60 Years

IAEA Atoms for Peace and Development

Nuclear model parameter optimisation with TALYS

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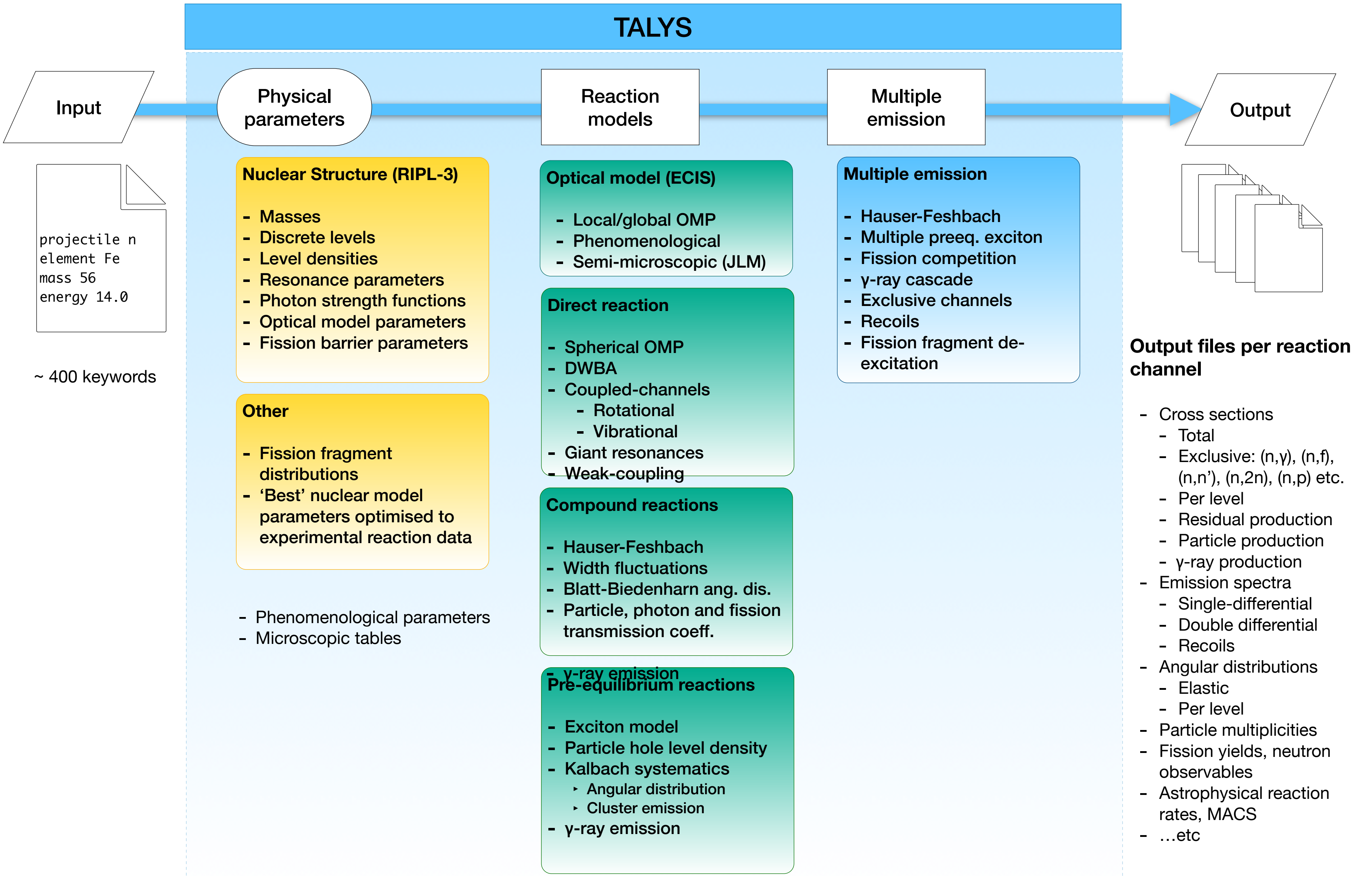
NDS library, November 3 2022

Introduction

- TALYS covers
  - All nuclides
  - All projectiles
  - 0-200 MeV
- 6000-7000 citations in all possible fields: neutron fission, medical isotope production, astrophysics, fusion, activation, etc.
- Objective: make the code globally better, regardless of the application
- Global good prediction: better physics, global optimisation to experimental data
- Global good description: nuclide-by-nuclide optimisation to experimental data


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
- Weak-coupling
Compound reactions
- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.
- γ-ray emission
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

Prediction of reality

Microscopic global models

Phenomenological global models

Micro/pheno models with adjusted parameters

Micro/pheno models with unphysical parameters or functions

Direct normalisation of model output to experimental data

Description of reality = exp. data

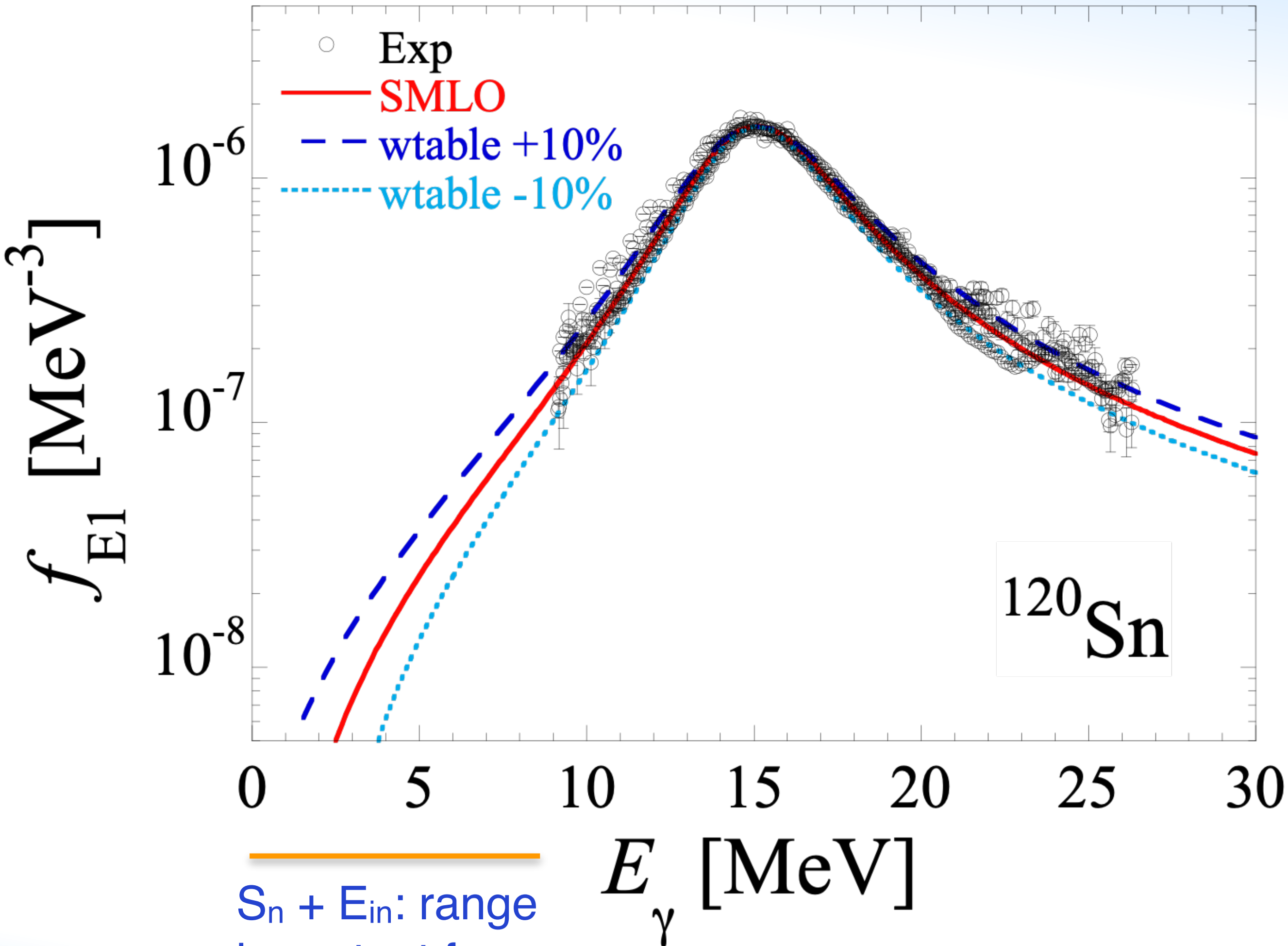
TALYS Application to (n, γ) cross sections

- 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

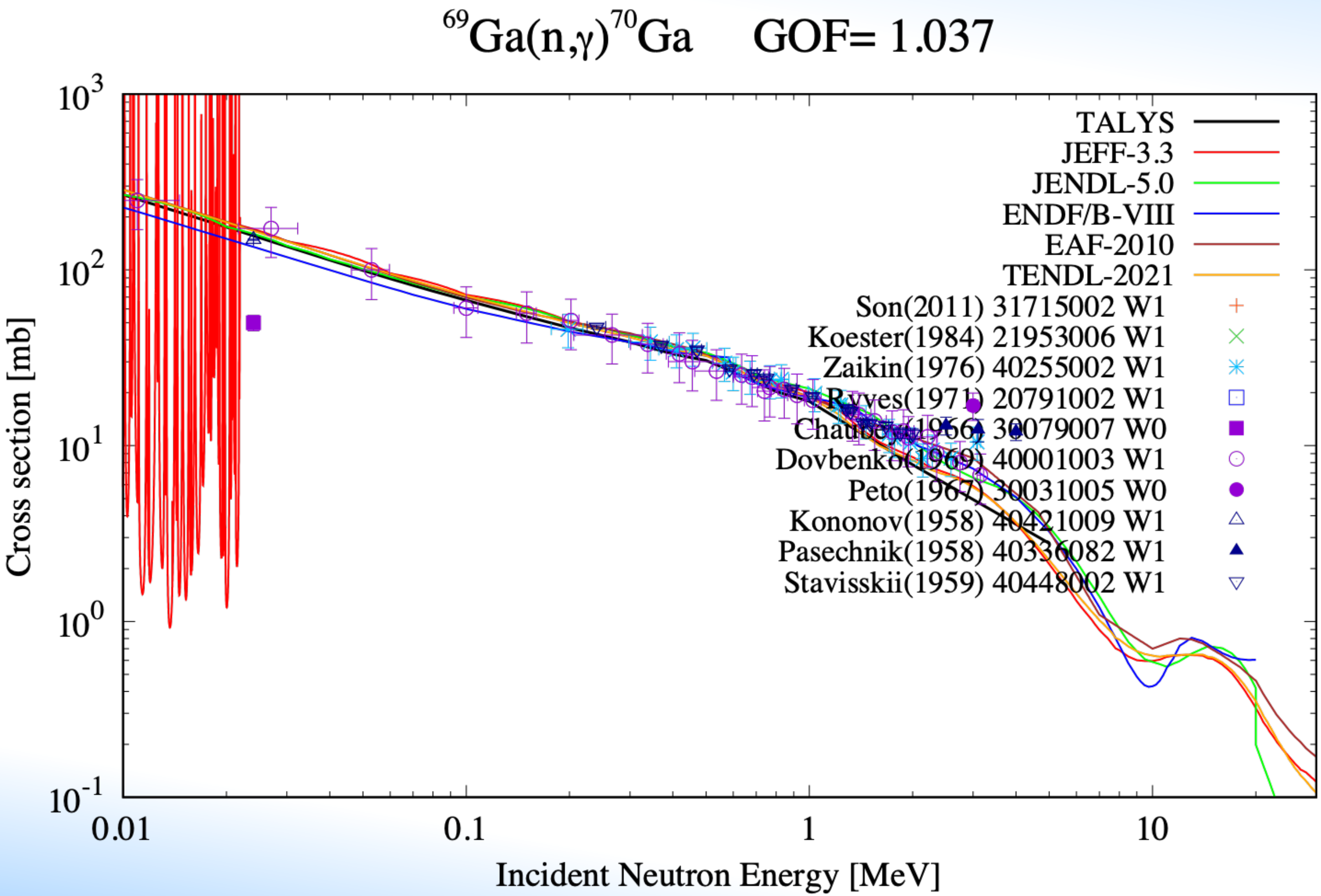
Adjusted width parameter does not affect original photon strength function very much



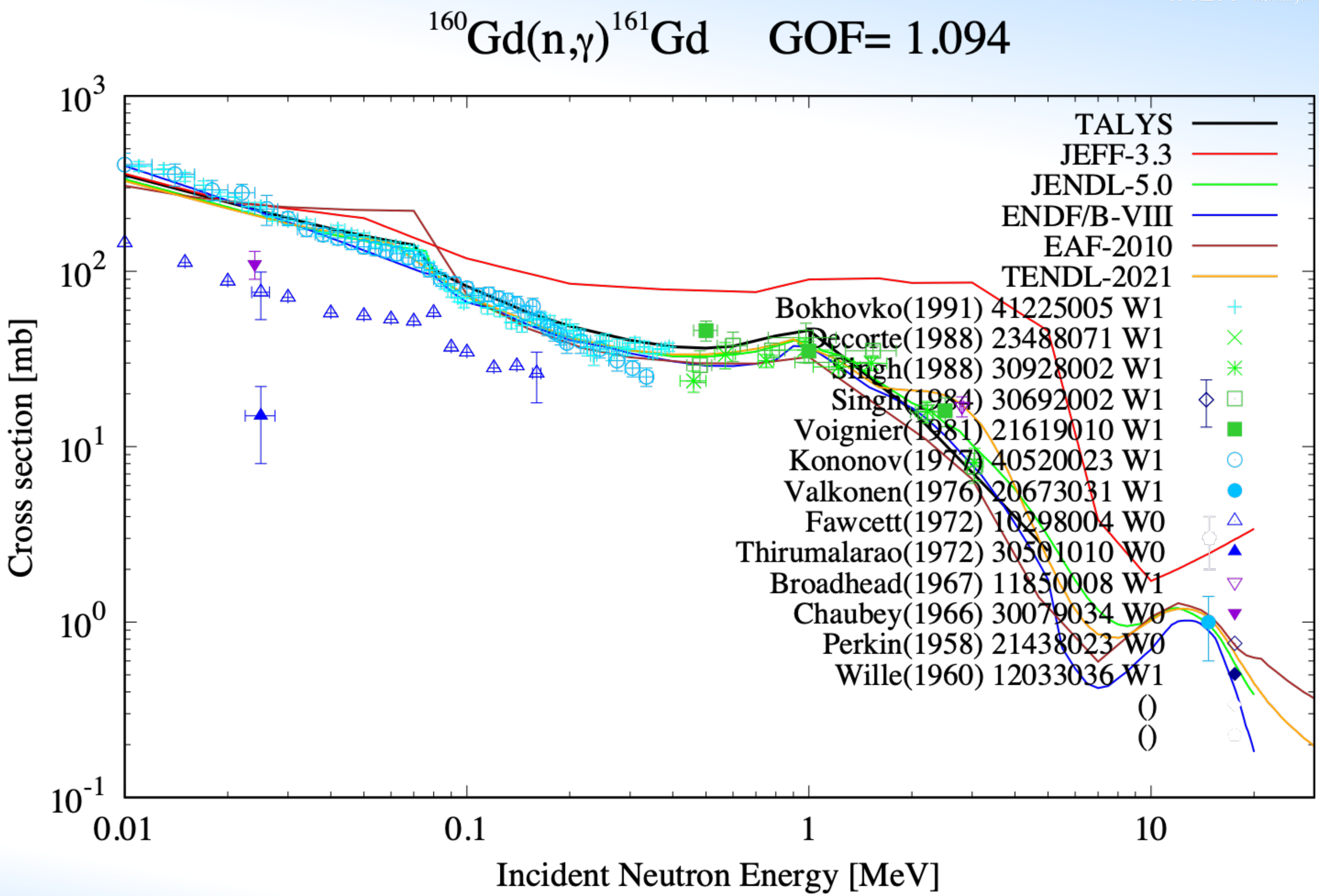
$S_n + E_{in}$: range important for (n,γ)

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

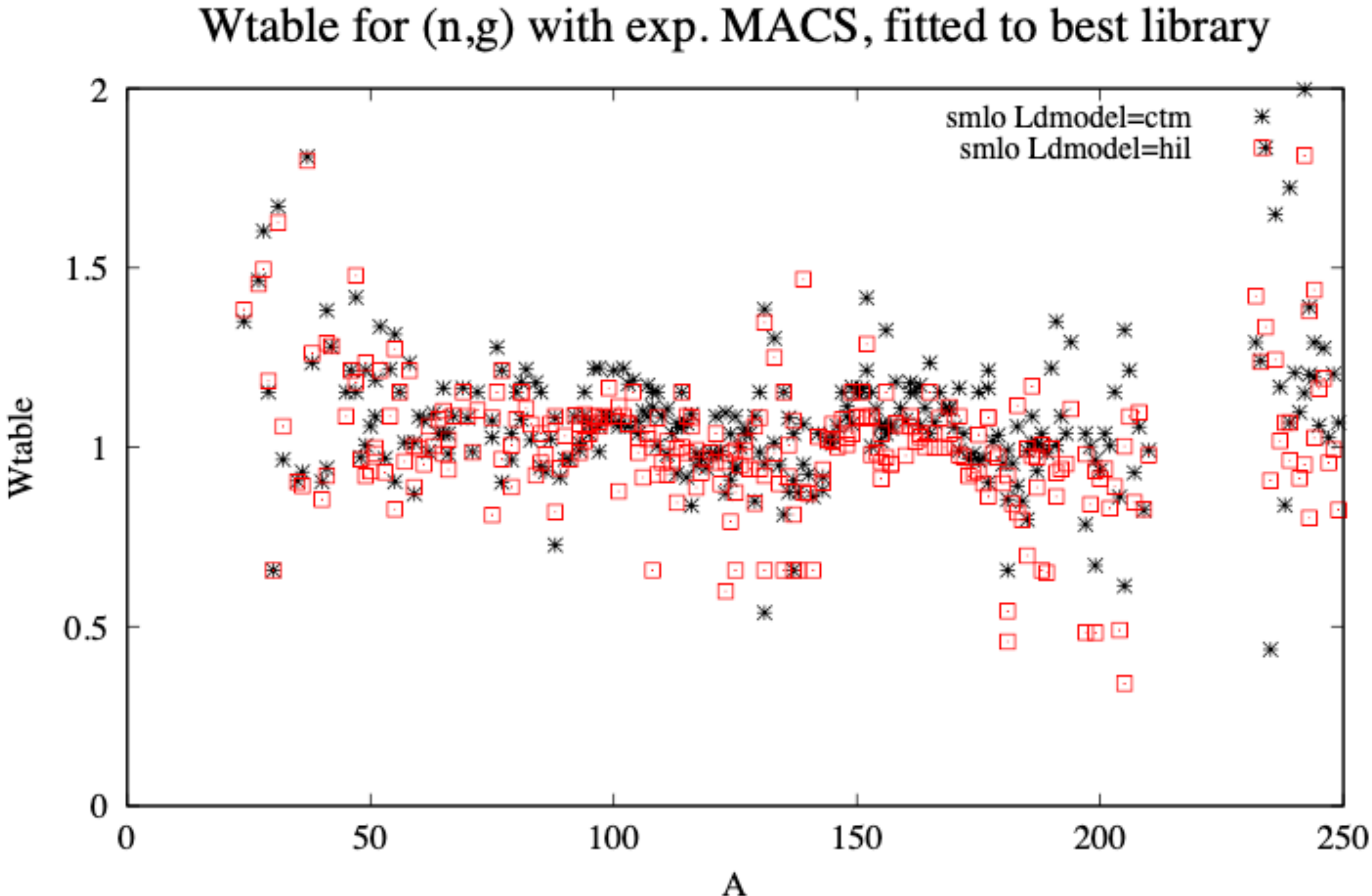
Optimization to included exp. data



W0: weight 0



$^{160}Gd(n,\gamma)^{161}Gd$ GOF= 1.094
Cross section [mb]
Incident Neutron Energy [MeV]
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


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%

TALYS optimisation to EXFOR

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- 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 files available
  - Optimization of TALYS parameters to all cross sections
    - Use of XC5 format of EXFOR (V. Zerkin)
    - Dimension reduction
    - Same parameter set for all nuclides

8400 JSON outlier/inlier files, one per EXFOR subentry


```
{
    "Subentry"    : "A0001004",
    "Author"      : "Skakun",
    "Year "       : 1975,
    "Projectile"  : "p",
    "Target Z"    :   48,
    "Target A"    :  111,
    "Target state": "0",
    "X4 Reaction" : "48-CD-111(P,N)49-IN-111,,SIG",
    "Evaluations" :
    [
        {
        "Evaluator"   : "Arjan Koning",
        "Date"        : "2022-06-05",
        "Weight"      :    0,
        "Comment"     : [
                        " Excluded from evaluation: graphical outlier"
                        ]
        },
        {
        "Evaluator"   : "Erwin Alhassan",
        "Date"        : "2019-11-08",
        "Weight"      :    0,
        "Comment"     : [
                        " Erwin Alhassan (PSI, 2018)  0",
                        " (1 -> accept and 0 -> reject)",
                        " Reasons for inclusion/exclusion",
                        " 1) Experimental data set not consistent with other experiments such as Takacs (2005) between about 10 - 15
 MeV (The cross sections are systematically lower)"
                        ]
        },
        {
        "Evaluator"   : "Natalie Gaughan",
        "Date"        : "2019-03-15",
        "Weight"      :    1,
        "Comment"     : [
                        " IAEA-TECDOC-1211 - Data selected"
                        ]
        }
    ]
}
```


So far: 1 user

TALYS parameters for optimization

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)

TASMAN code (AK): Nelder-Mead optimisation.
Number of TALYS trials: N(parameters) x 20

Fitting all actinides at the same time

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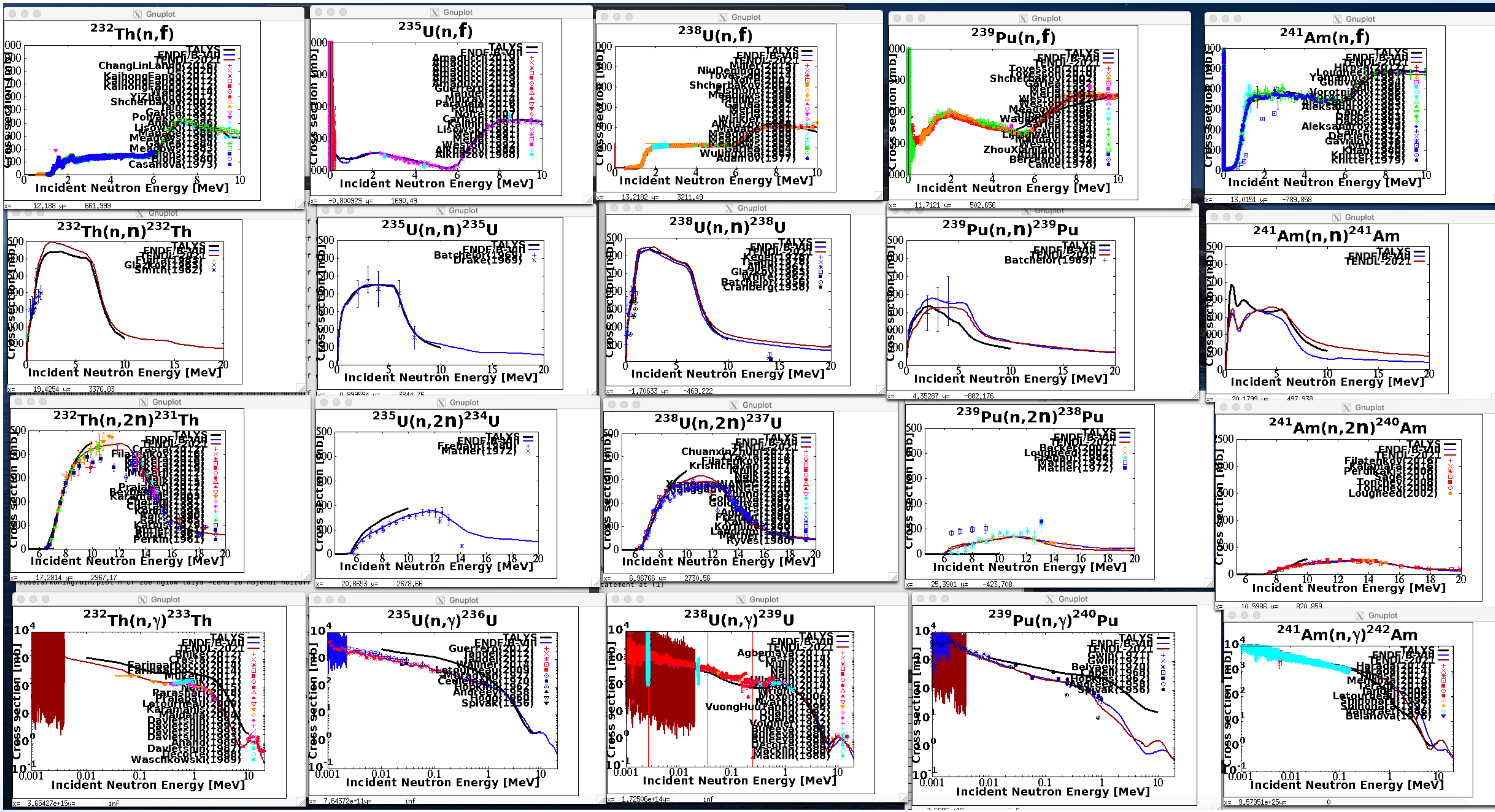
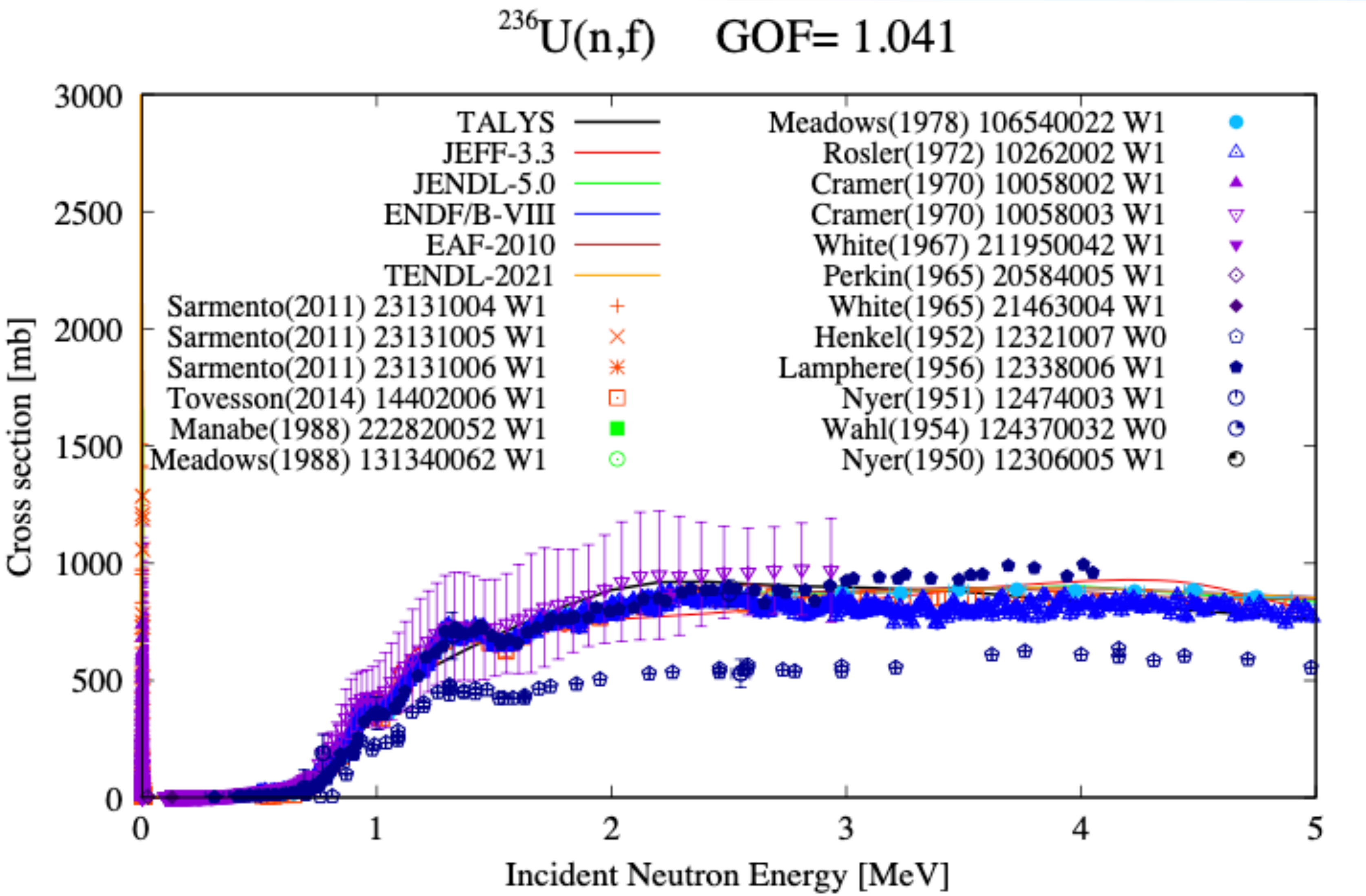
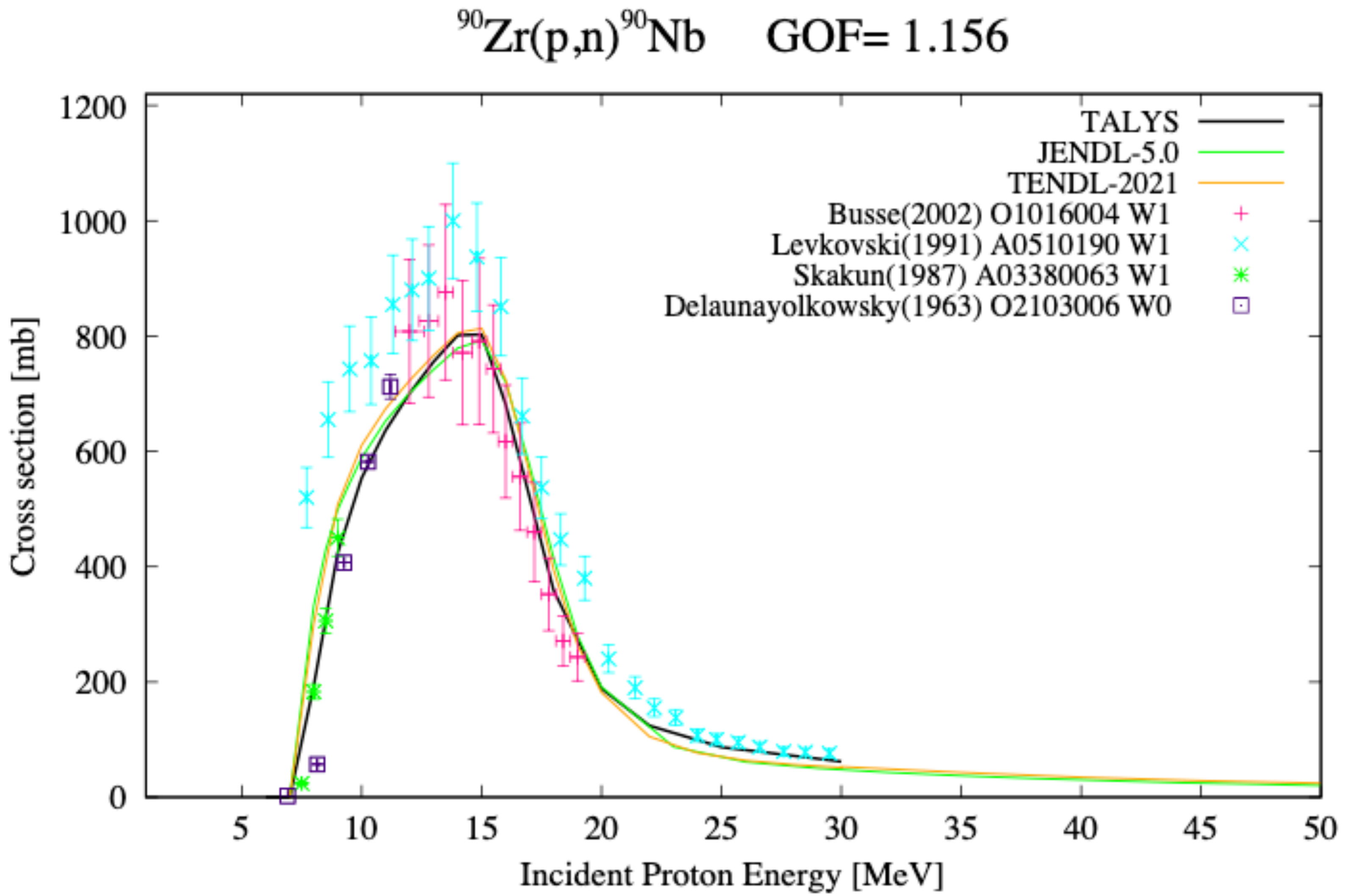


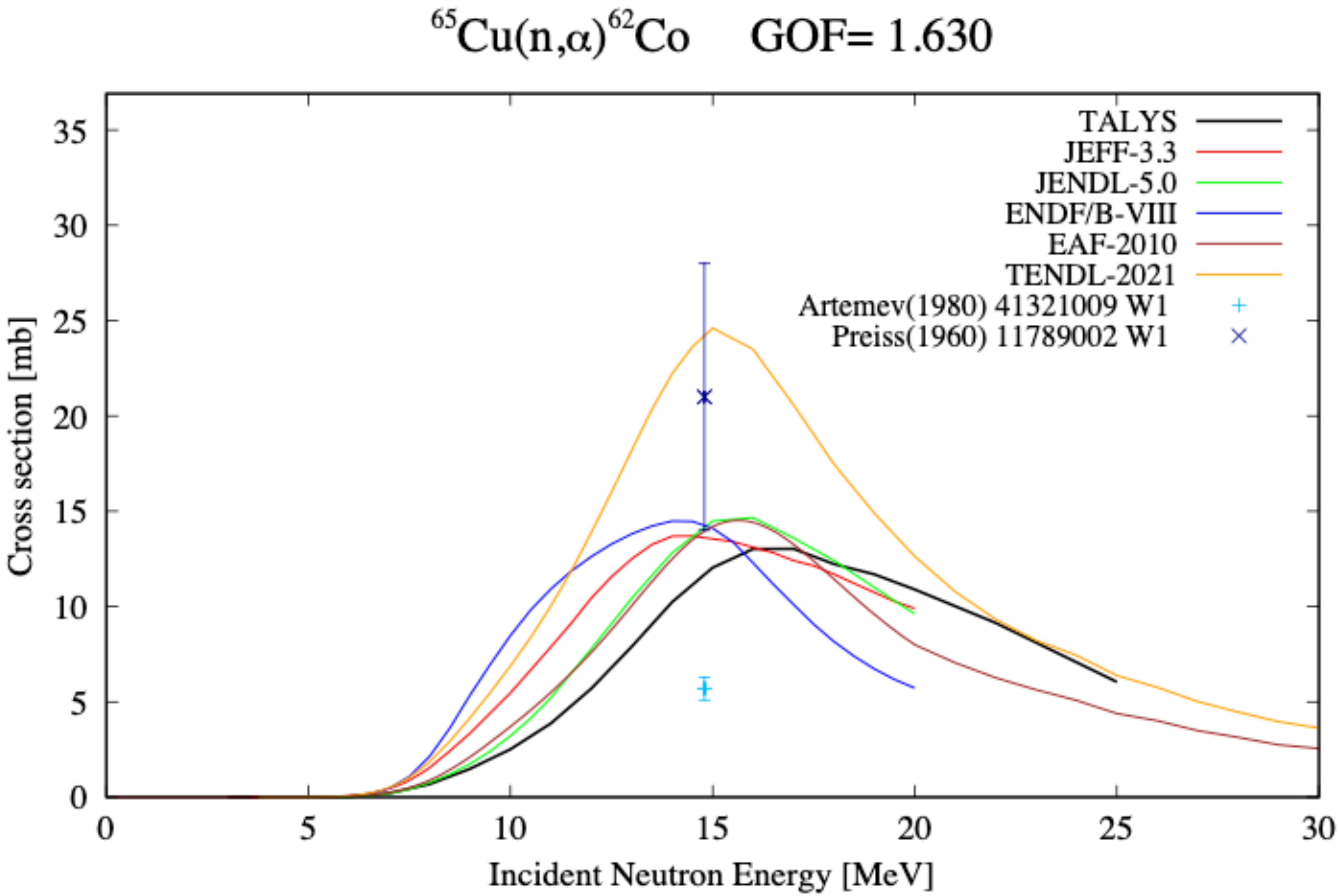
Fission: WKB (Sin, Capote) + HFB level densities (Hilaire, Goriely)



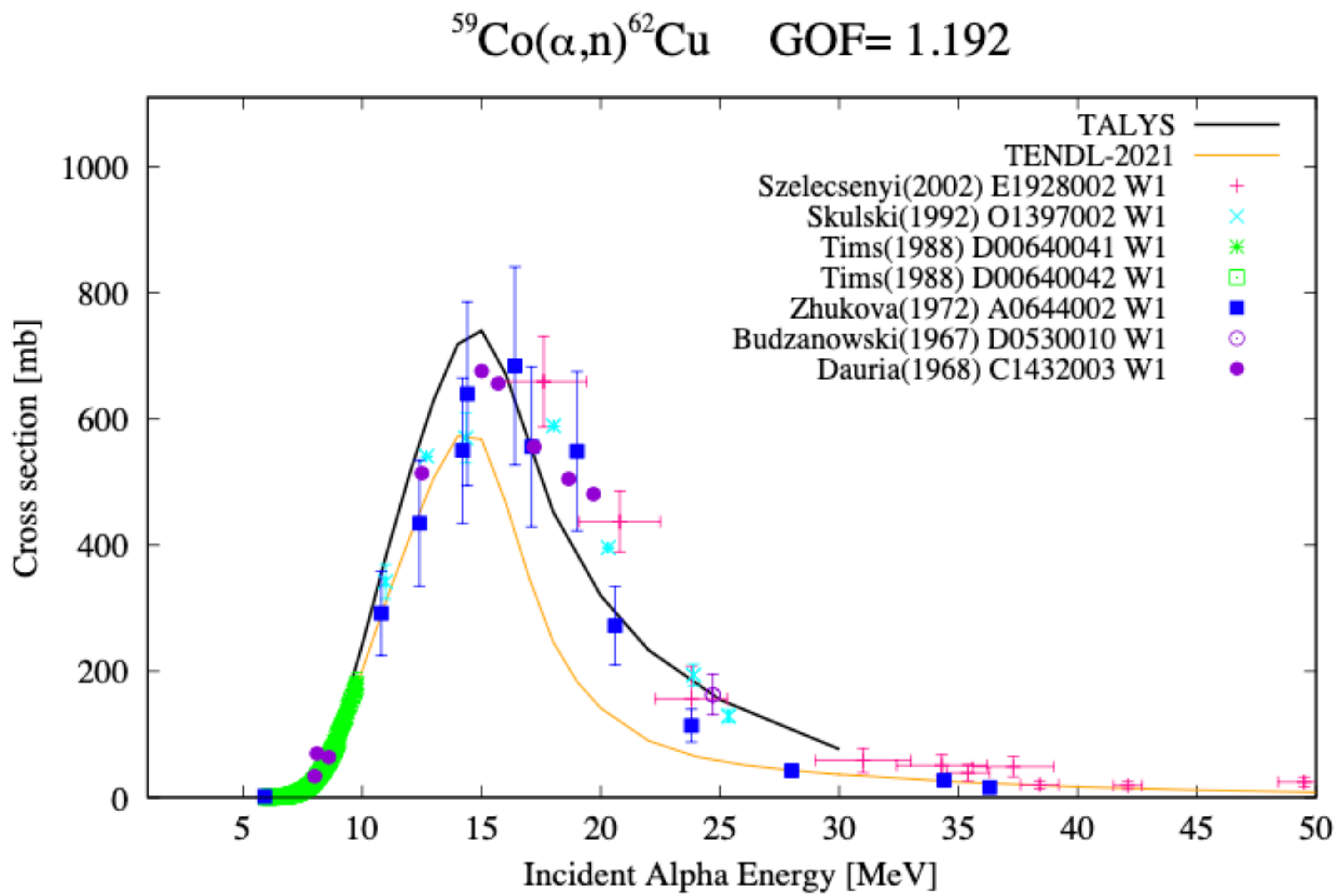
(p,n): several nuclides with JENDL-5 evaluation



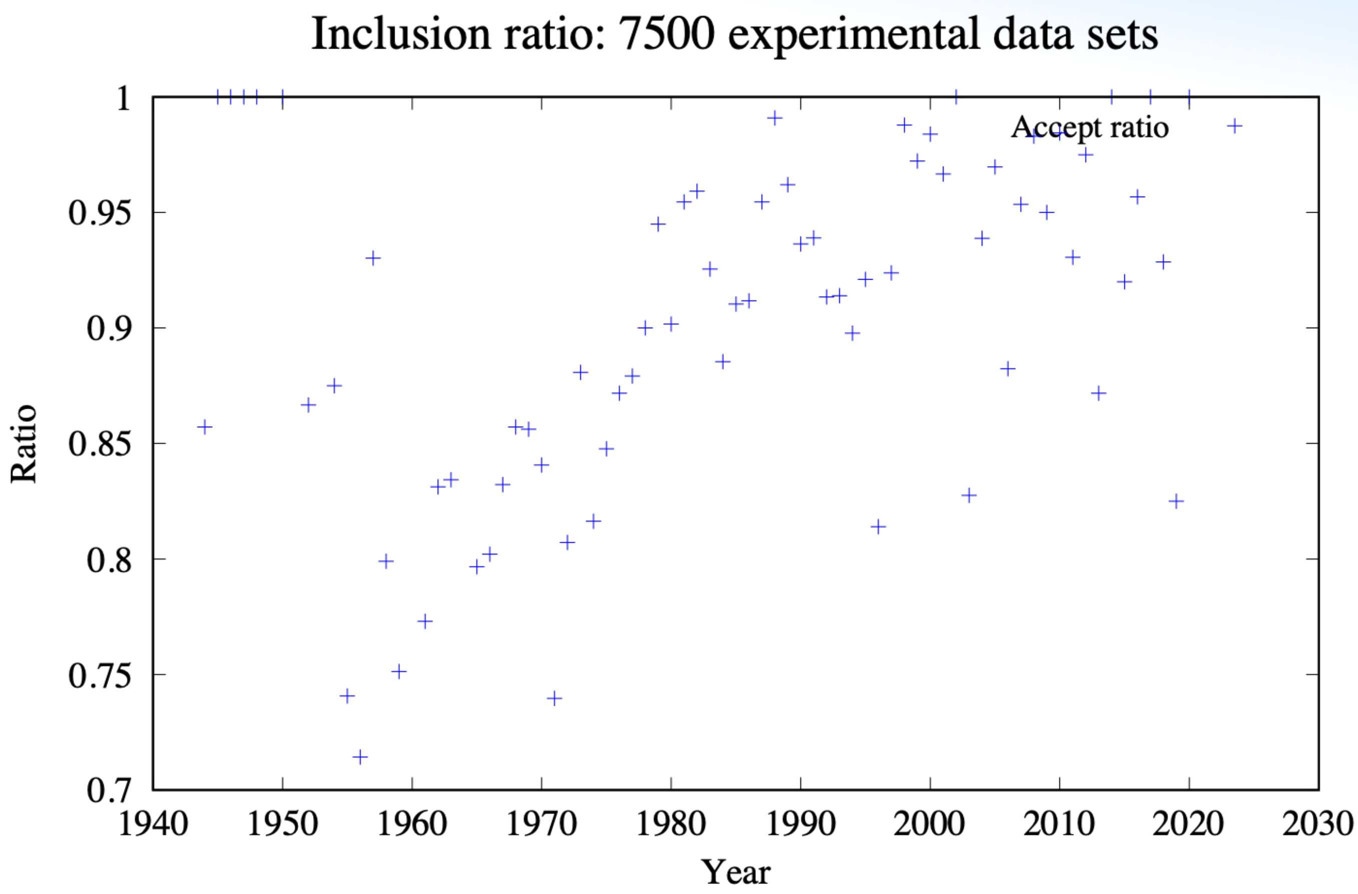
Segal's law: A man with a watch knows what time it is.
A man with two watches is never sure.



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

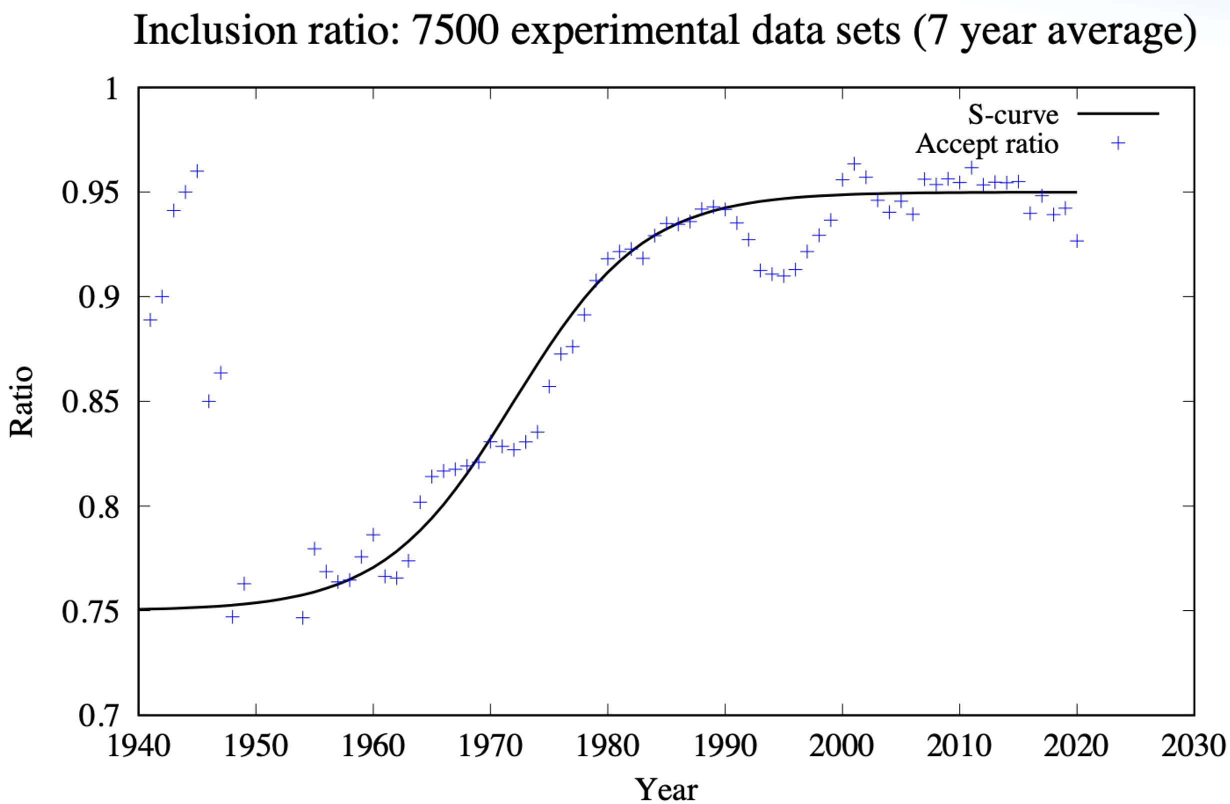


Outlier assignment



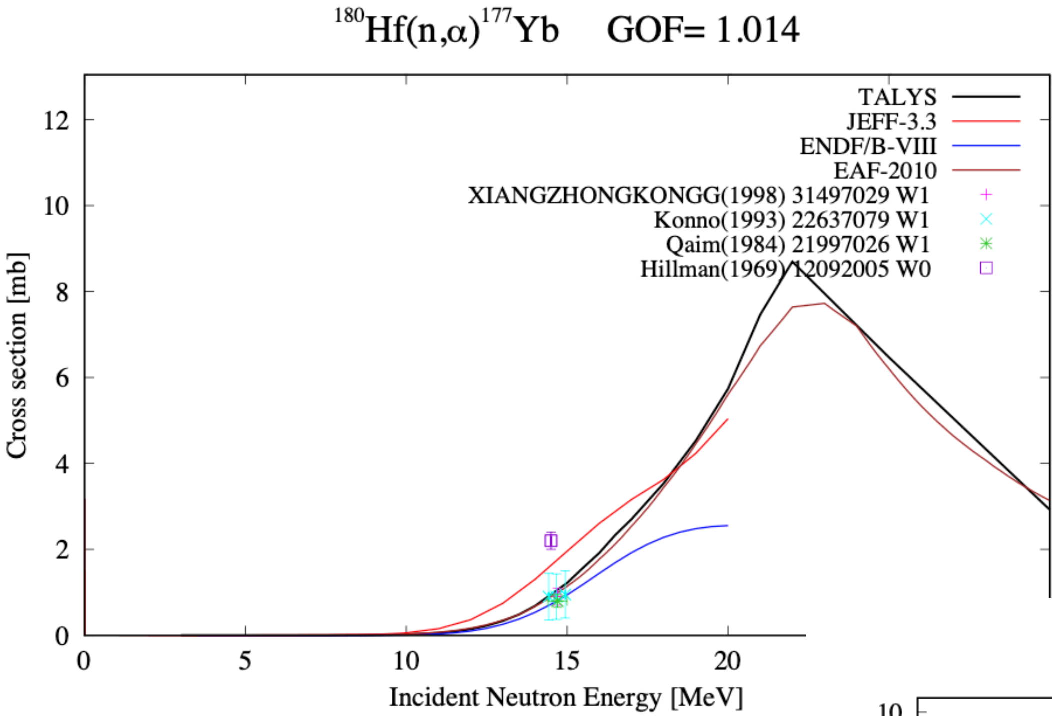
Summed over all (n,g), (n,f), (n,n'), (n,2n), (n,p), (n,a), (p,n), (g,n), (a,n), (d,n) reactions we could mine from EXFOR. 6500 accepts, 1000 rejects

Outlier assignment: a learning curve?

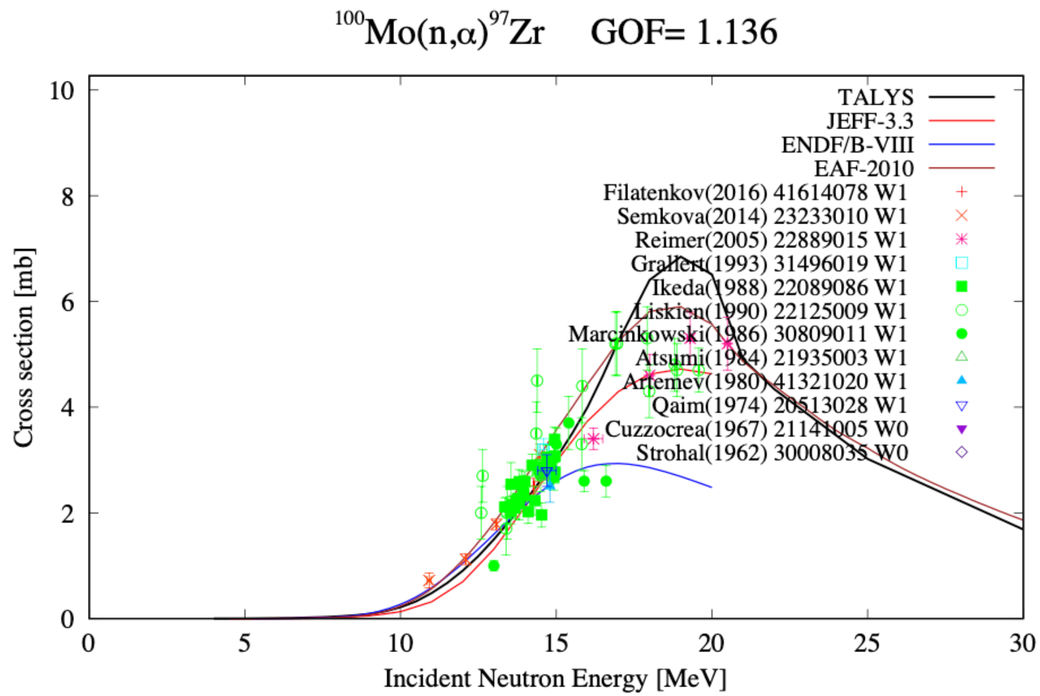


Other analyses possible:

- 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



rv(α)	Cstrip(α)	$g_{ph}(0)$	ctable(α)



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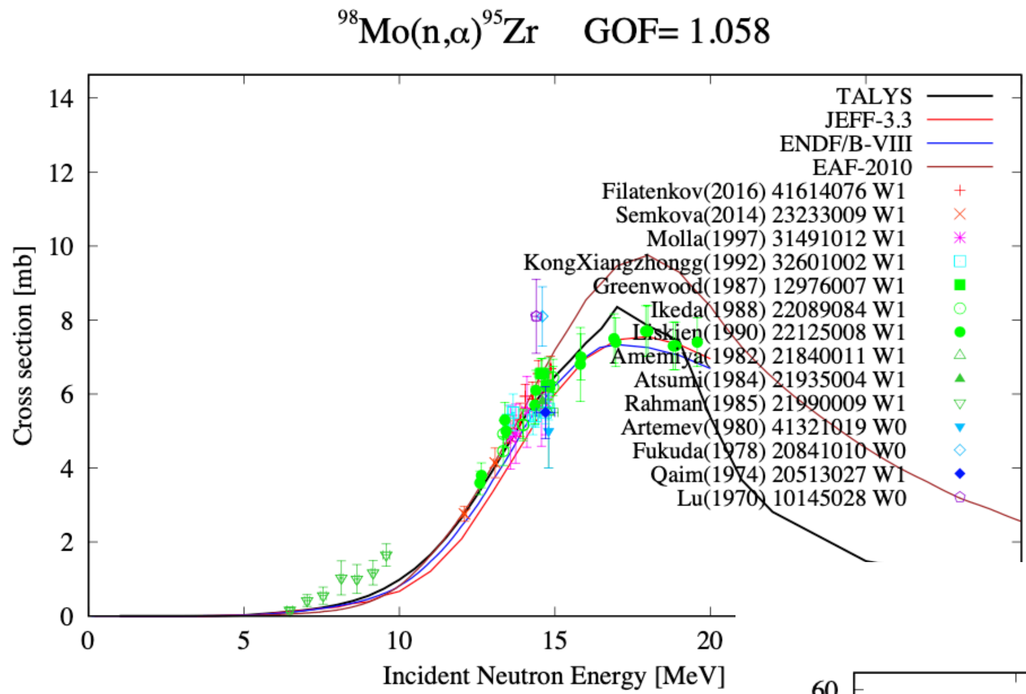
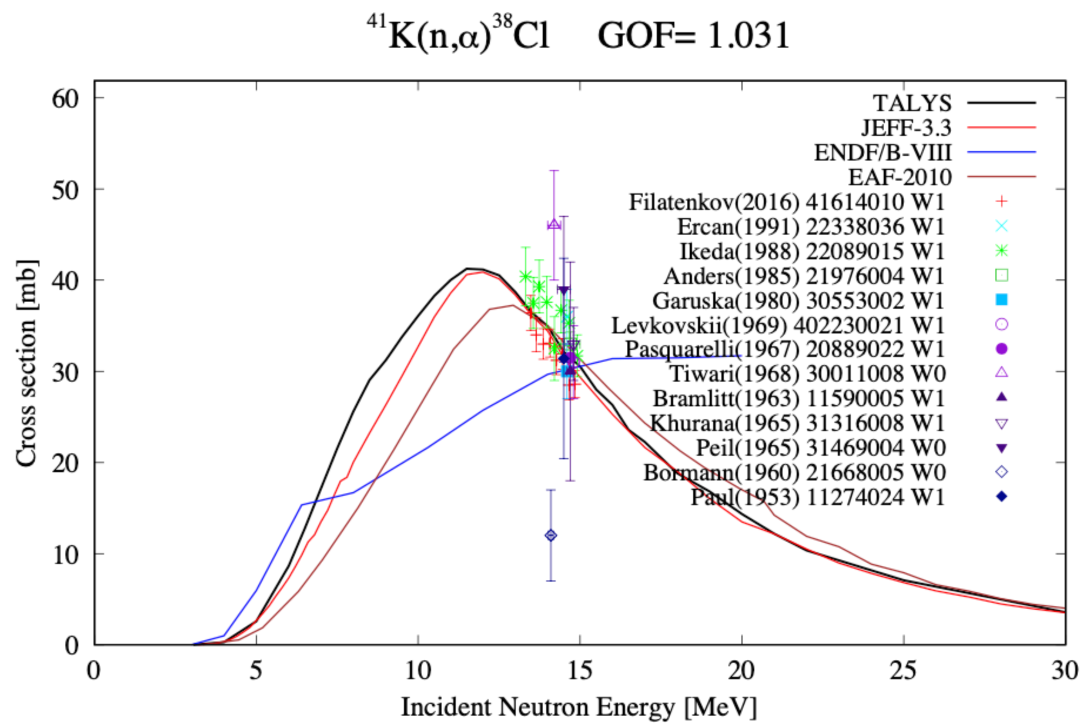


rv(α)	Cstrip(α)	$g_{ph}(0)$	ctable(α)



Can ML help here for unmeasured nuclides?

```
#Fitted parameters for (n,a)
#alphaomp     6
#ldmodel      5
#colenhance n
#nuclides    163
```

# Z	A	rv-a	cstrip	gadjust-0	ctable-a
4	9	1.00000	1.00000	1.00000	0.00000
5	10	0.21085	2.21082	1.64359	1.66936
5	11	0.11639	4.20759	1.67975	2.86544
6	12	0.48959	0.02787	1.21481	-0.44030
6	13	1.14567	1.21152	0.28736	1.64602
7	14	0.92861	0.31371	1.20199	-0.44030
8	16	1.11293	8.86975	0.84572	-0.92541
8	17	0.96495	2.43752	1.01593	-1.75192
8	18	0.22696	7.14760	0.90733	3.71203
9	19	0.89539	0.81826	1.10131	0.89627
10	20	0.91654	0.22750	1.38561	0.48796
10	21	0.95587	1.78427	1.20656	-0.34957
11	23	0.96817	0.53236	1.12941	0.17828
12	24	0.15974	2.96245	1.98147	-4.79352
12	25	0.29923	2.89807	1.63549	-7.02134
12	26	1.01241	1.33169	1.04872	0.34515
13	26	1.01873	0.76462	1.02671	-0.22364
13	27	1.02951	0.57233	1.14429	0.33124
14	28	0.96387	1.50342	1.25148	-2.66615
14	29	1.00194	1.35584	0.96969	0.90763
14	30	0.97181	2.11276	0.89030	-0.29783
15	31	1.04834	0.63263	1.01261	-0.08361
16	32	1.02006	0.36600	1.01089	-1.45398
16	33	0.27283	1.43855	2.22639	0.41495
16	34	0.97253	5.25031	1.13227	-0.07678
17	35	0.81829	0.89638	1.17646	-1.32655
17	36	0.99394	0.87904	1.08989	0.15246
17	37	0.93518	0.78168	0.83646	1.06129
18	36	0.45342	0.90863	0.94192	0.69087
18	40	0.85430	3.04631	1.36767	-0.46891
19	39	1.04509	1.20812	0.94896	-1.08482
19	41	1.01116	0.57316	1.04658	-0.24002
20	40	0.98171	0.22697	1.08368	-0.08800

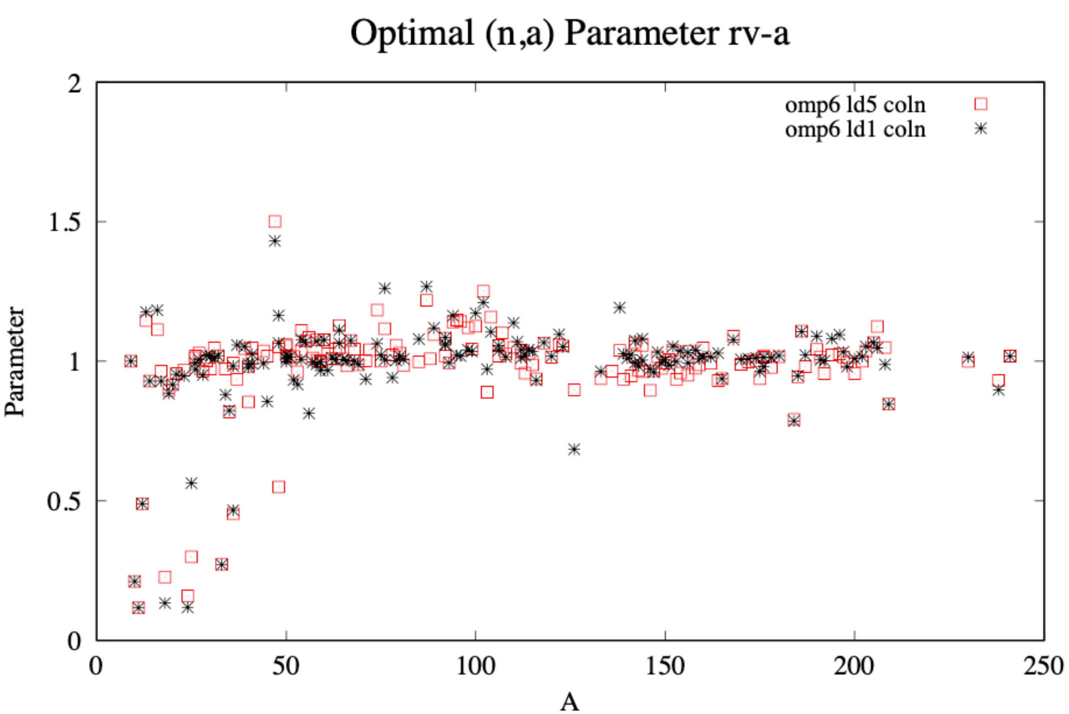
Can we discover trends that a human can not see?

We know that for $A < 20$ the physics of TALYS is not good enough

Are 160 nuclides enough to select a 20% training set?

Can an ML algorithm be predictive for nuclides at or close to the valley of stability?

Optical model parameter rv(a) for 2 different level density models



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Summary

- Trying to put human knowledge and opinions in consistent metadata
- Part of the objective to make TALYS more predictive and more descriptive (zeroing in on the truth)
- Accessible experimental database essential
- “Standard” optimisation with Nelder-Mead done for each reaction and target nuclide: scripts running scripts running search code running TALYS
- Per reaction channel: scattered parameters for up to 5 dimensions, for typically 200 nuclides, looking for trend and parameter guesses for unmeasured nuclides closed to the measured ones

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Thank you!