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TALYS for charged-particle cross sections: Predictive power and parameter fitting

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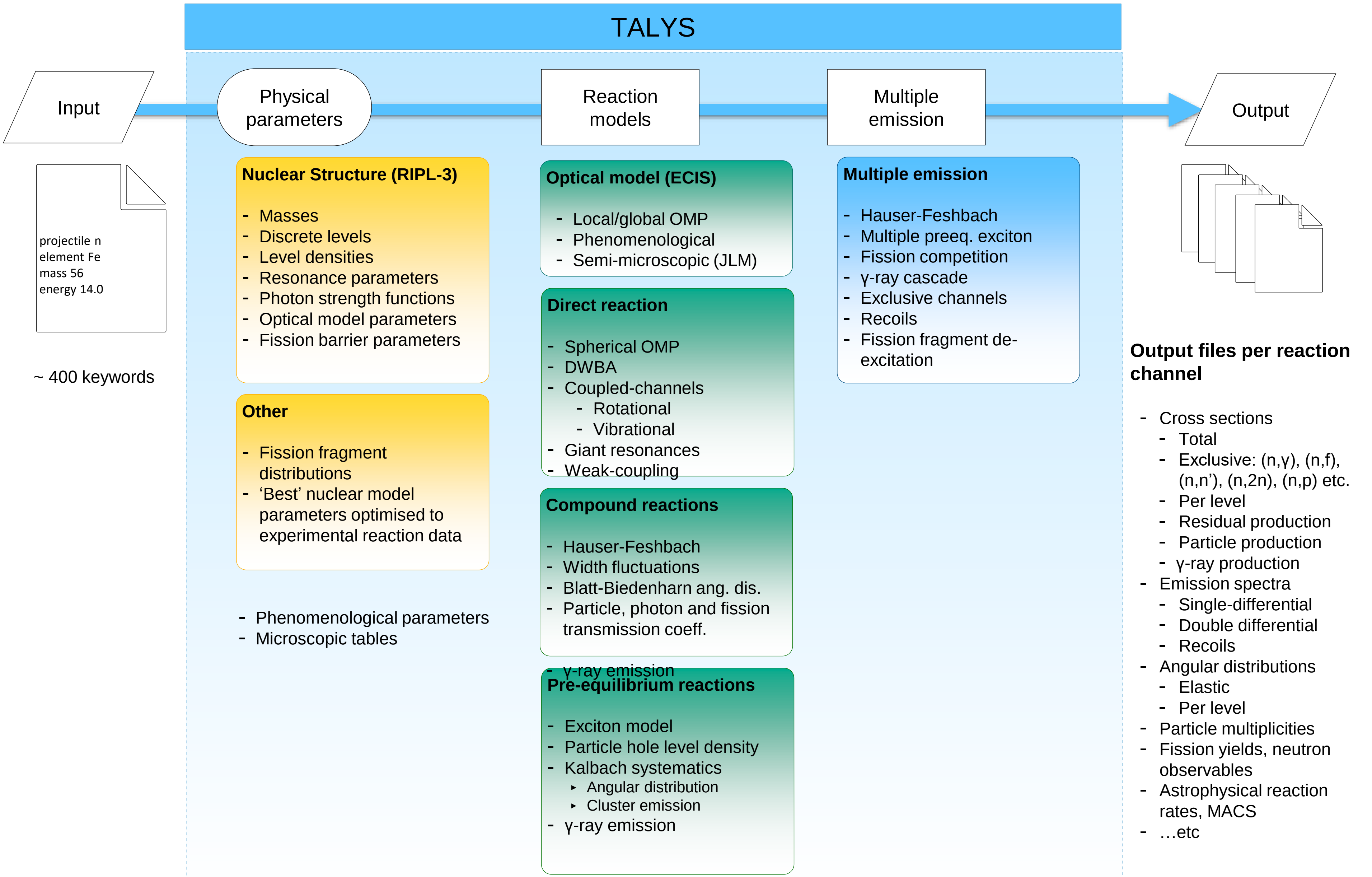
Introduction

- TALYS
- Global assessment of experimental data and outlier assignment
- Consistent and automated parameter fitting
- Special case: Th232(p,x)Ac225
- Conclusions


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

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Review

TALYS: modeling of nuclear reactions

This is now the basic reference for TALYS

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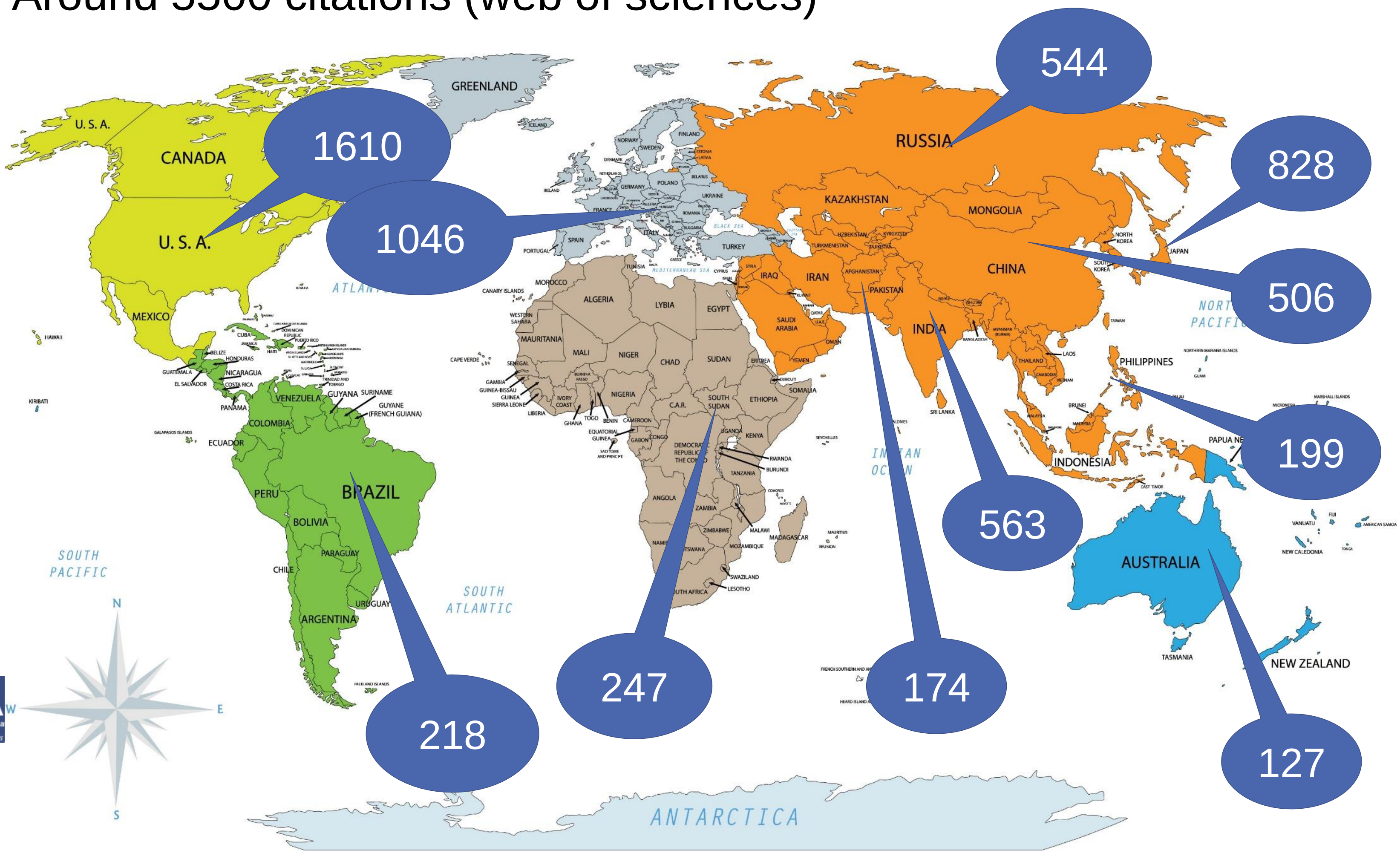
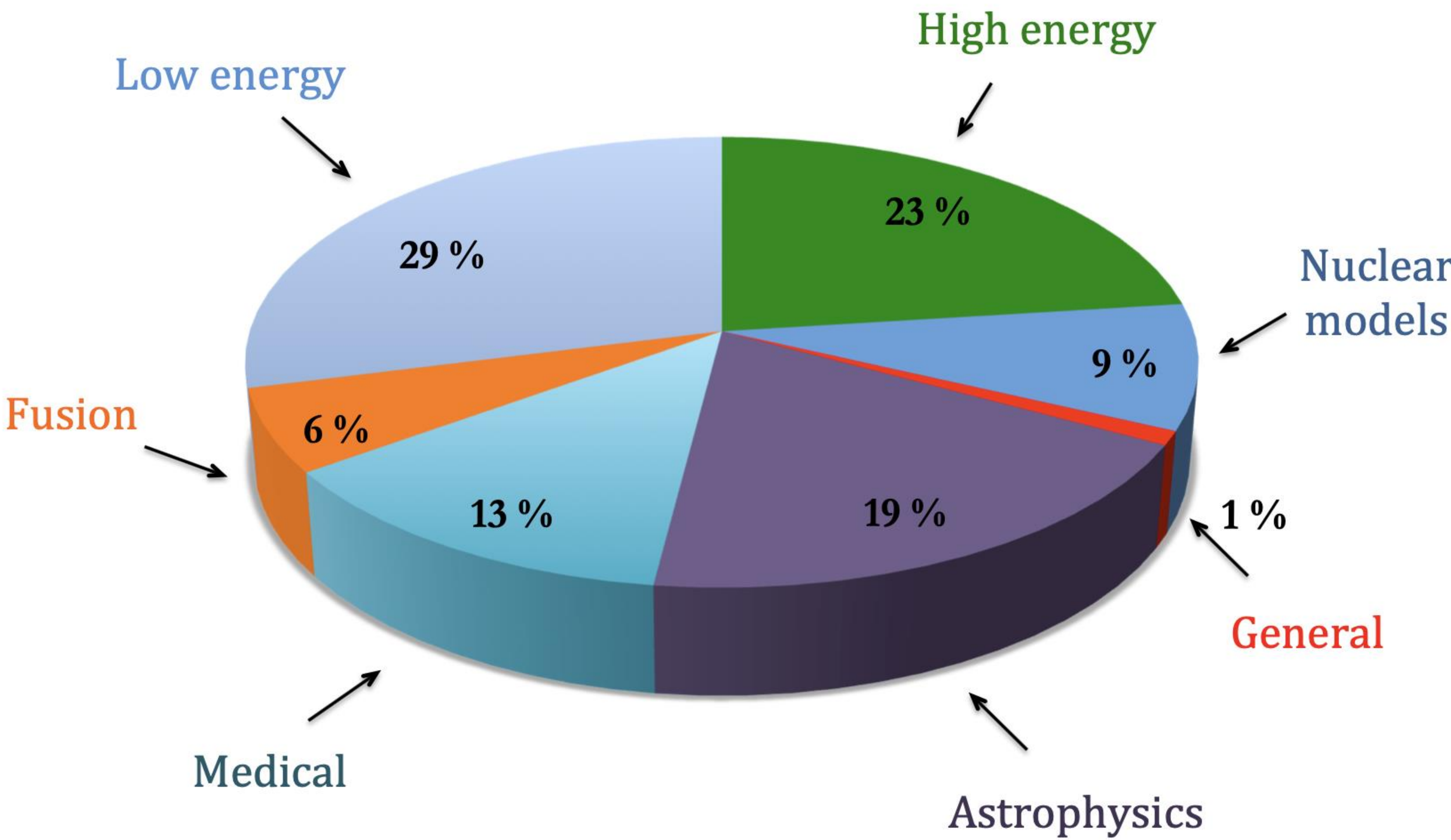
Communicated by Nicolas Alamanos

Abstract TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. A general overview of the implemented physics and capabilities of TALYS is given. The general nuclear reaction mechanisms described are the optical model, direct reactions, compound nucleus model, pre-equilibrium reactions and fission. The most important nuclear structure models are those for masses, discrete levels, level densities, photon strength functions and fission barriers. A wide variety of nuclear reactions simulated with TALYS will be demonstrated, ranging from low-energy neutron cross sections, astrophysics, high-energy charged particle reactions and other reactions. TALYS is a nuclear reaction software which aims to give a complete description of nuclear reaction observables, and to be an important link between fundamental nuclear physics and applications.

TALYS around the World (status 2022)

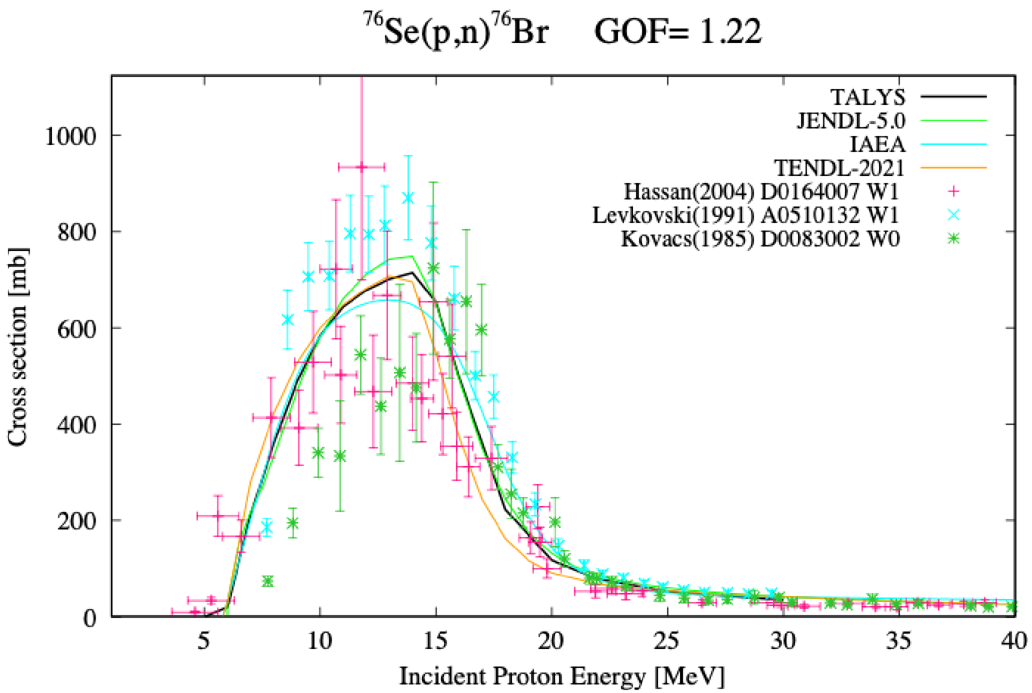
- Around 5500 citations (web of sciences)




High energy
23 %
Low energy
29 %
Nuclear models
9 %
Fusion
6 %
13 %
19 %
1 %
General
Medical
Astrophysics

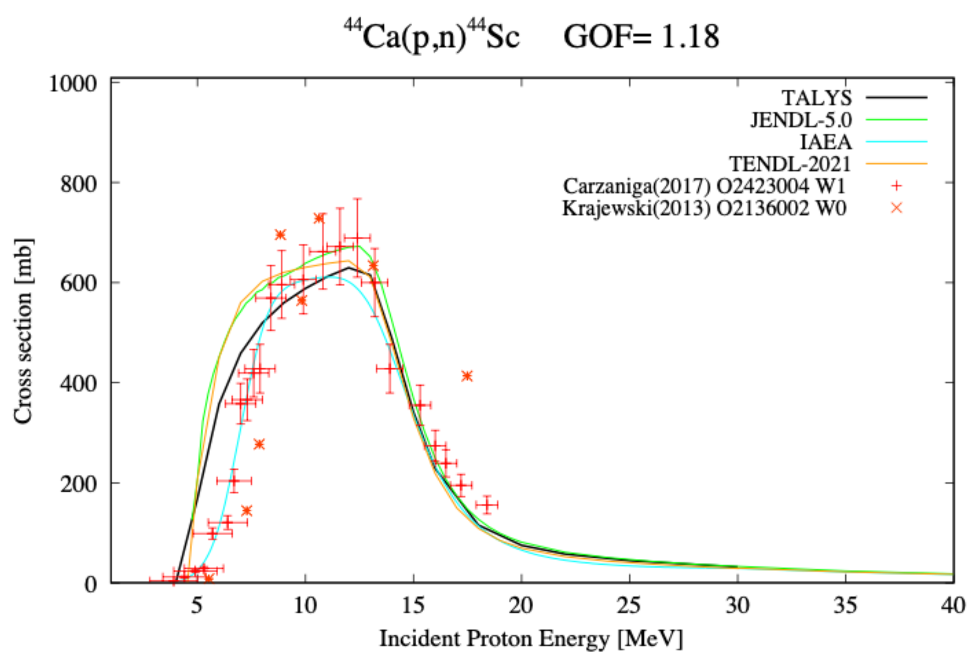
Zero-ing in on the truth

- Run TALYS for all projectiles, nuclides and energies with global settings
- Compare with the **entire** EXFOR database
  - Computational access to EXFORtables: directory-structured database with E-dE-xs-dxs data per measurement (from XC5 file, Viktor Zerkin)
  - Automatic normalisation to new monitor and decay data
  - Assign outliers in EXFOR (Exforcism)
    - comparison with nuclear data libraries,
    - comparison with TALYS
    - comparison with other experimental data sets
    - quantify historical evaluator's opinion in consistent metadata
- Assess predictive power of TALYS as a function of energy, reaction channel and mass range
- Zoom in on specific reaction channel with automated optimisation, varying a restricted set of TALYS parameters



W0: outlier-by-eye

Challenge: EXFOR data may be hidden under different reaction identifiers. Completeness of experimental data from EXFOR to EXFORtables not ensured, some data sets may be missing.



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

EXFOR outlier assignment

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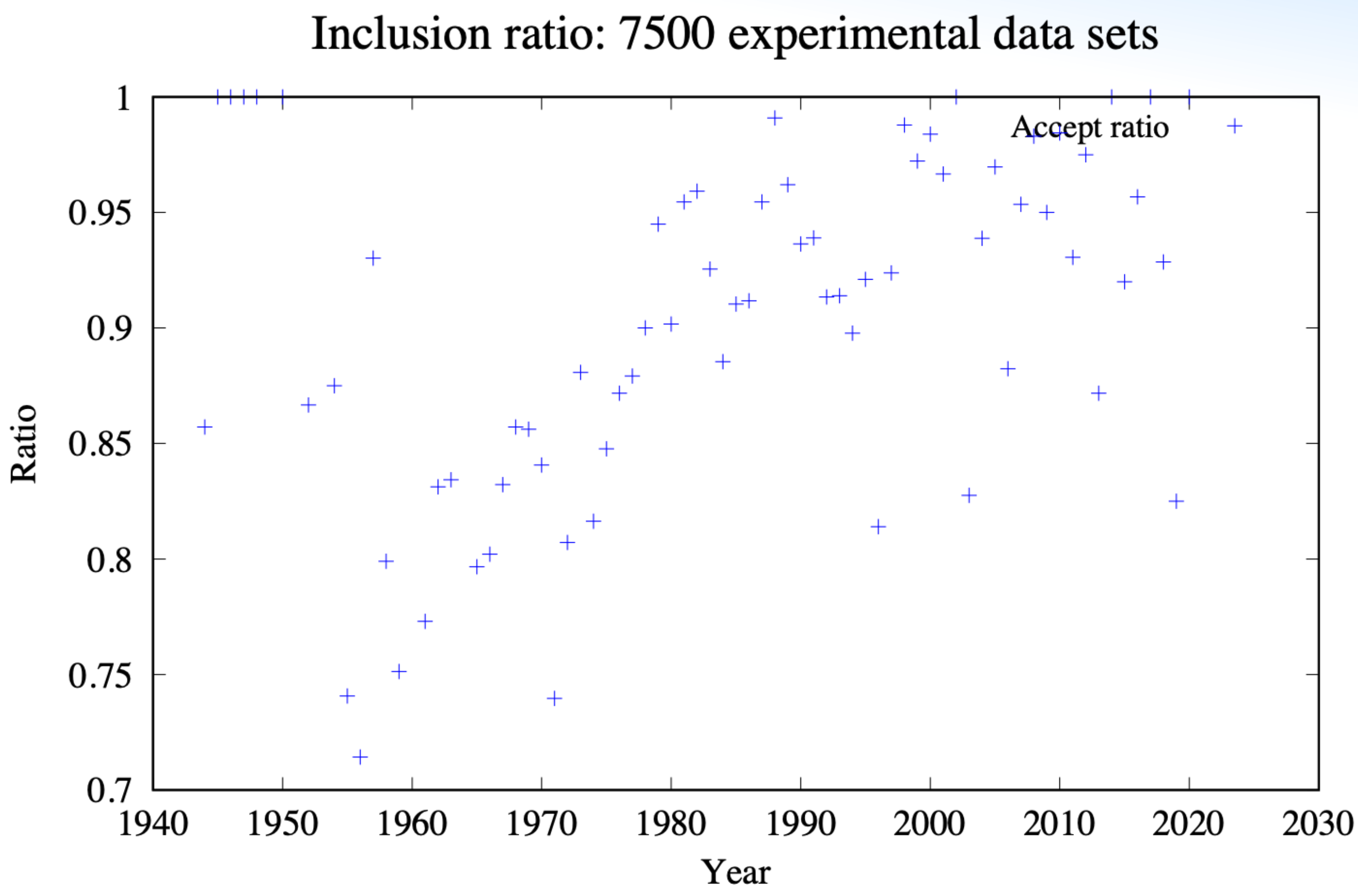
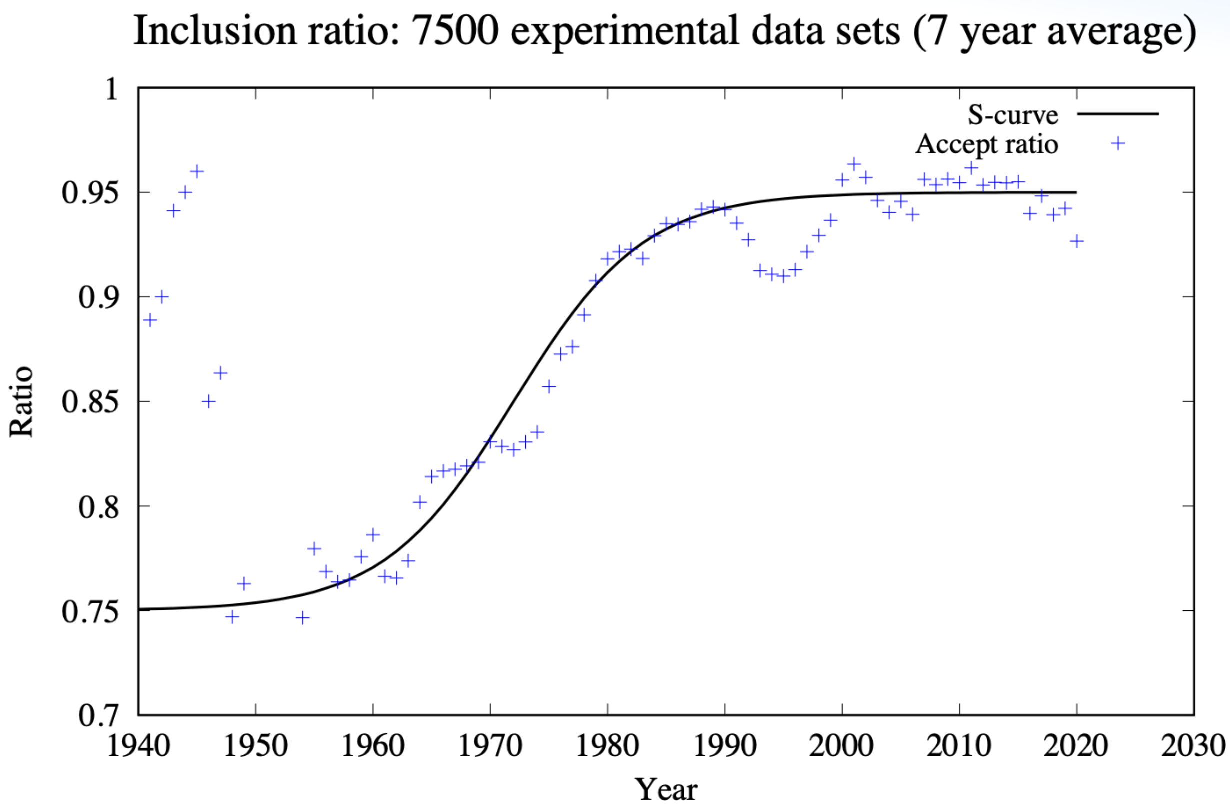


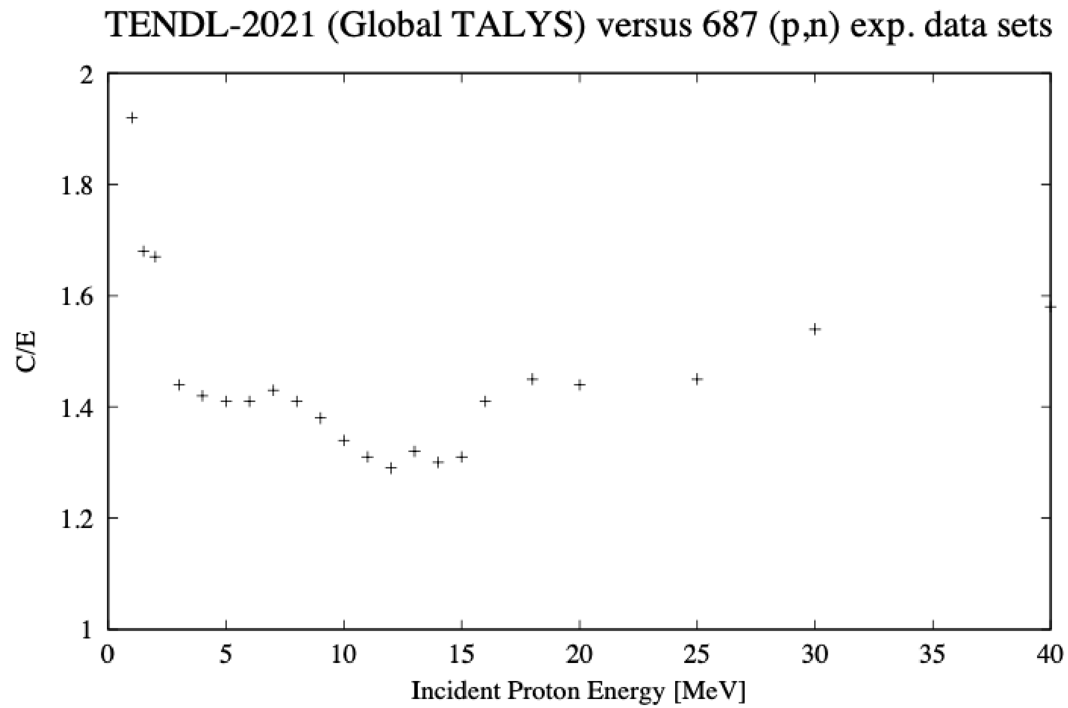
Summed over all (n,g), (n,f), (n,n'), (n,2n), (n,p), (n,a), (p,n), (g,n), (a,n), (d,n) reactions we could mine from EXFOR. 6500 accepts, 1000 rejects

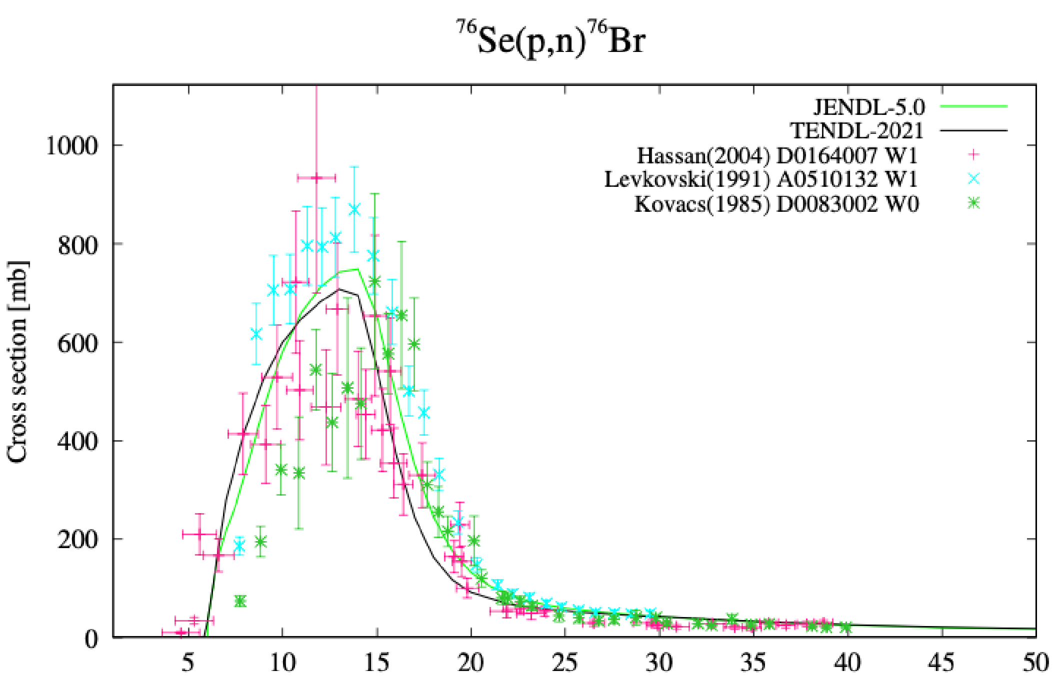
EXFOR outlier assignment: a learning curve?



Other analyses possible:

- per reaction channel
- per author, co-author, lab, etc (probably should not publish THAT)
- per incident energy (e.g. 14 MeV)
- re-insert this as prior in the next Bayesian update





Global predictive power for (p,n): ~30% around the peak

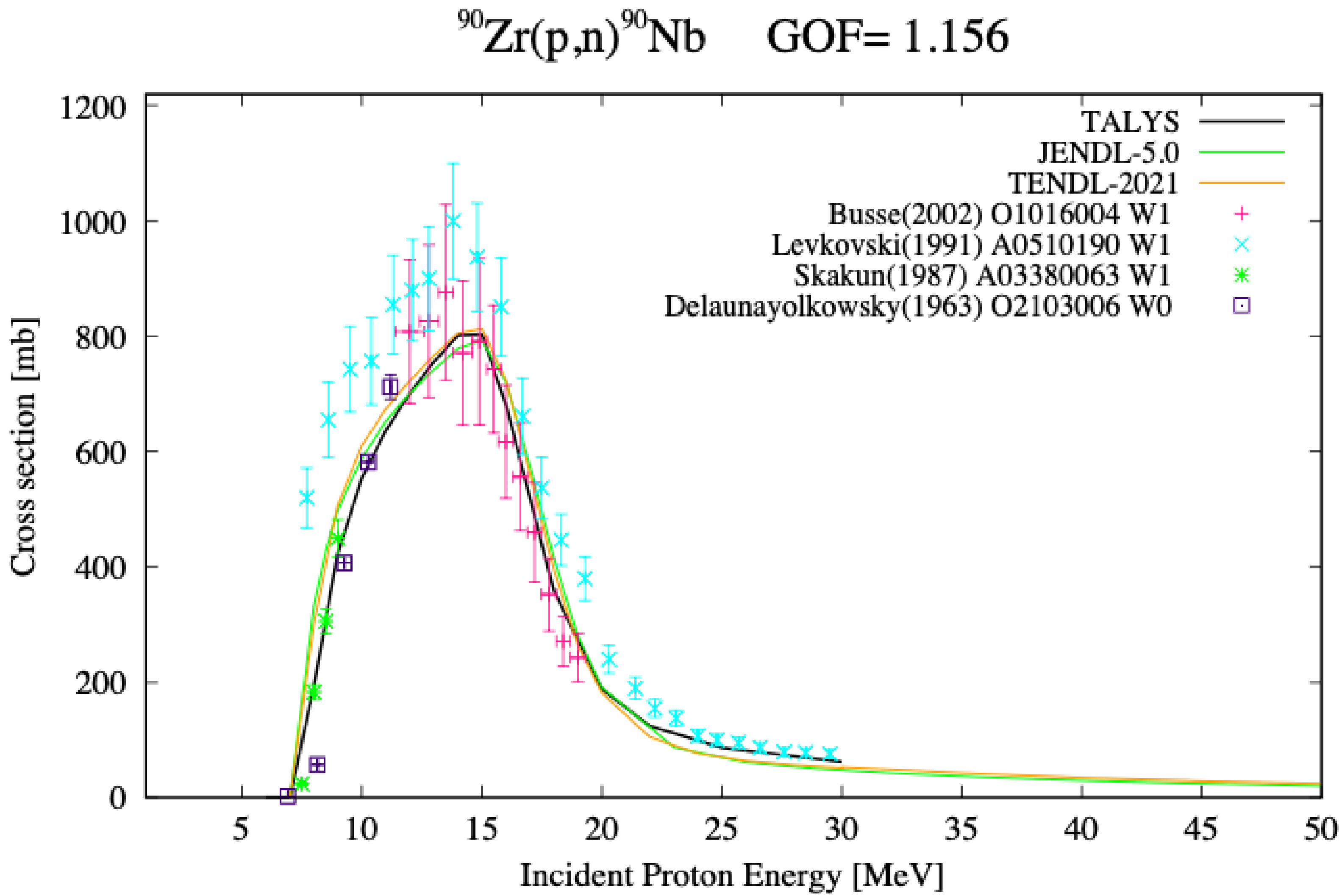
(p,2n): ~40%
(alpha,n): ~45%
(d,n): ~60%

Common trend for all threshold reactions. Relative deviation is

- Large near threshold (> 2)
- Small near peak
- Larger in the tail

Global predictive power is energy dependent

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

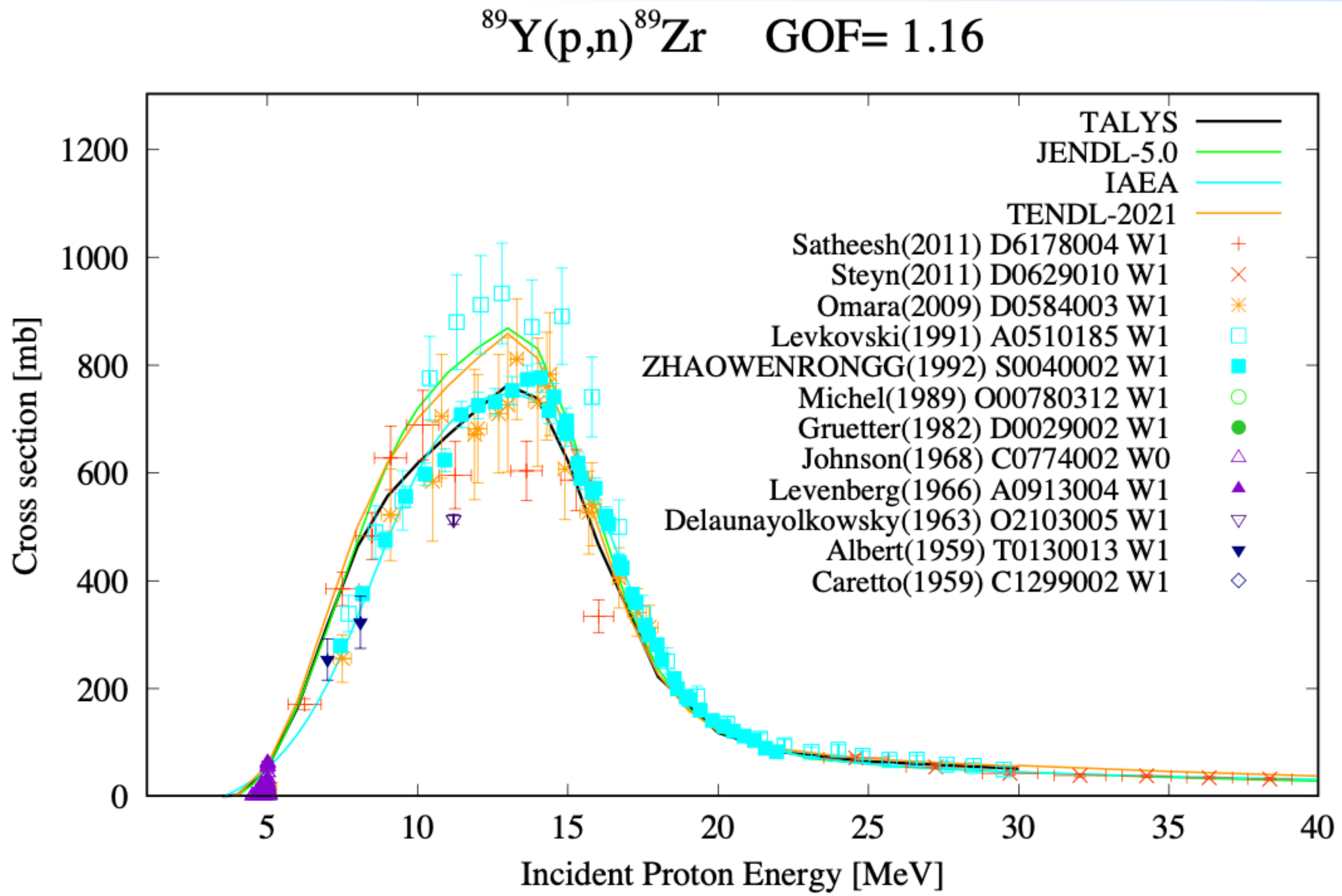


TALYS parameters for optimization

Reaction	Nuclides in EXFOR	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

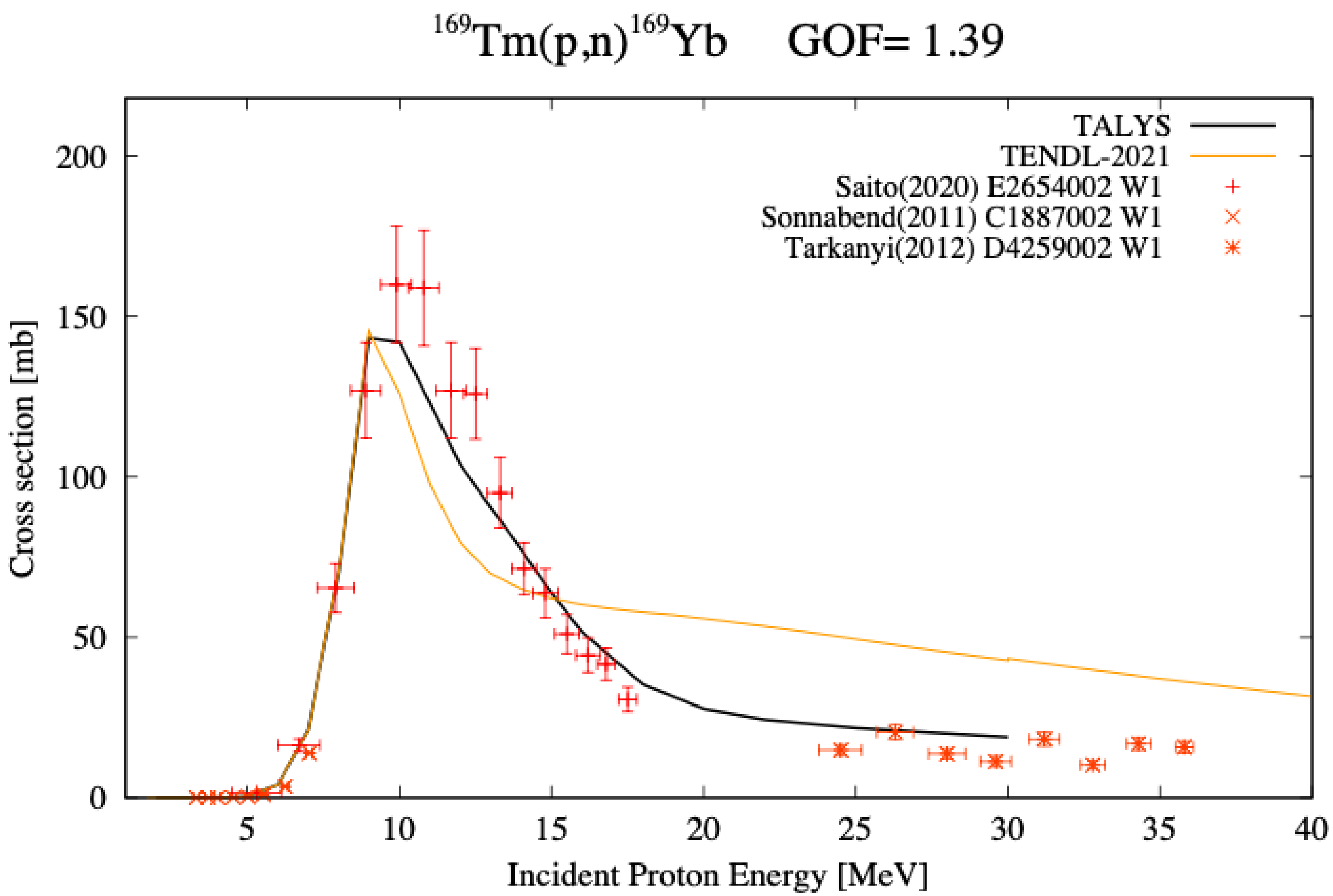
Automated fit (excluding outliers)




```
rvadjust      p    0.92464
rwdadjust     p    0.99070
rvadjust      n    1.00842
gadjust        40  90    1.11250
gadjust        40  89    1.10842
ctableadjust   40  89    0.65147 0
```

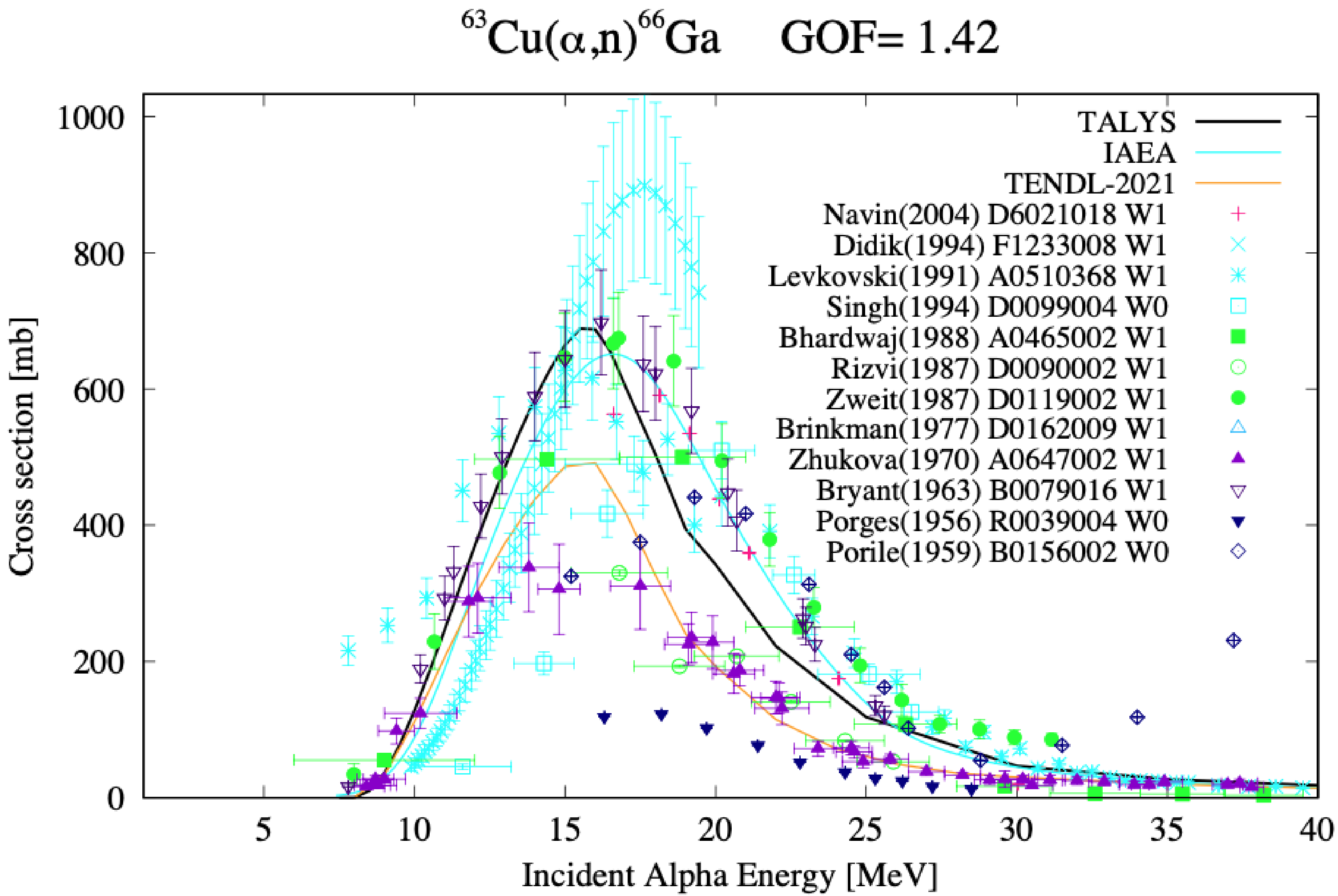
142 nuclides

Sometimes significant differences




```
rvadjust       p     0.97574
rwdadjust      p     0.87606
rvadjust       n     1.02987
gadjust         70 170     1.18983
gadjust         70 169     0.92669
ctableadjust    70 169     0.31802 0
```

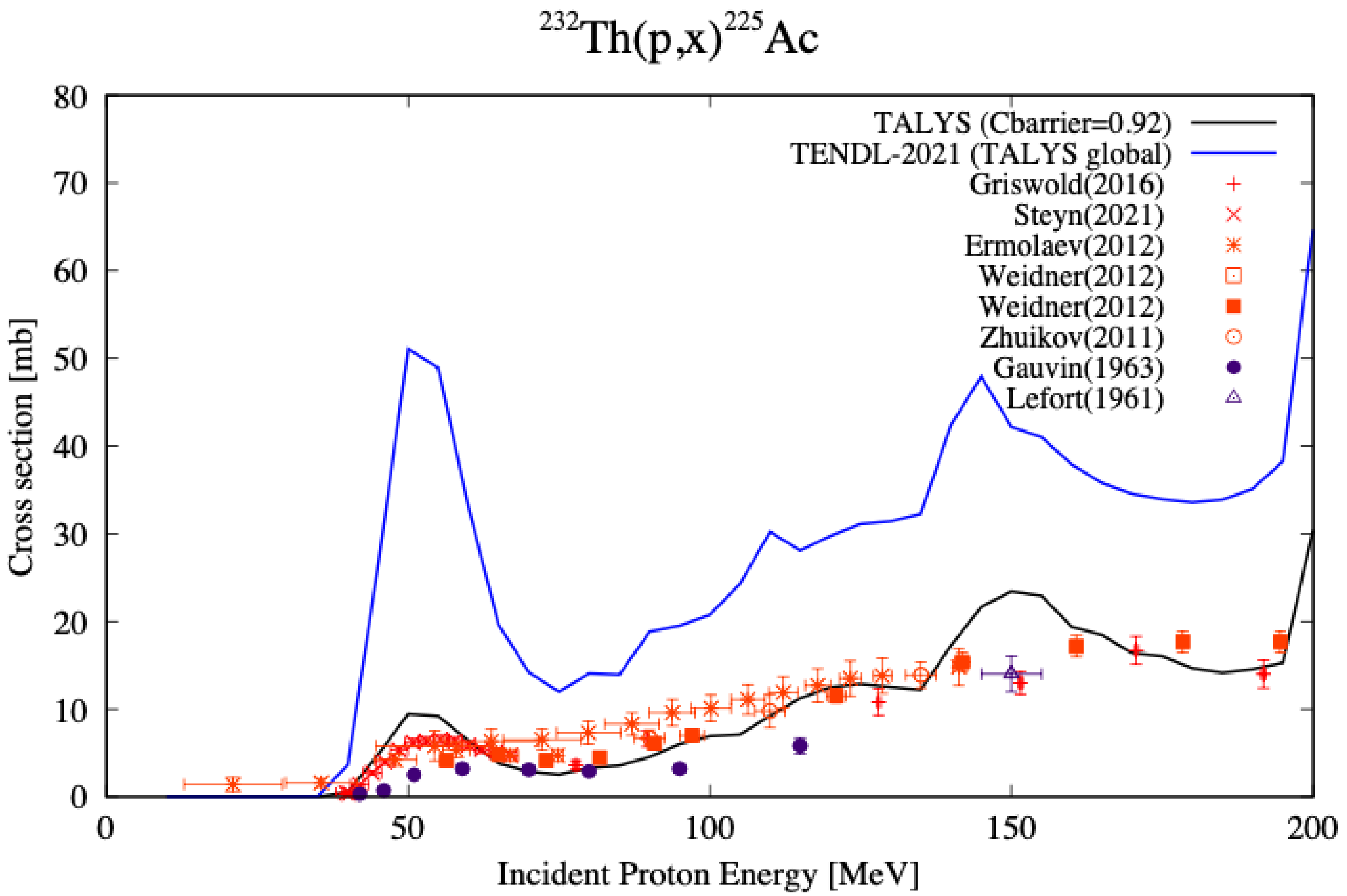
TENDL-2023 will have optimised fits




```
rvadjust      a     1.00307
rwdadjust     a     0.93064
rvadjust      n     1.01999
gadjust        31   67      0.98591
ctableadjust   31   66      0.88253 0
```

93 nuclides

Actinides: uncertainty due to fission

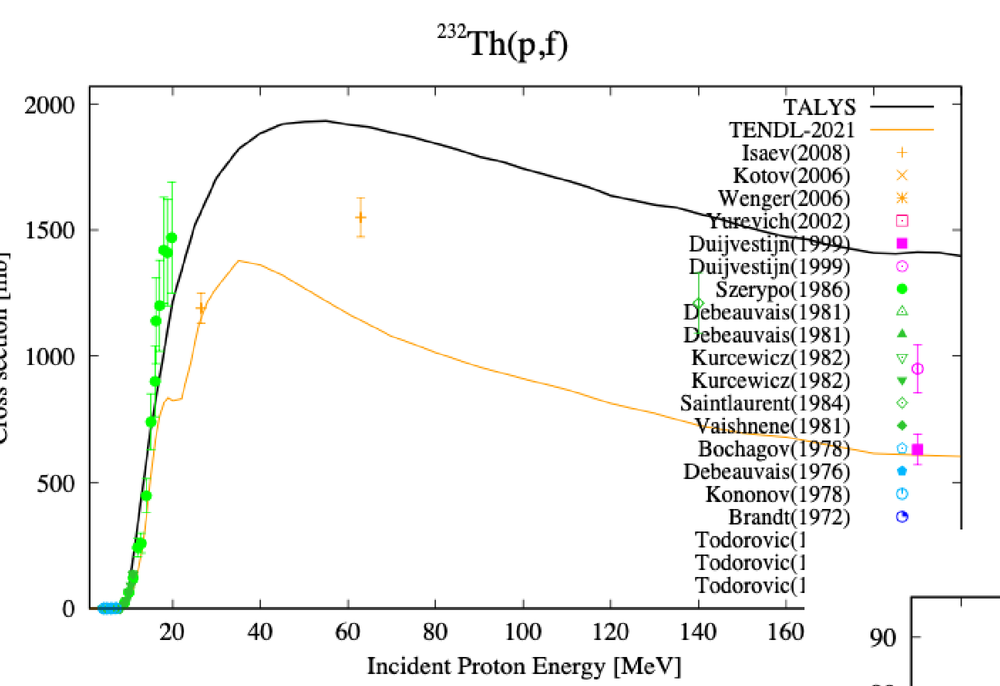


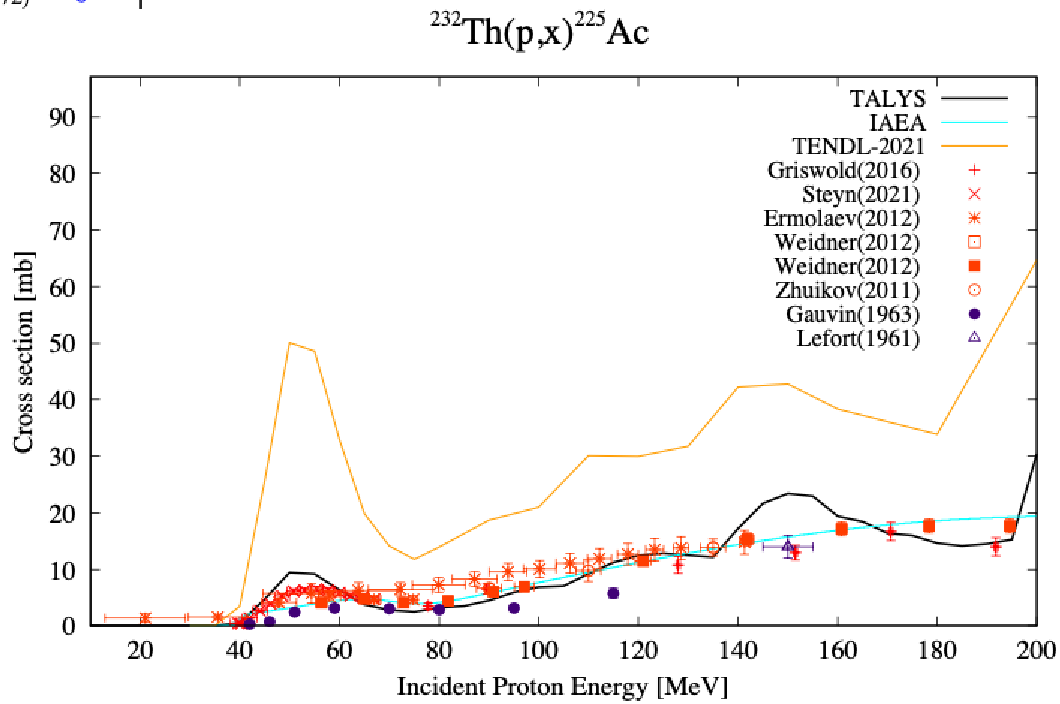
TALYS input file:

```
projectile p
element Th
mass 232
energy 10. 200. 5.
partable y
bins 100
Cbarrier 0.92
```

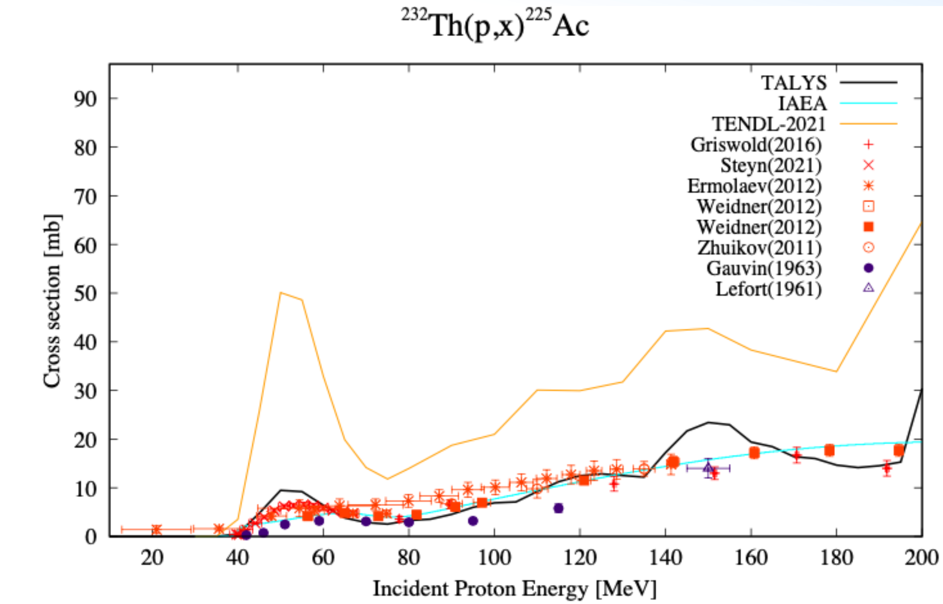
TALYS-2: one parameter ‘Cbarrier’ to reduce/increase all fission barriers

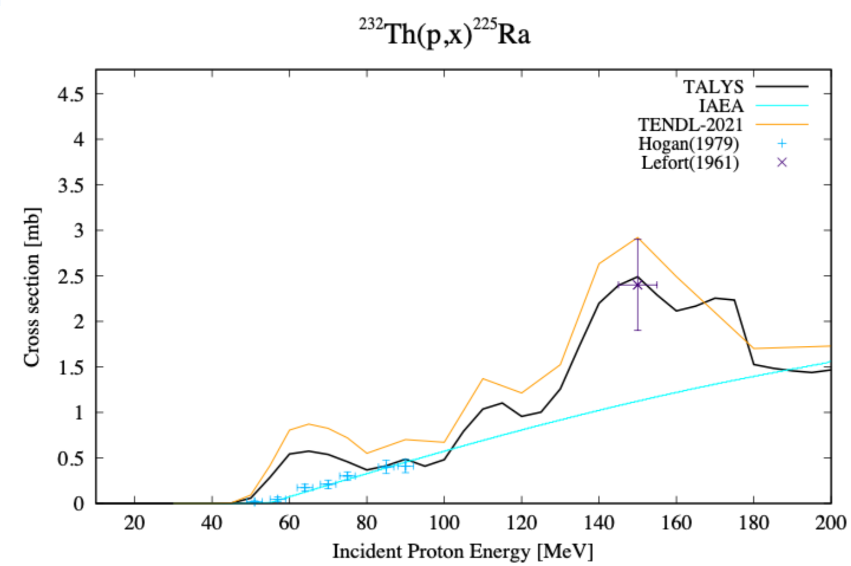
Th232(p,f) could be higher compared to TENDL-2021

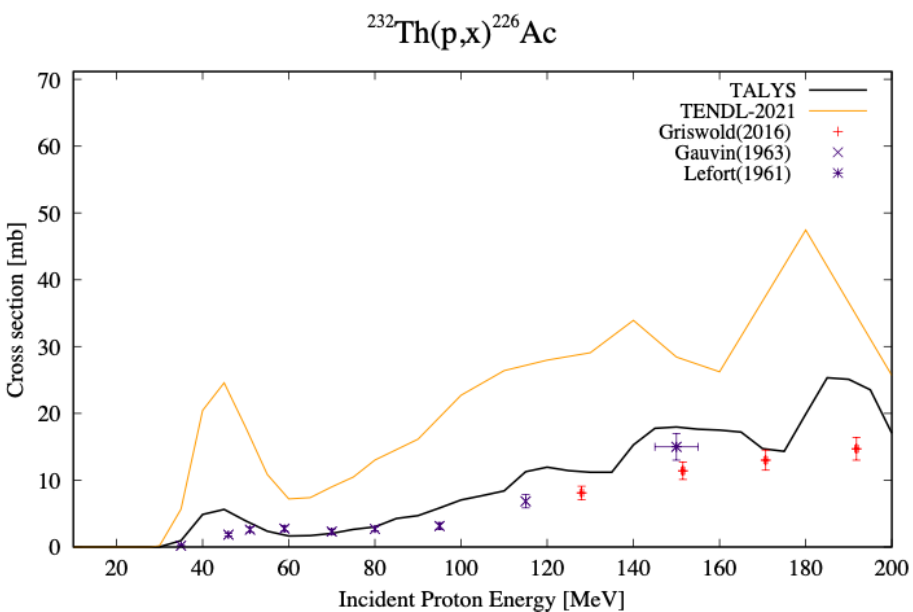


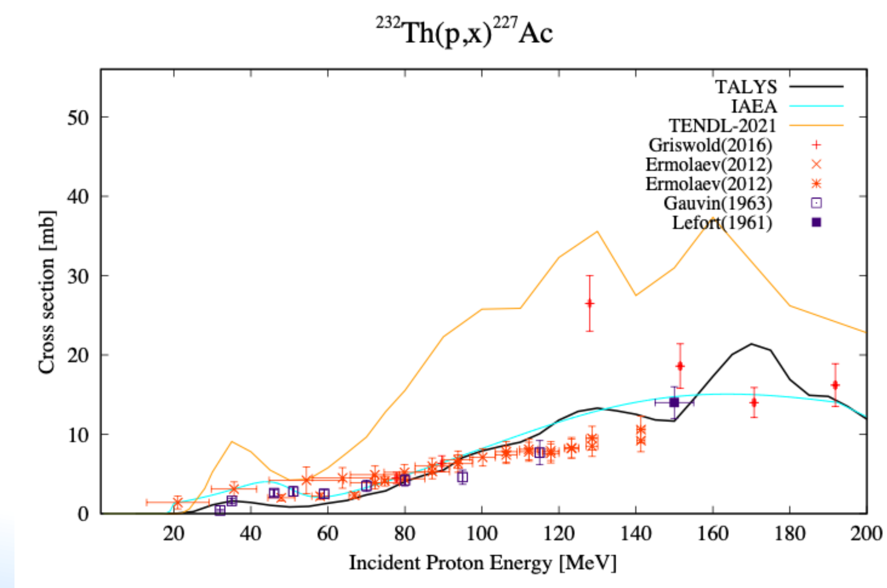


Consistency with neighbouring channels

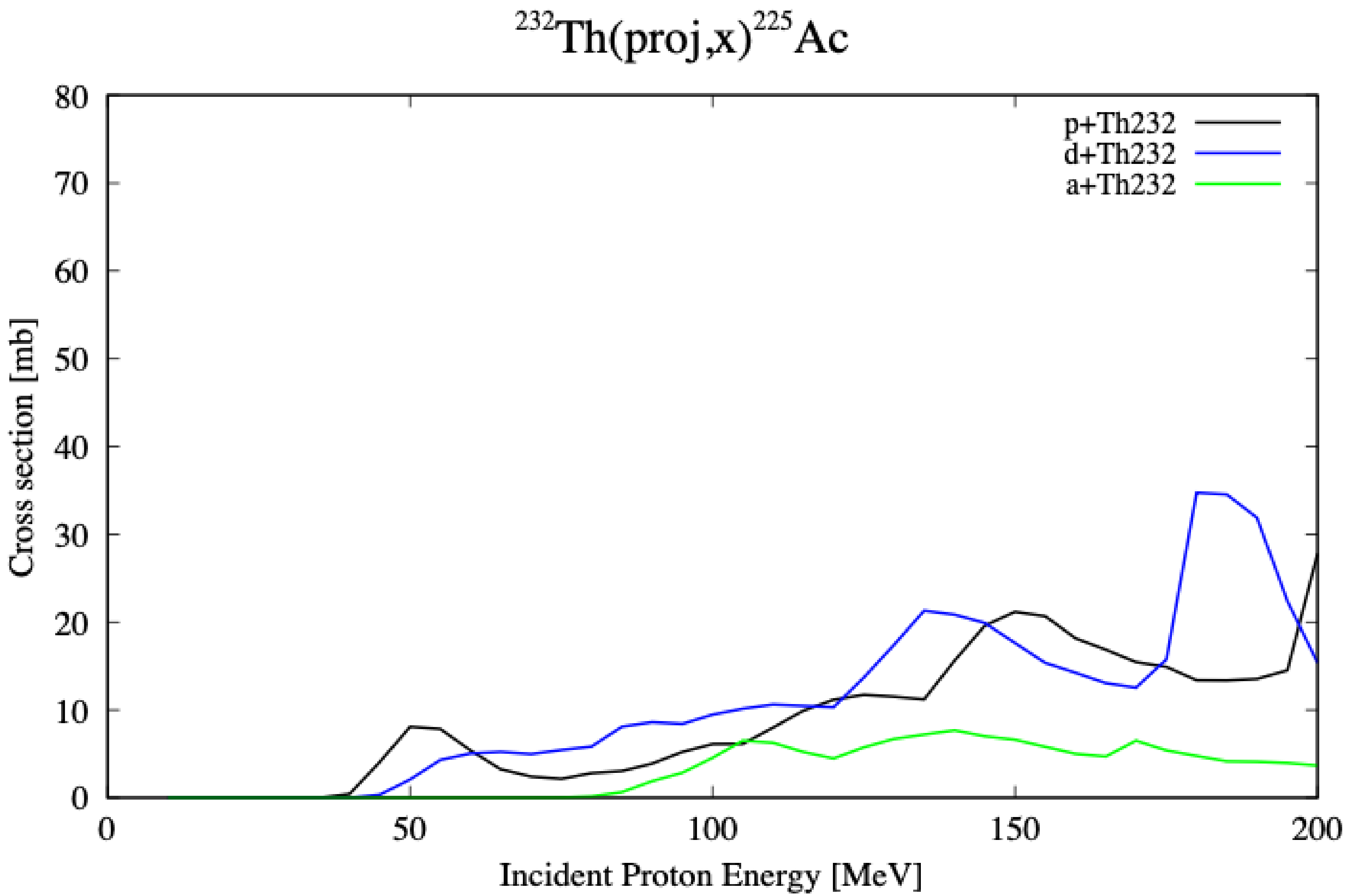








Other projectiles?



Conclusions

- TALYS a stable and well-tested (thanks to you!) tool for reasonable to good predictions up to 200 MeV
- TALYS-2 will be released in December 2023
- Automated optimisation to many reaction channels with a relatively small number of TALYS parameters
  - Requires computational access to entire EXFOR database at once
  - Requires extensive outlier database
- TENDL-2023 will contain optimised excitation functions

Thank you!