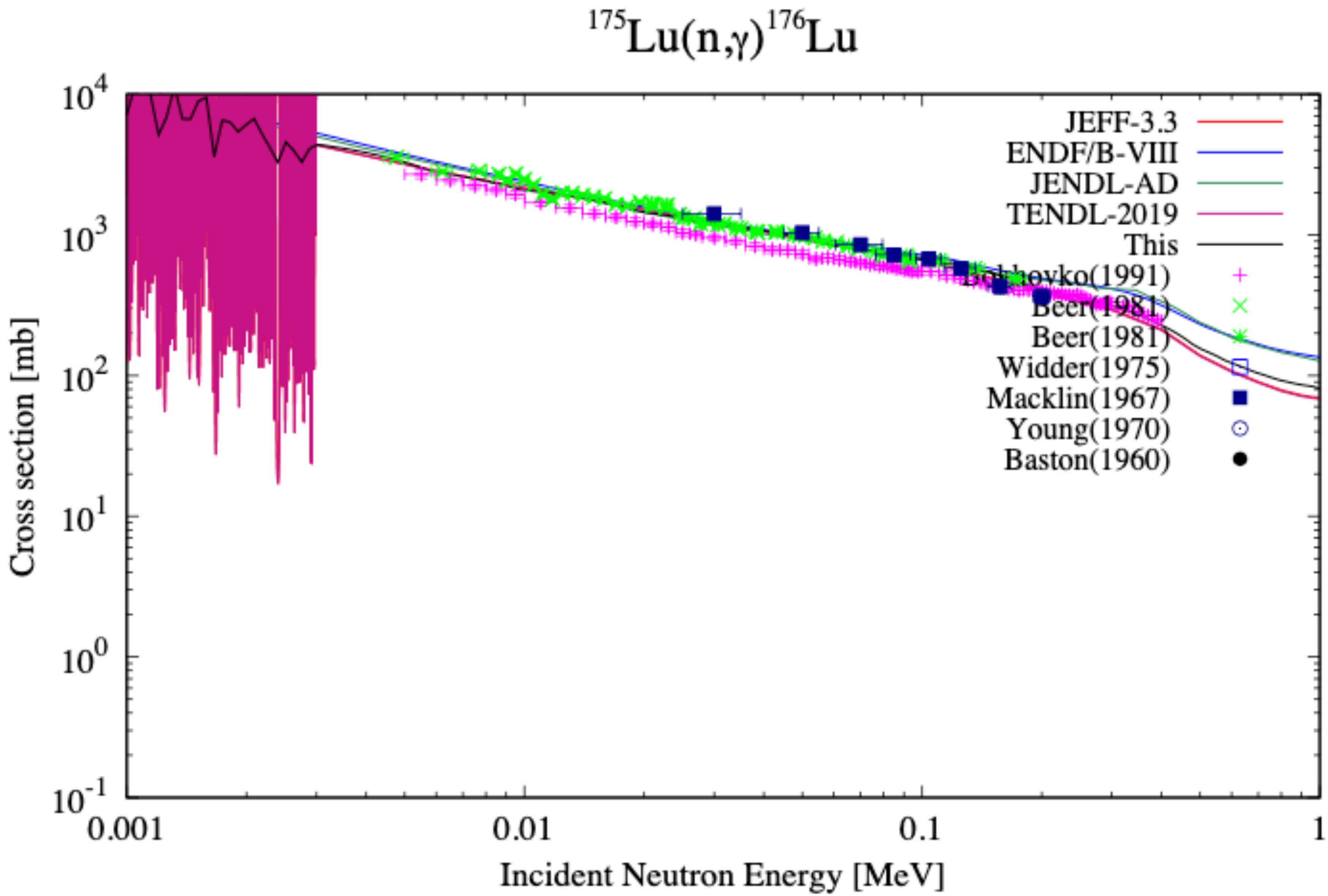


S_n + E_{in}: range important for (n,γ)

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


Wtable for (n,g) with exp. MACS, fitted to best library
smlo Ldmodel=ctm
smlo Ldmodel=hil
Wtable
A
0
0.5
1
1.5
2
0
50
100
150
200
250

F_{rms} : 12%


$^{175}Lu(n,\gamma)^{176}Lu$
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-3.3
ENDF/B-VIII
JENDL-AD
TENDL-2019
This
Beer(1981)
Beer(1981)
Widder(1975)
Macklin(1967)
Young(1970)
Baston(1960)
0.001
0.01
0.1
1

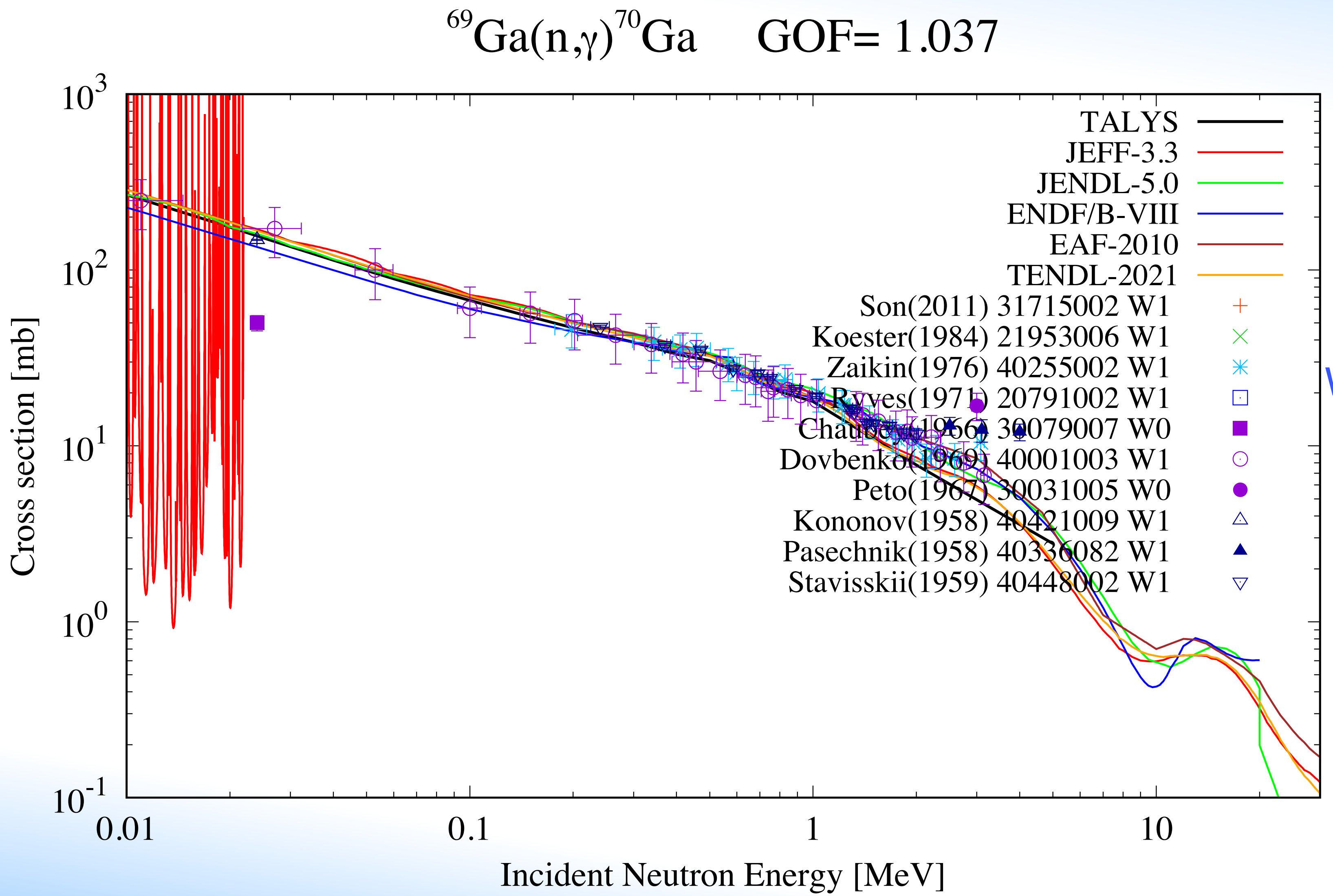
Towards TENDL-2023: TALYS optimisation to EXFOR

- Two birds with one stone:
  - Exforcism (flag evil data in EXFOR)
    - Add to current database of experimental ‘outliers’ by Alhassan, Gaughan and Dzysiuk
    - ‘Graphical’ outliers
    - Full JSON file soon to be released
  - Optimization of TALYS parameters to all cross sections
    - Use of XC5 format of EXFOR (V. Zerkin)
    - Dimension reduction
    - Same parameter set for all nuclides

TALYS parameters for optimisation

Reaction	Nuclides	Parameter	Parameter	Parameter	Parameter	Parameter	Parameter
(n, γ)	278	wtable					
(n,f)	34	vfiscor	betafiscor	ctable(1)	ptable(1)	ctable(2)	ptable(2)
(n,n'), (n,2n), (n,p)	210	rv(p)	g_{ph}(0)	g_{ph}(n)	ctable(n)	ctable(p)	
(N,α)	157	rv(α)	Cstrip(α)	g_{ph}(0)	ctable(α)		
(p,n)	142	rv(p)	rwd(p)	rv(n)	g_{ph}(0)	g_{ph}(n)	ctable(n)
(γ,n)	77	wtable	ftable	etable			
(α,n)	93	rv(α)	rwd(α)	rv(n)	g_{ph}(0)	ctable(α)	
(d,n)	40	rv(p)	rwd(p)	rv(n)	g_{ph}(0)	g_{ph}(n)	ctable(n)

Optimization to included exp. data



W0: weight 0

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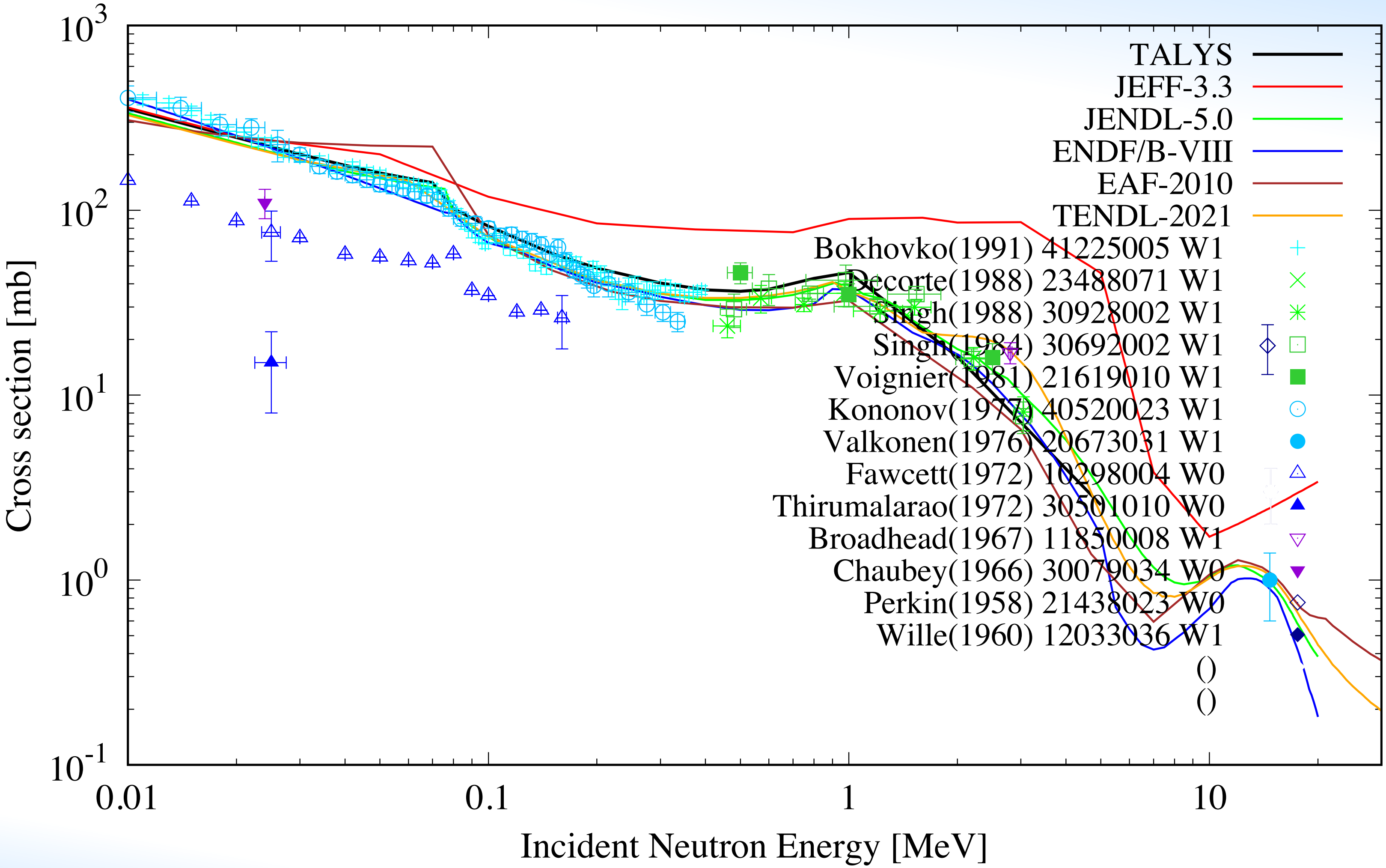
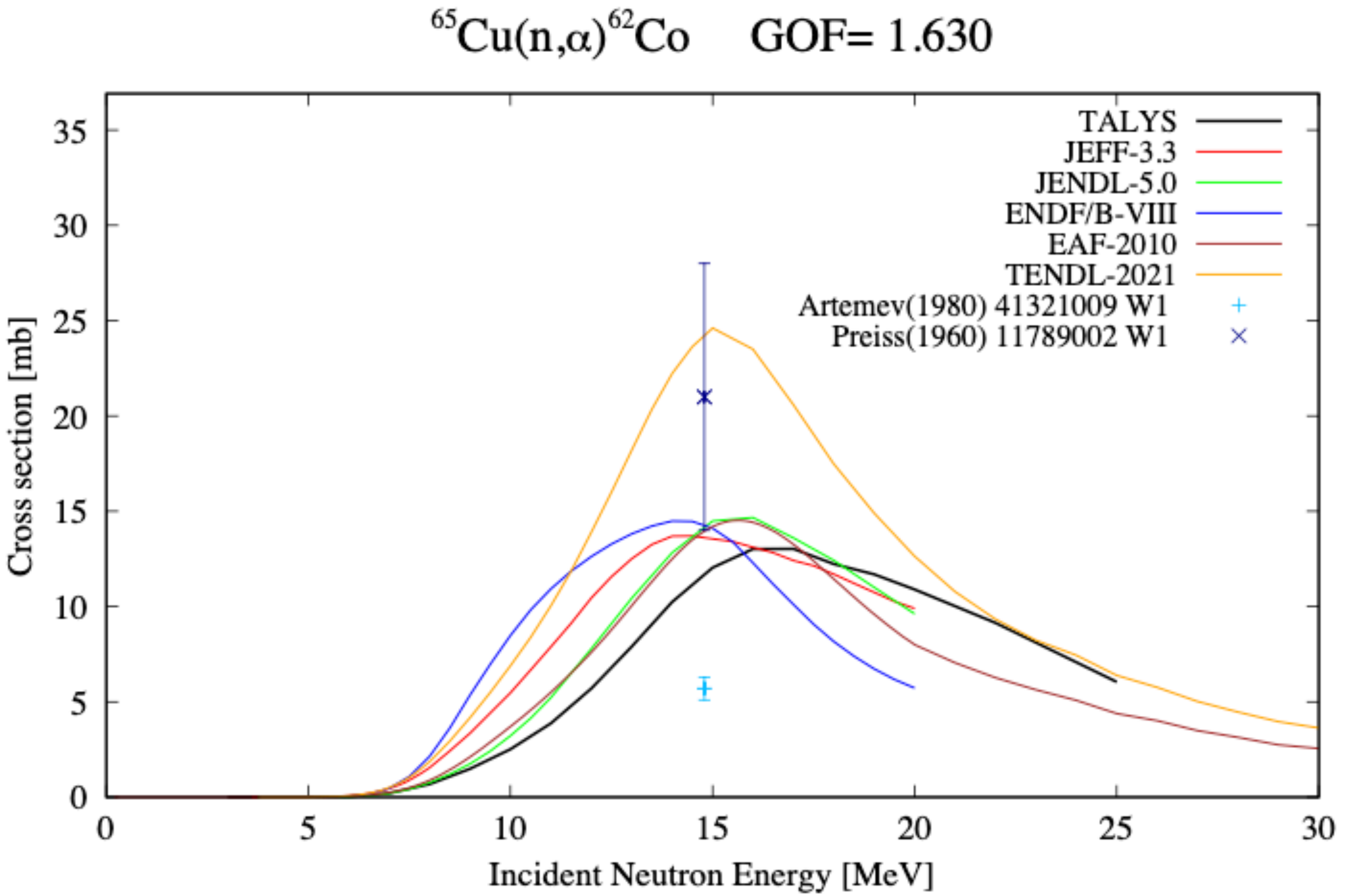
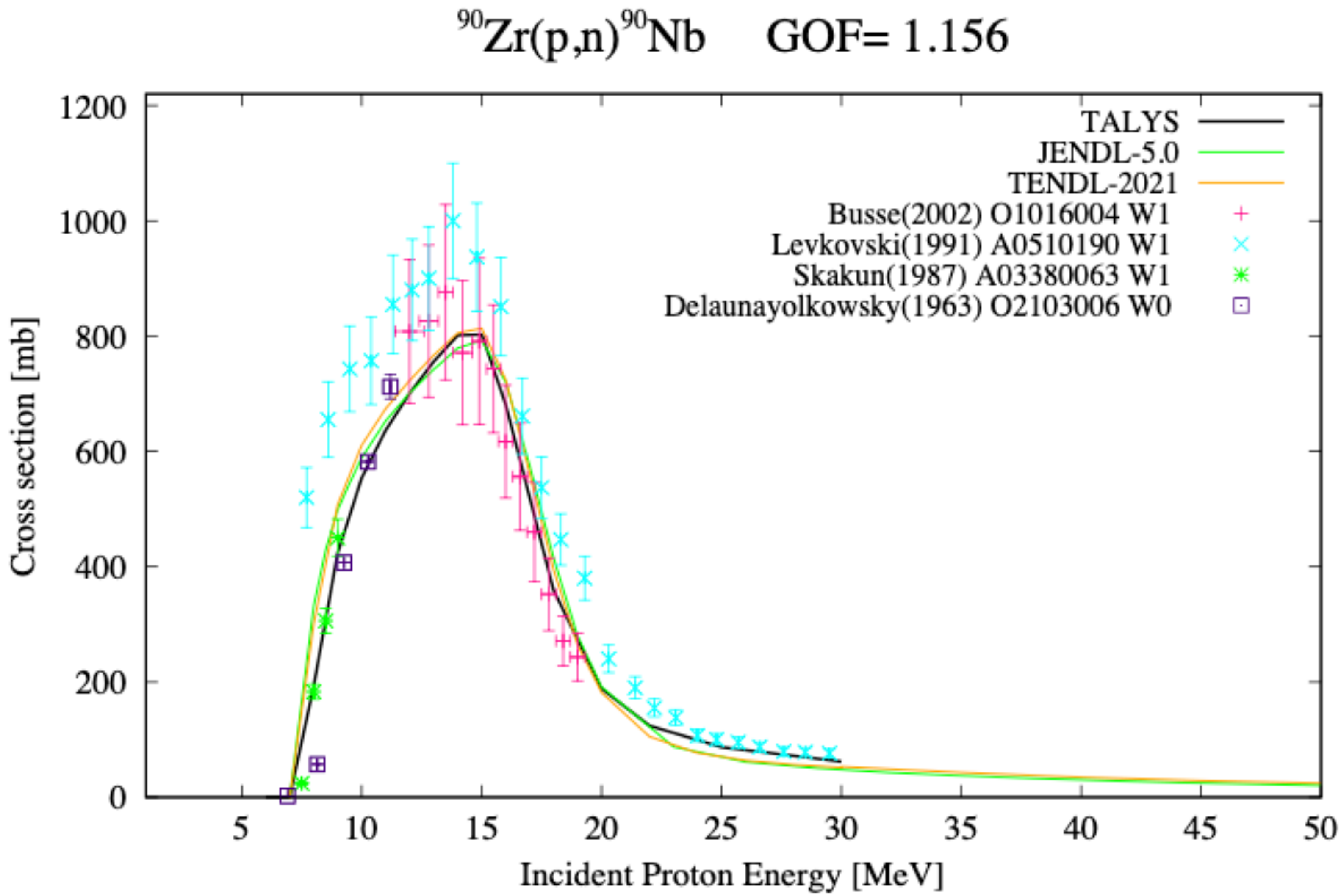
$^{160}Gd(n,\gamma)^{161}Gd$ GOF= 1.094



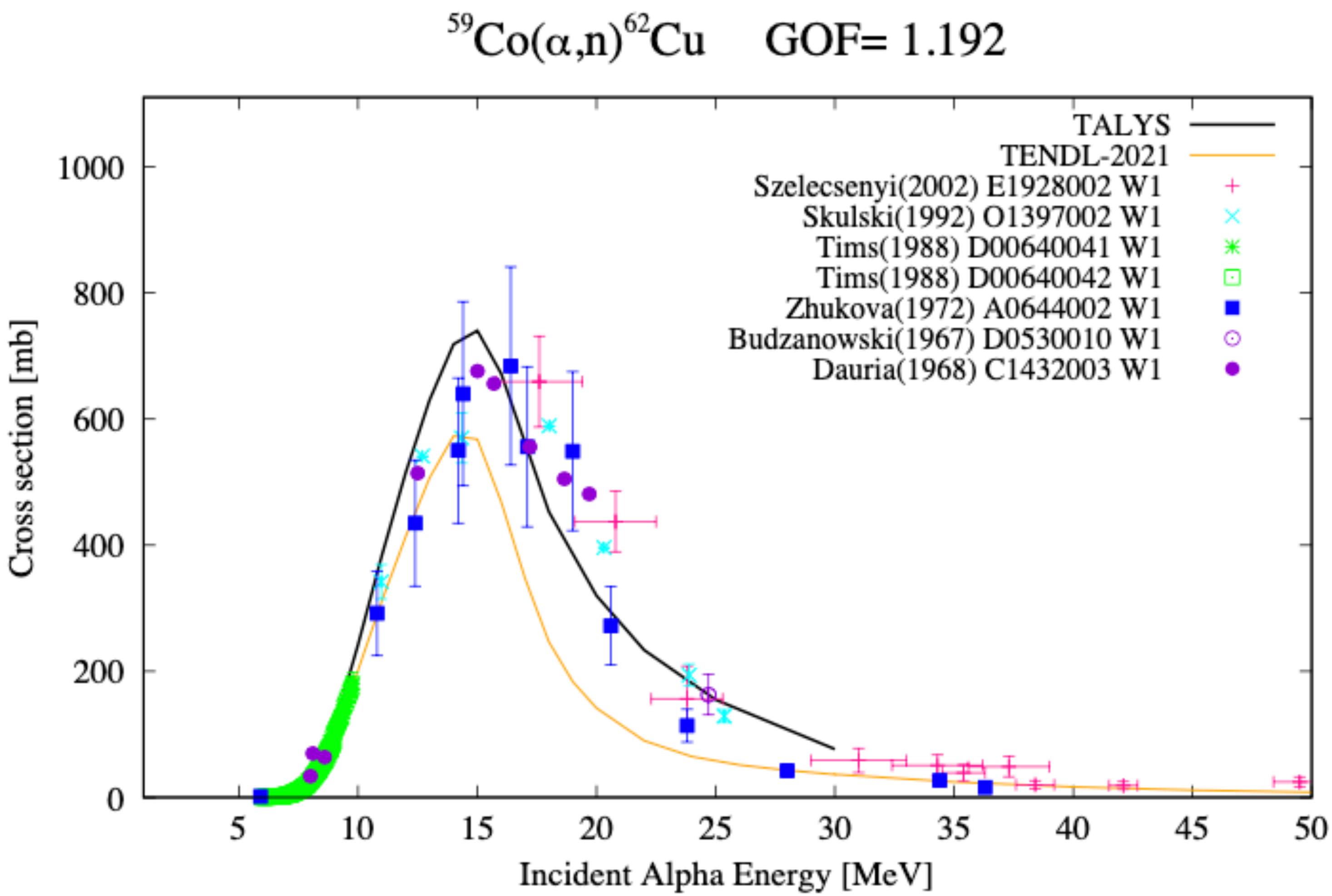
Segal's law: A man with a watch knows what time it is.
A man with two watches is never sure.



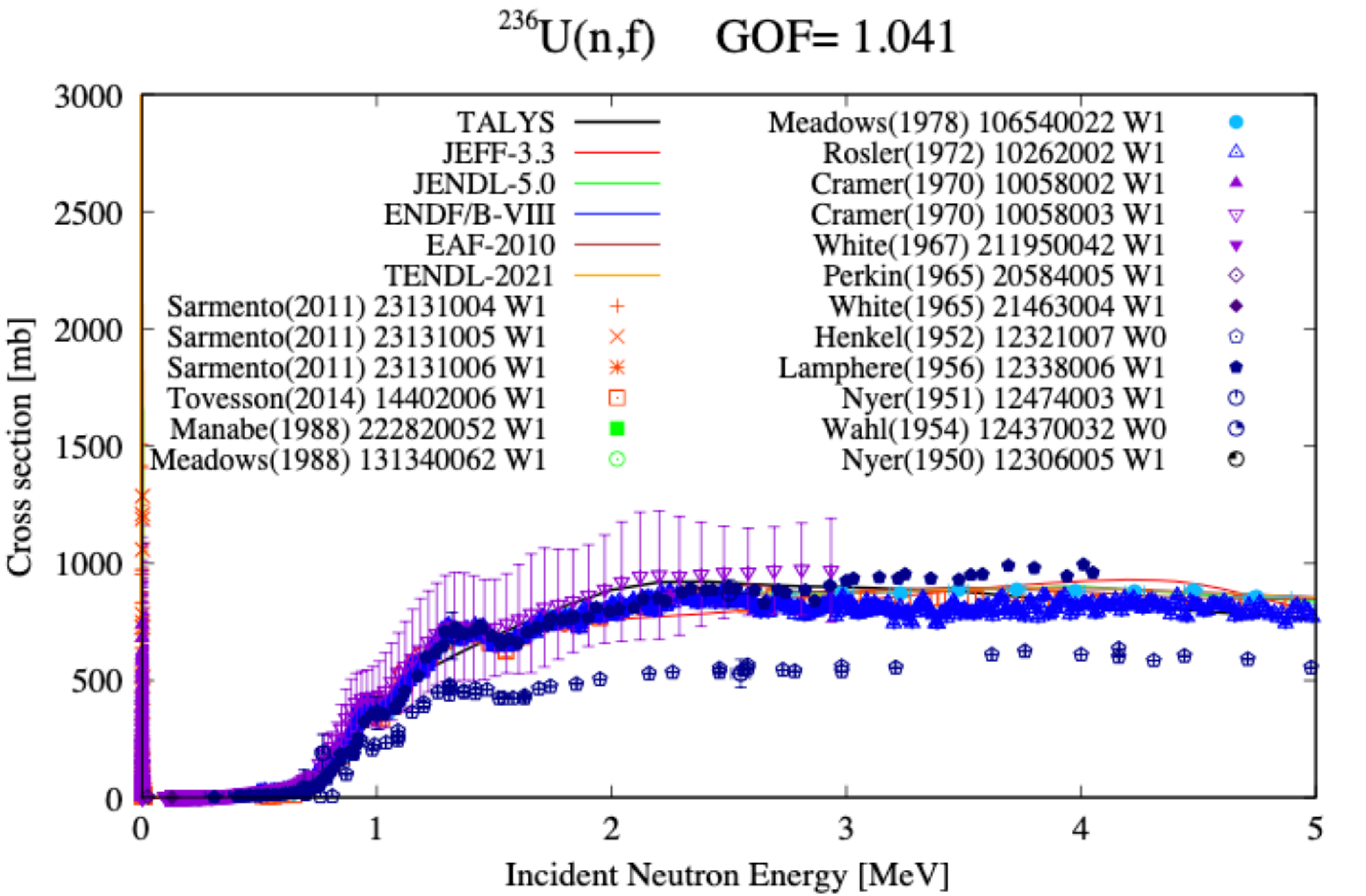
(p,n): several nuclides with JENDL-5 evaluation



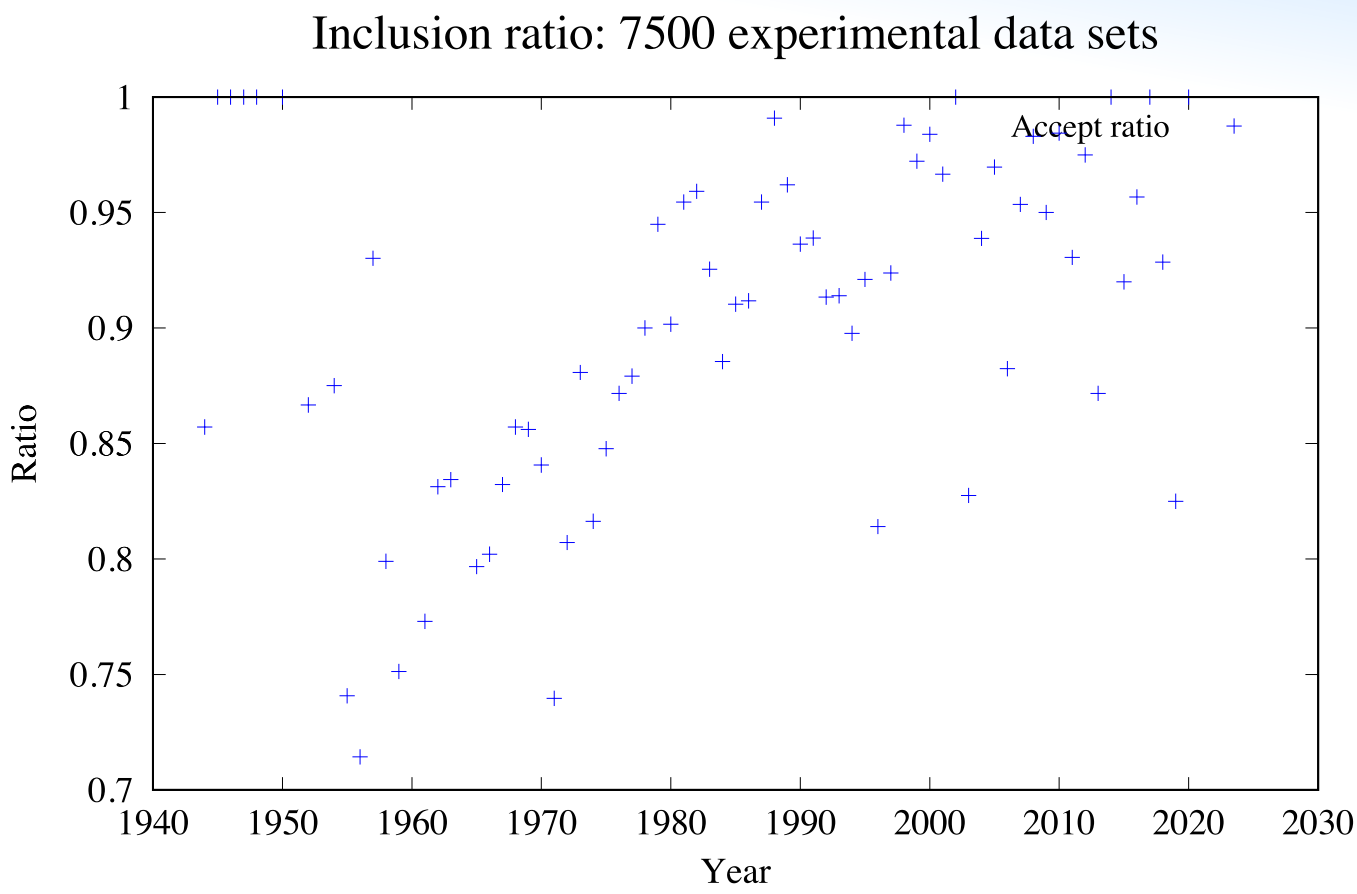
(α,n): TENDL rules! (OK OK, because there is nothing else for A > 20)



Fission: WKB (Sin, Capote) + HFB level densities (Hilaire, Goriely)

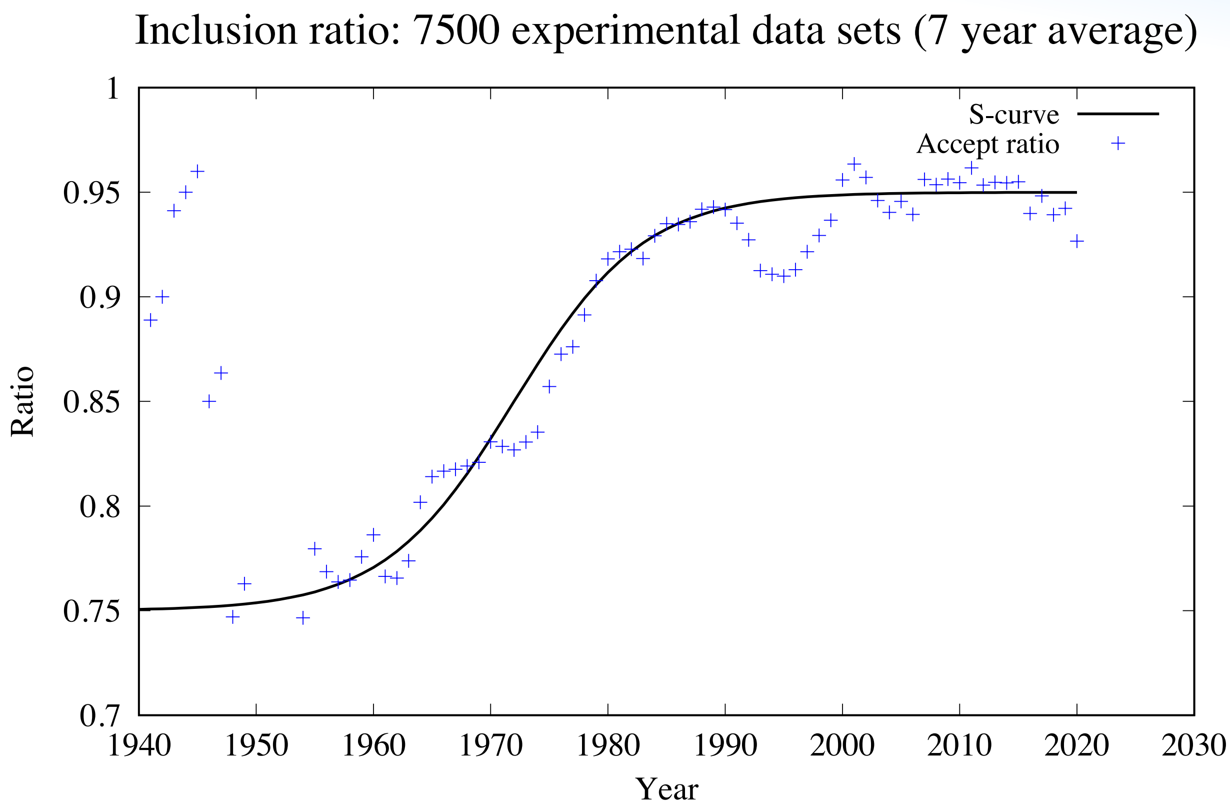


Outlier assignment



Summed over all (n,g), (n,f), (n,n’), (n,2n), (n,p), (n,a), (p,n), (g,n), (a,n), (d,n) cross sections for all nuclides

Outlier assignment



Other analyses possible:

- per reaction channel
- per author, co-author, lab, etc
- per incident energy (e.g. 14 MeV)
- re-insert this as prior in the next Bayesian update

The power of Total Monte Carlo

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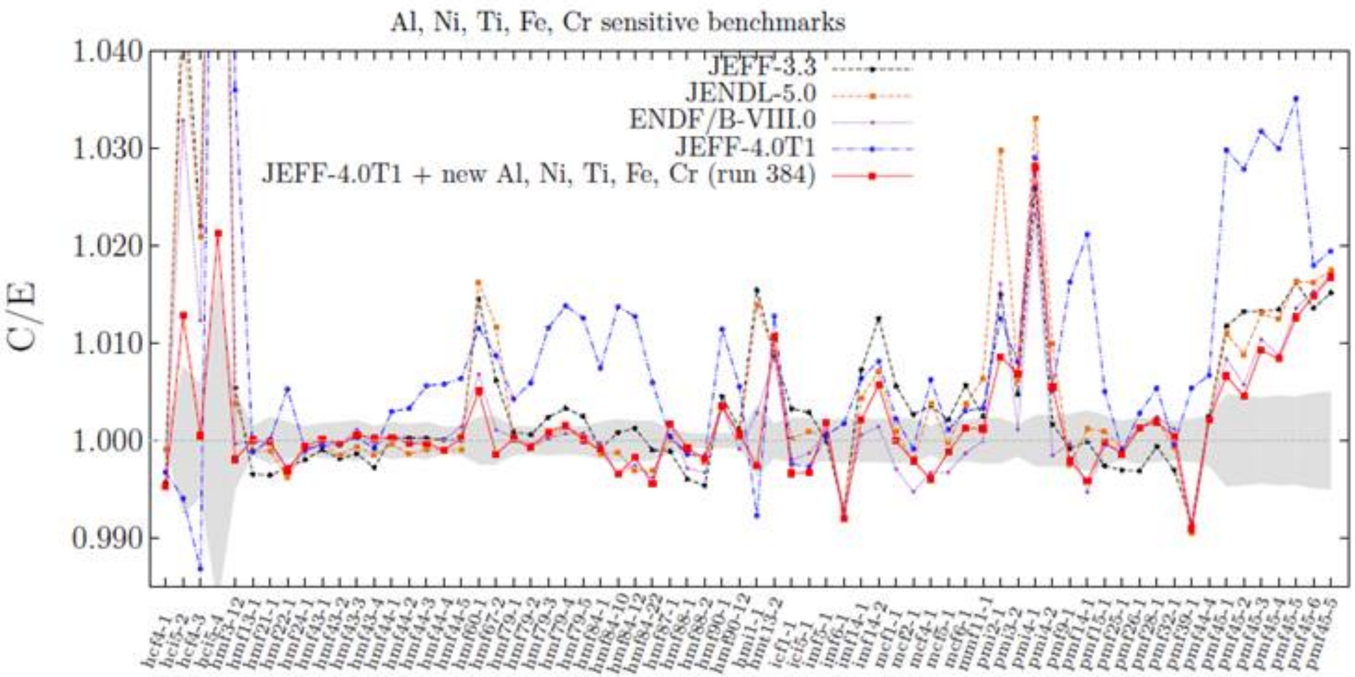
- Suboptimal performance of TENDL-2021 (—> JEFF-4.0T) for Al, Ti, Cr, Fe, Ni benchmarks
- Solution: Sample all resonance parameters and TALYS parameters inside uncertainty bands
- Produce 2000 random ENDF files for all of them and choose the best combination



JEFF-3.3 $\chi^2 = 9.9$
JEFF-4.0T0 $\chi^2 = 14$
JEFF-4.0T1 $\chi^2 = 23$
JEFF-4.0T1+new $\chi^2 = 5.6$
ENDF/B-VIII.0 $\chi^2 = 5.9$
ENDF/B-VIII.0+Inden $\chi^2 = 5.4$
JENDL-4.0 $\chi^2 = 13$
JENDL-5.0 $\chi^2 = 11$

- Procedure is automated for any benchmark (D. Rochman and A.J. Koning, How to randomly evaluate nuclear data: a new method applied to Pu-239, Nucl. Sci. Eng. 169(1), 68 (2011).
- Challenges:
  - analyse why this particular combination is the best one
  - what is the quality beyond criticality benchmarks?

Other TENDL developments

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- Bypassing ENDF-6: TAGNDS, with Caleb Mattoon
- Direct feeding into the Medical isotope Browser nds.iaea.org/mib
- Automated fitting to all cross sections from EXFOR, including actinides, use of ML to estimate TALYS parameters for neighbouring nuclides
- Include EGAF for thermal capture gamma lines
- To have integral validation as automated as evaluation (‘validation on the spot’) (> 2030)
- 517 citations in 2021-2022 on very different subjects

Summary

- TALYS-1.96 released 30 December 2021. TALYS-2.0 will follow. All satellite software for TALYS (TASMAN: statistics, optimisation and uncertainties, TEFAL: ENDF formatting), autotalys to GitHub
- TENDL-2021 was released end of December 2021:
  - Improved fast neutron cross sections thanks to new photon strength functions and semi-automated EXFOR fitting
  - Improved nuclear data for incident charged particles and photons
- Strong collaboration with JEFF-4:
  - Improved resonance parameters, in this case from CEA-Cad, are inserted into the T6/autotalys evaluation system

For each isotope:

2010: Use TENDL, if you have nothing else

2020: Use TENDL, unless you have something better

2030: ~~Explain why you don't use TENDL~~ don't know yet

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Thank you!