IAEA

From nuclear data to nuclear energy applications

Arjan Koning

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Contents

- Nuclear data: some essential databases
- Nuclear reaction simulation: TALYS
- Towards nuclear energy applications
  - From photon strength functions and level densities to fission products
  - From isomeric branching ratios to decay heat for fusion
- Summary

Nuclear data landscape

Number of target nuclides:
Stable: 287
τ > 1 year + stable: 407
τ > 1 day + stable: 675
τ > 1 hour + stable: 995
τ > 1 sec + stable: 2854

Nuclides with EXFOR cross sections:
(n,tot): 347
(n,el): 223
(n,γ): 402
(n,f): 32
(n,n'_1): 176
(n,2n): 198
(n,p): 212
(n,α): 169

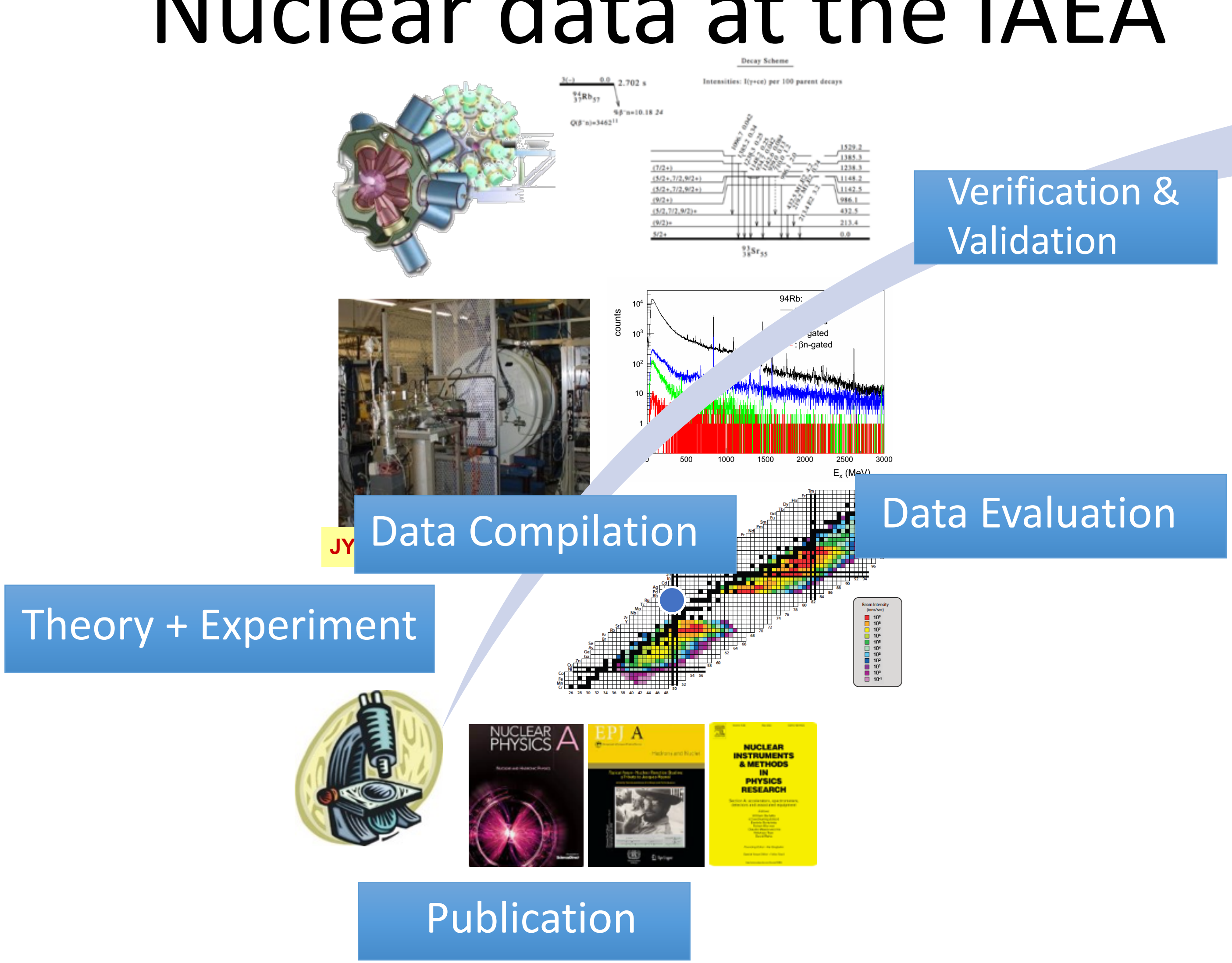
Exp. nuclear structure:
Discrete levels: ~1200
Masses: 2550 (3558)

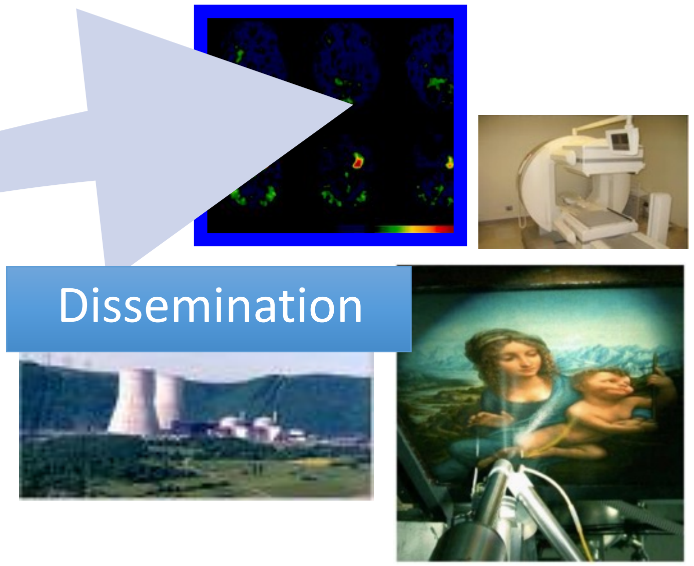
Nuclides in nuclear data libraries:
ENDF/B-VIII.1: 495
JENDL-5.0: 667
JEFF-4.0: 547
TENDL-2023: 2854

Material	Experimental data	Nuclear models	Evaluation/Validation
(1) The Big Three: $^{235,238}U$, ^{239}Pu	High-quality measurements (< 2 % for important channels), directly (cor)related with neutron standards More than 10-20 exp. data sets in same energy range	Models overruled by experimental data for important channels: complete normalization of model results	Need for reliable experiment-based covariance data Direct feedback from integral measurements: criticality, reactor systems, inventory, etc.
(2) Important coolants and structural materials: H, C, O, Fe	Many experimental data sets for many channels uncertainty < 10% (dosimetry reactions < 3 %)	Precise nuclear model calculations with many parameters to interpolate between measurements	Sometimes differential data overruled by data with better integral performance
(3) Other coolants and structural materials: N, Na, Al, Si, Ti, V, Cr, Mn, Ni, Cu, Zr, Mo, W, Pb, Bi,...		Parameter adjustment for well-measured channels	
(4) Other important actinides: ^{232}Th, ^{233}U, $^{240-242}Pu$	Many experimental data sets for only the most important channels	Models used for almost all secondary distributions (angles, spectra, photons, etc.)	Isolated benchmarks available for transport or activation analyses
(5) Important fission products: ^{99}Tc, ^{103}Rh, ^{129}I,....			
(6) Breeding materials and reflectors: Li, Be,...		Model calculations with a few parameters adjusted to the few exp. data sets	
(7) Absorbers: Gd, Hf,...			
(8) Minor actinides: $^{241,242m,243}Am$, ^{237}Np,....	Experimental data only available for (low energy) total, elastic, capture (resonance parameters) and a few other channels		Global covariance estimates
(9) Remaining materials (natural isotopes): P, S, Cl, Ca,....			Automatic production of data libraries
(10) Remaining long-lived nuclides ($\tau > 1$ year)			
(11) Medium long-lived nuclides (1000 sec. ¡ $\tau < 1$ year)	(Almost) no experimental data	Complete reliance on nuclear models, preferably microscopic	(Almost) no integral experimental data
(12) Short-lived nuclides ($\tau < 1000$ sec.)			Astrophysics

D. Rochman and A.J. Koning, TENDL-2011: TALYS-based Evaluated Nuclear Data Library, PHYSOR2012

Nuclear data at the IAEA

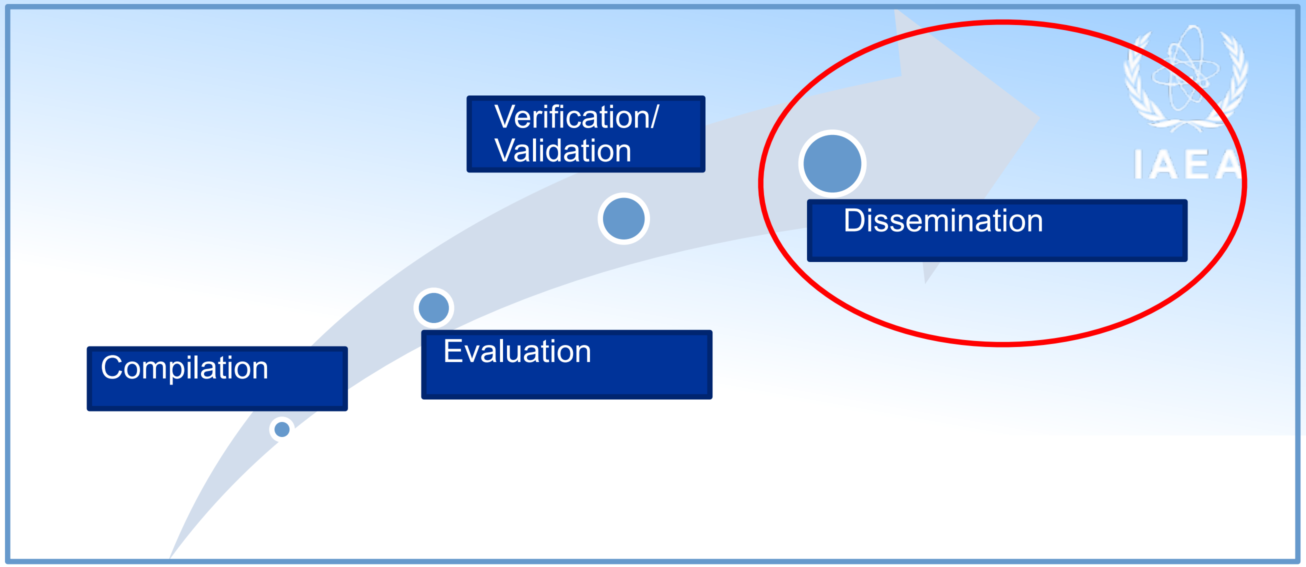




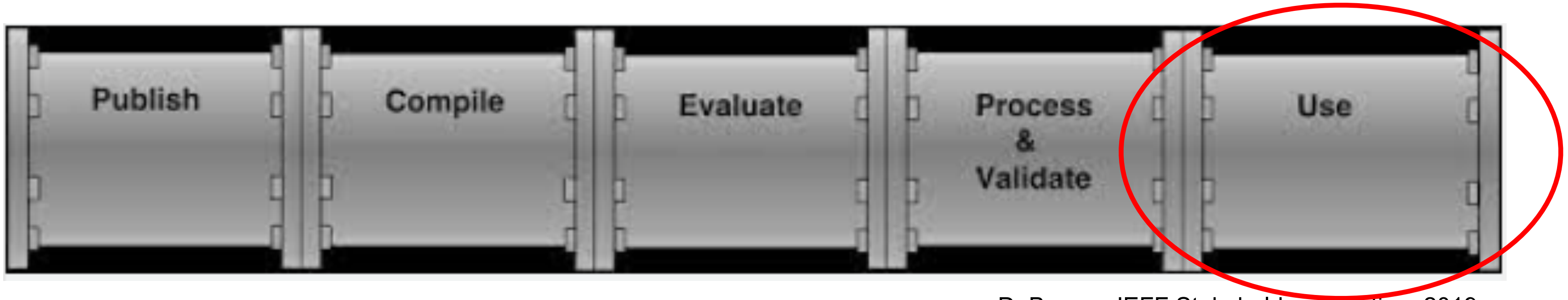
Applications:

organised
complete
recommended
traceable
easily retrievable

Nuclear Data



Nuclear Data Pipeline



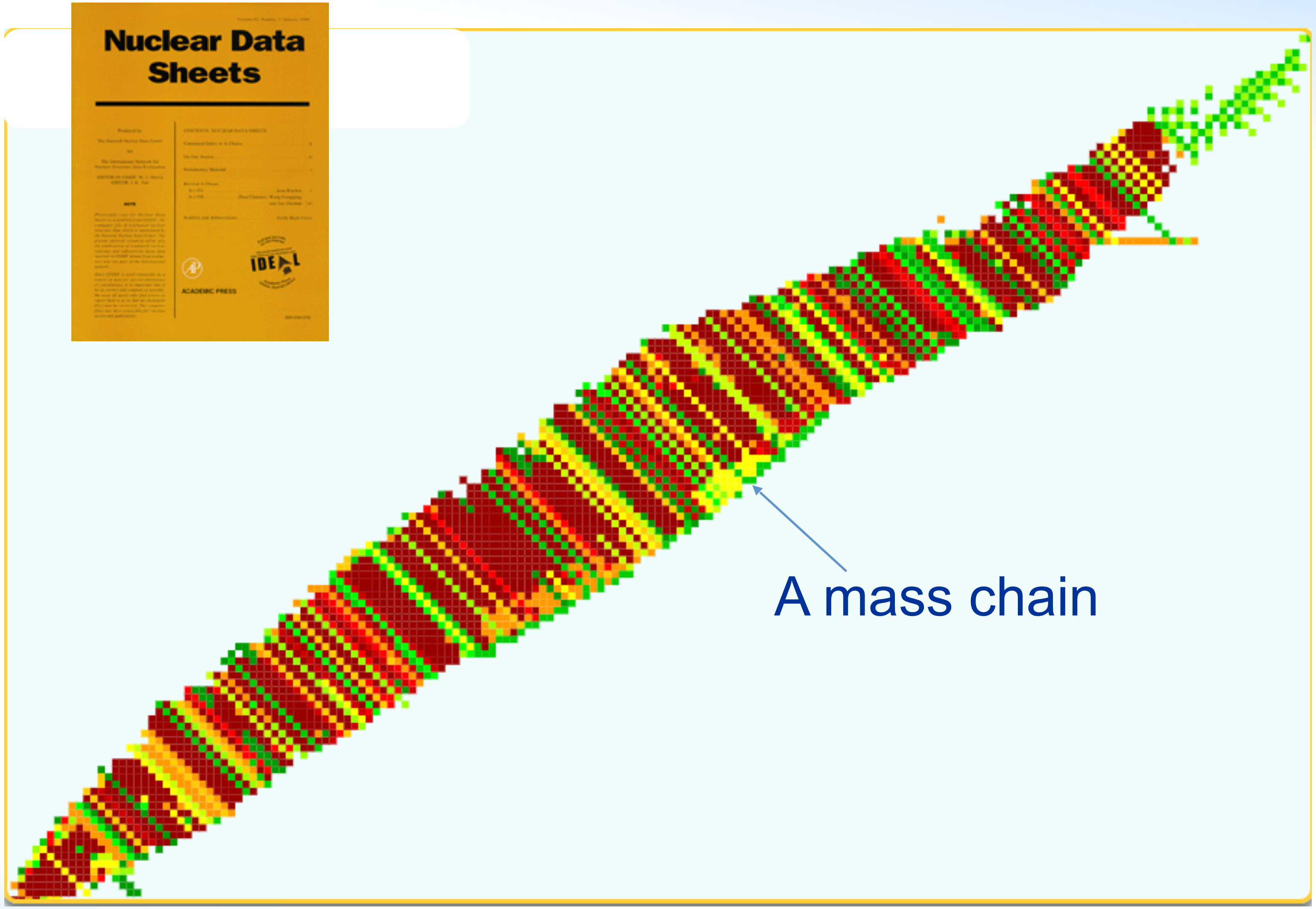
D. Brown, JEFF Stakeholders Meeting, 2019

Unless measurements go through the nuclear data pipeline and are incorporated in the nuclear databases they ARE NOT USED

Evaluated Nuclear Structure Data File (ENSDF)

- 298 mass chains
- 3421 nuclides
- 19697 datasets

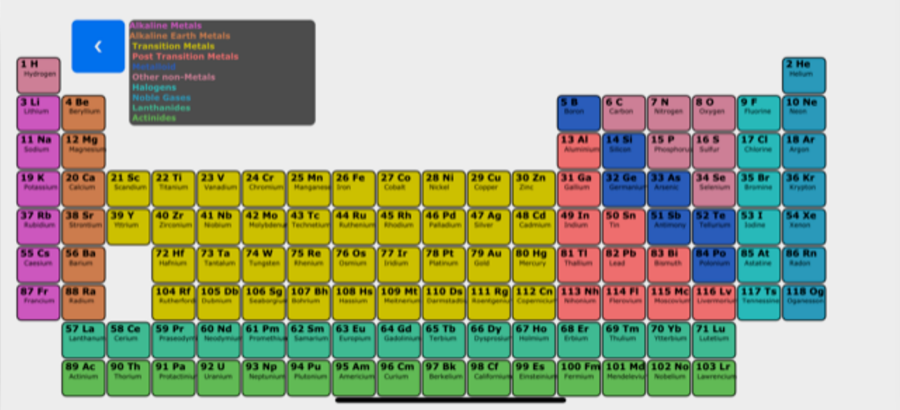
- Levels, spins, parities, band structure
- Multipolarities, mixing ratios, conversion coefficients
- Half-lives, transitions strengths, emission energies and probabilities
- Level schemes

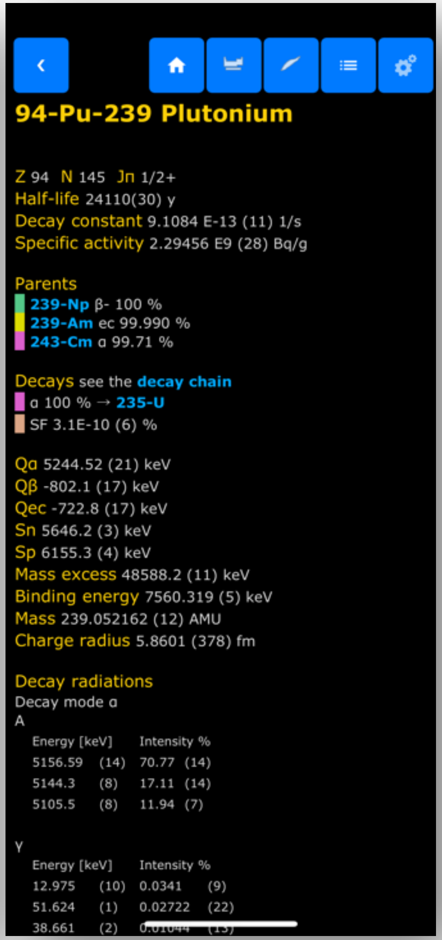


Isotope Browser – for Mobile Devices

- App for Mobile Devices
  - Properties of over **4,000 isotopes**
  - **No internet** connection needed
  - **~180,000** downloads, **4.8** ⭐
  - **11 languages** (Arabic, Chinese, English, French, Spanish, Russian, Japanese, Slovenian, Italian, Trad. Chinese, German)
  - **Regularly updated** with new features and data

Available for both
- Android
- Apple

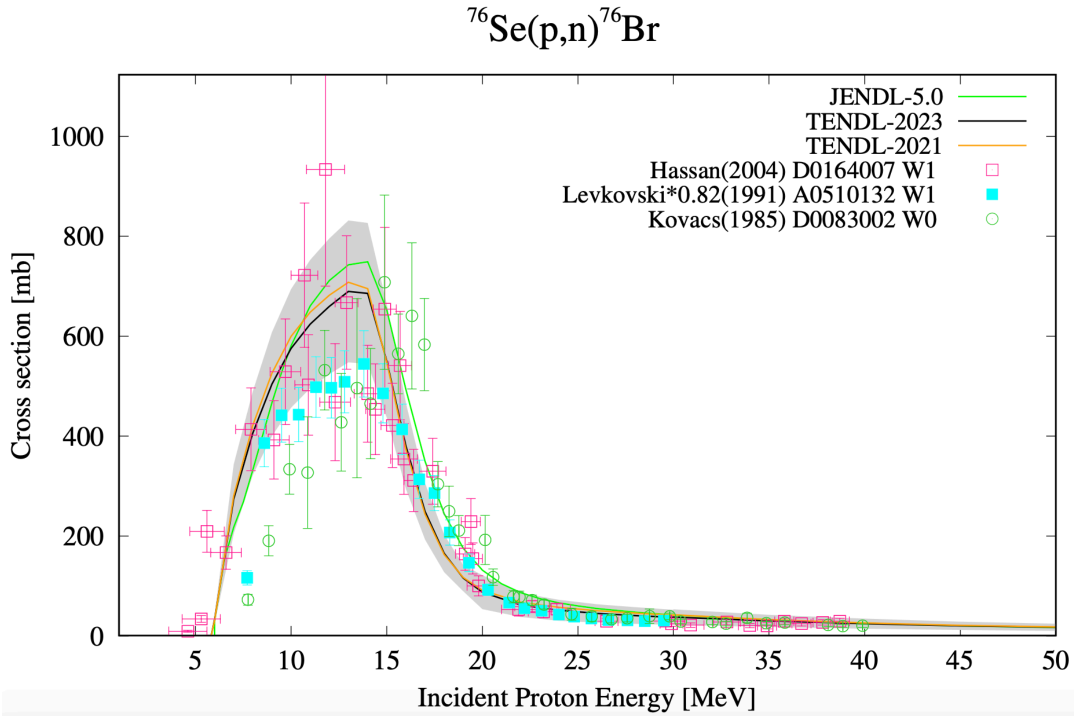


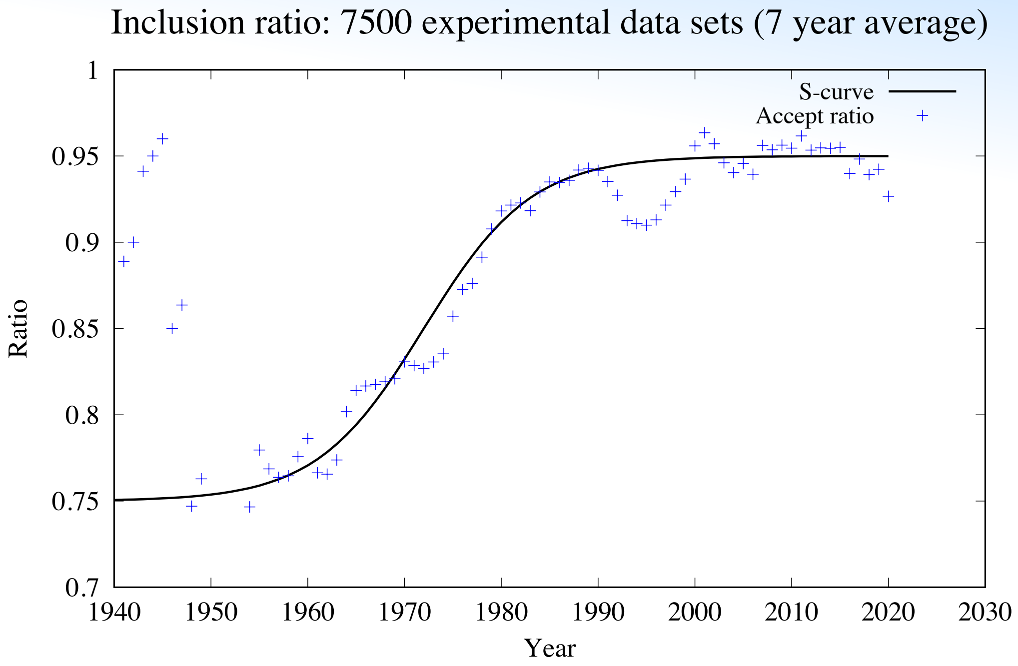


EXFORCISM: flag evil experimental data sets from the EXFOR database as outlier

Koning, Dzysiuk, Alhassan, Gaughan
Scanned 12 000 EXFOR data sets for neutrons up to alpha particles. Cross sections only.
Outliers based on comparison with other exp. data, nuclear data libraries and TALYS:

- Visual,
- Rms goodness-of-fit
- reading papers (Dzysiuk, Alhassan)





Essential for automated parameter optimisation with TALYS

My subjective statement:
~1960: 25% of exp. data sets not included
> 2000: 5% of exp. data sets not included

“New exp. data are better than old ones”

Eur. Phys. J. A (2023) 59:131
https://doi.org/10.1140/epja/s10050-023-01034-3

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Review

This is now the basic reference for TALYS

TALYS: modeling of nuclear reactions

Arjan Koning[1,a], **Stephane Hilaire**[2,3,b], **Stephane Goriely**[4,c]

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[2] DIF, CEA, Arpajon 91297, France
[3] Université Paris-Saclay, CEA, LMCE, 91680 Bruyères-le-Châtel, France
[4] Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine, CP-226, Brussels 1050, Belgium

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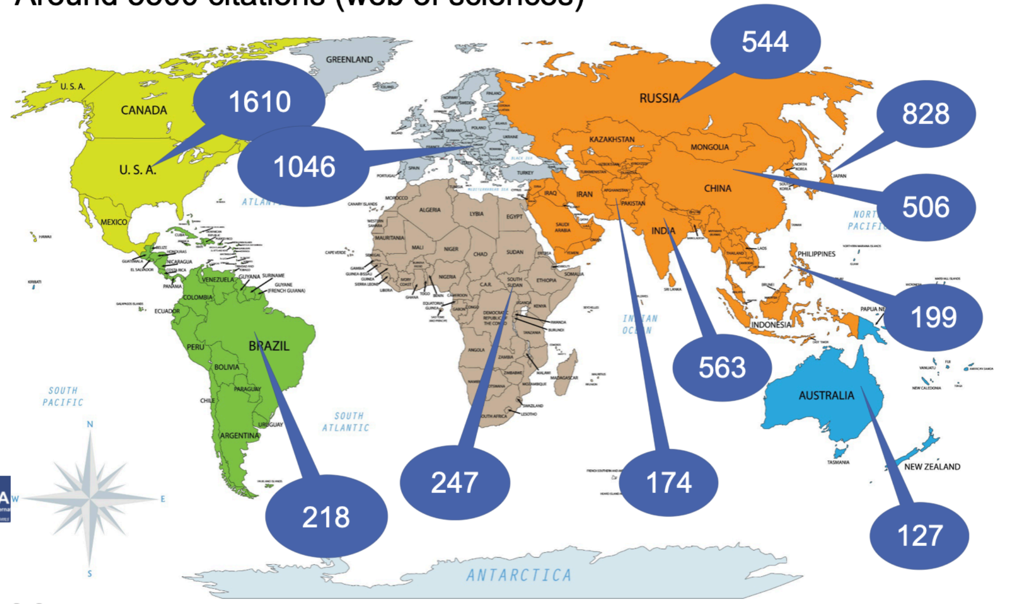
Communicated by Nicolas Alamanos

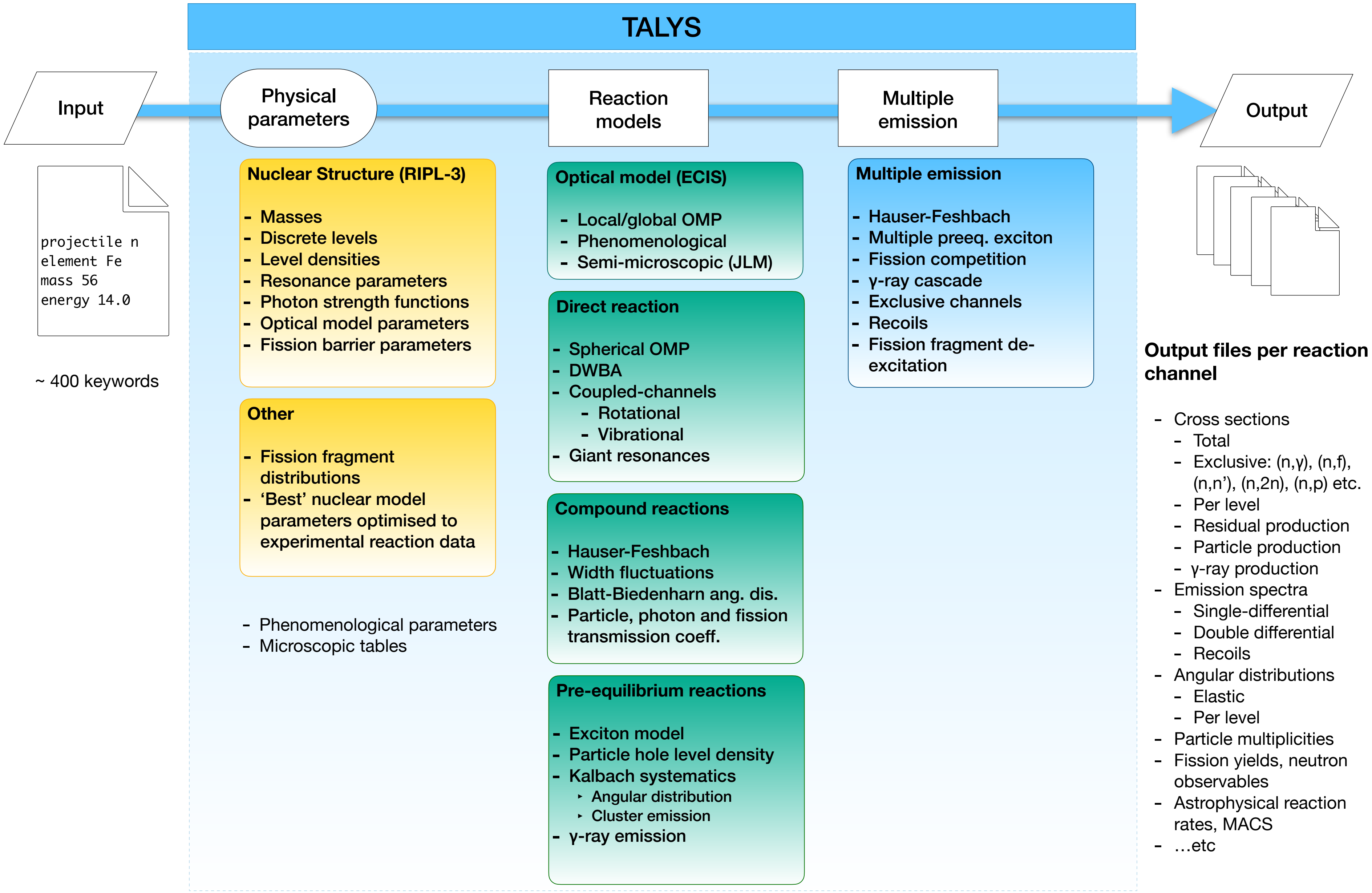
Abstract TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. A general overview of the implemented physics and capabilities 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)

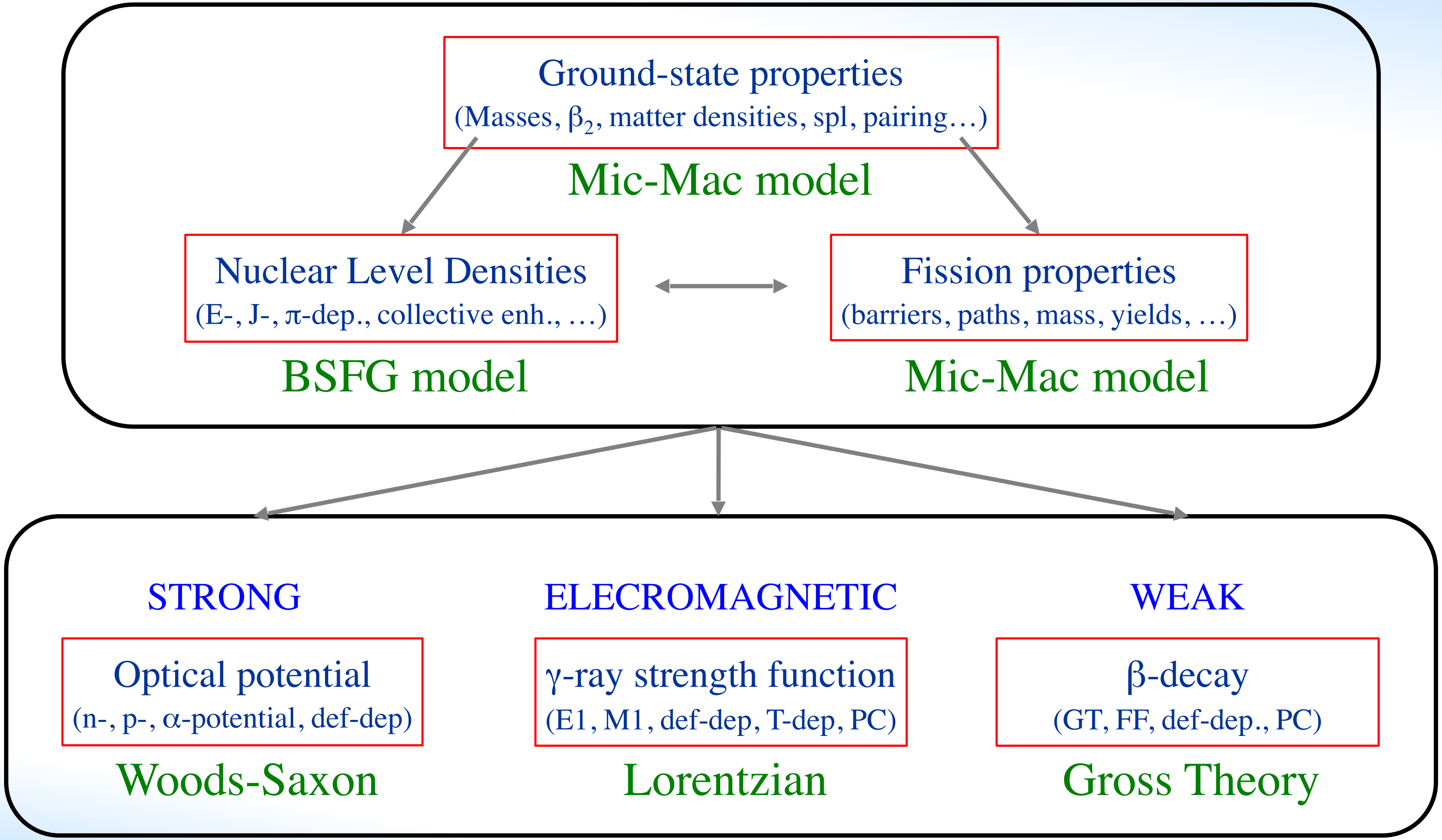
- Around 5500 citations (web of sciences)



Nuclear reaction models

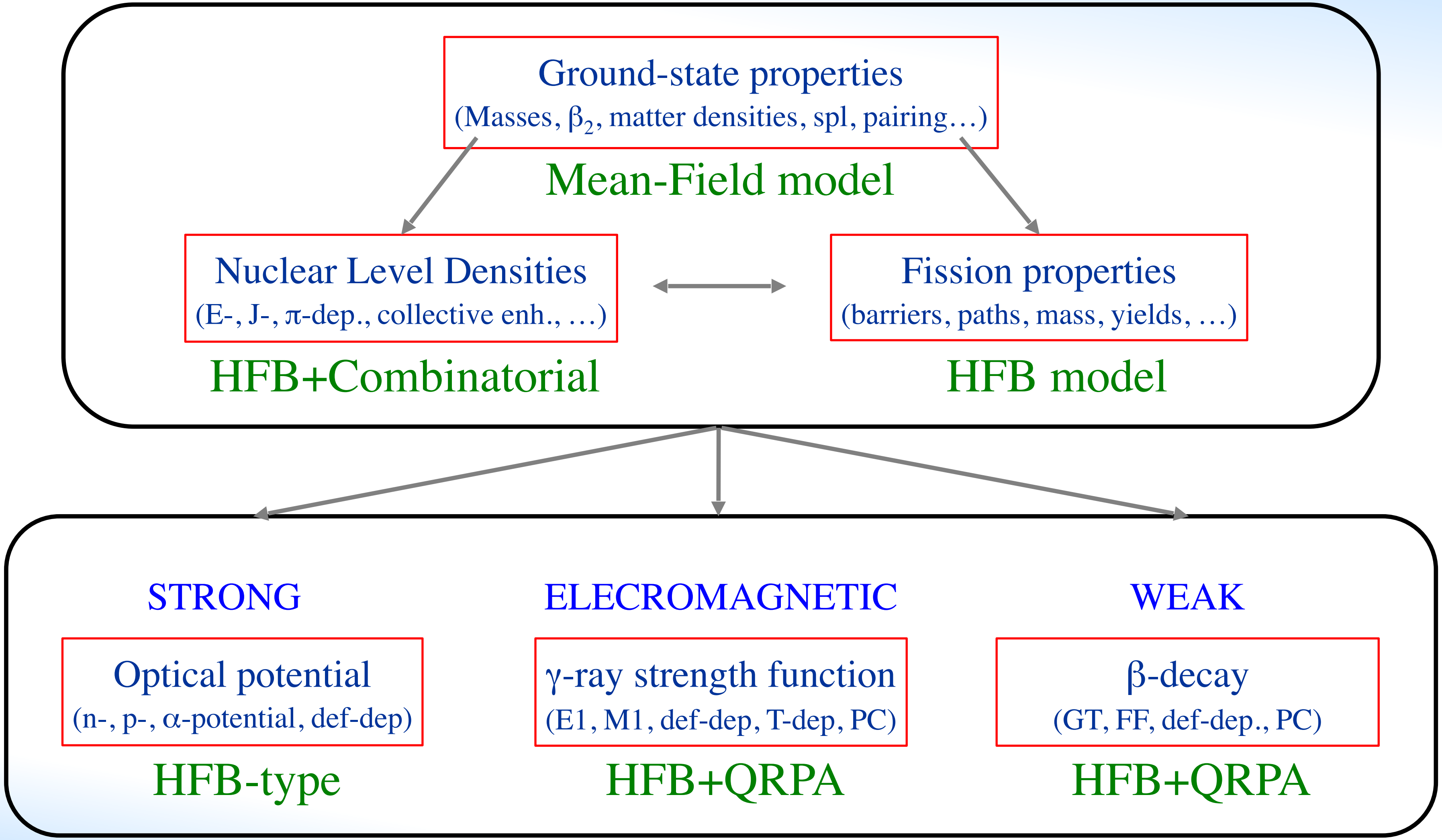


“Macroscopic” Nuclear Inputs



Most of this is implemented in the TALYS code

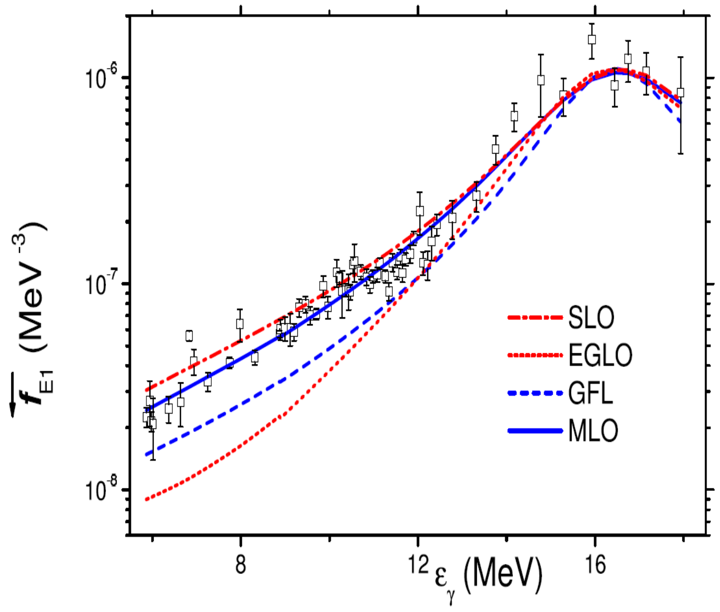
“Microscopic” Nuclear Inputs



Most of this is implemented in the TALYS code

Models of γ-ray strength function

- Standard Lorentzian (SLO)
- Lorentzian with *E*-dependent width
- Generalized Lorentzian with *T*- and *E*-dep. width: at the origin of GLO, EGLO, MLO, SMLO, …

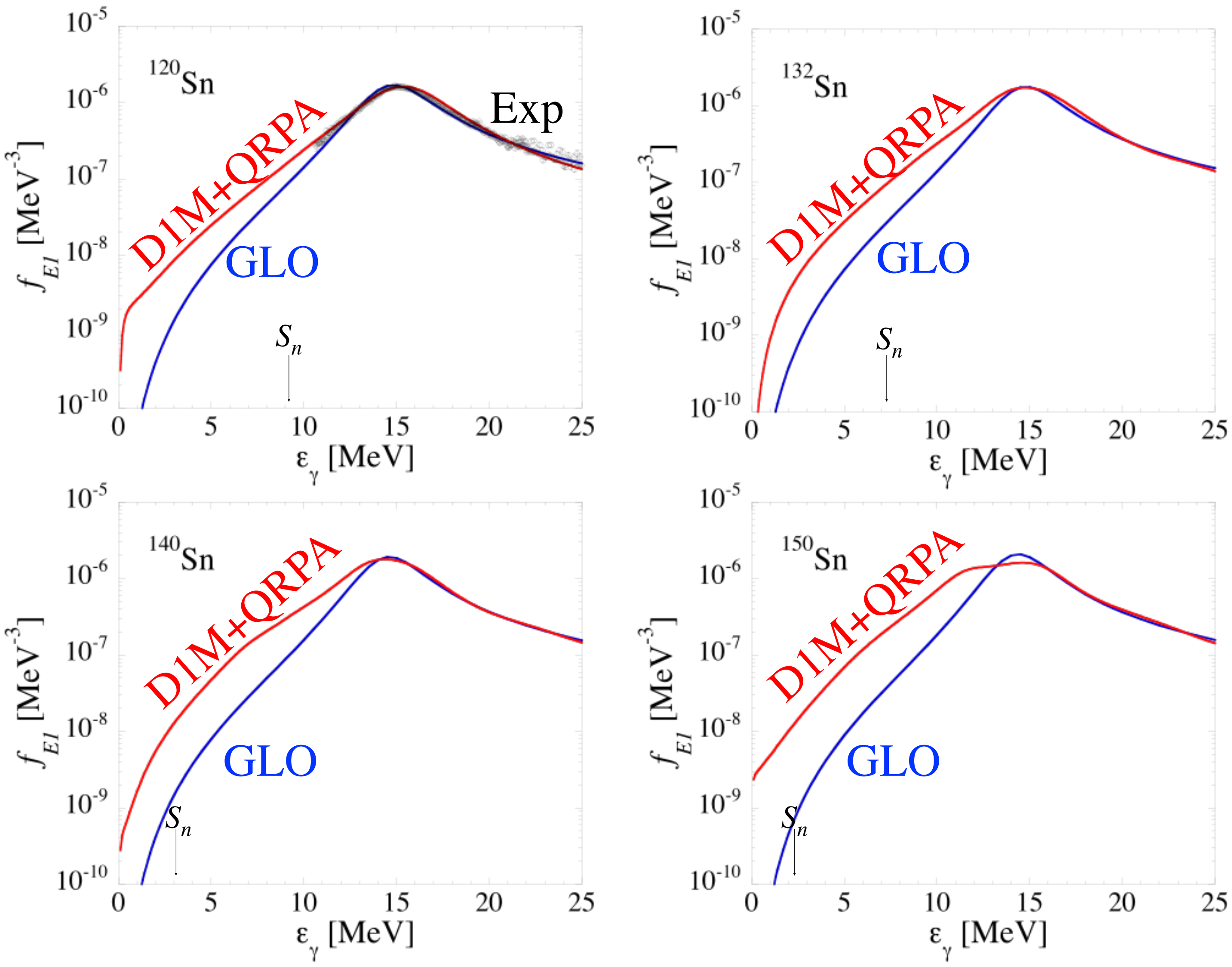


- Mean-Field + QRPA
  - ➢ Skyrme-HFB+QRPA
  - ➢ Gogny-HFB+QRPA
  - ➢ RMF+QRPA

Provided empirical corrections are made, QRPA calculations can accurately reproduce experimental data !

*Gogny-HFB QRPA E*1 strength function in n-rich Sn isotopes

GLO = Kopecky & Uhl (1990)



Essential for (n,γ) reactions: Photon strength functions

(From the TALYS manual)

strength

Model for $E1$ gamma-ray strength function, see Section 10. There are many possibiliti

Examples

strength 1 : Kopecky-Uhl generalized Lorentzian (GLO)
strength 2 : Brink-Axel Lorentzian (SLO)
strength 3 : Hartree-Fock BCS tables
strength 4 : Hartree-Fock-Bogoliubov (HFB) tables
strength 5 : Goriely hybrid model [53]
strength 6 : Goriely T-dependent HFB tables
strength 7 : T-dependent RMF tables
strength 8 : Gogny D1M HFB+QRPA tables
strength 9 : Simplified Modified Lorentian (SMLO) tables
strength 10: Skyrme-BSK27 HFB+QRPA tables
strength 11: D1M-Intra-E1 tables
strength 12: Shellmodel-E1 tables

Range

1 - 12

Default

strength 8

strengthM1

Model for $M1$ gamma-ray strength function. There are various possibilities. For tabulated values, the model numbers are consistent with those for E1.

Examples

strengthM1 1 : Standard Lotentzian with parameters from Eq. (10.15)
strengthM1 2 : Normalize the $M1$ gamma-ray strength function with that of $E1$ as $f_{E1}/(0.0588A^{0.878})$.
strengthM1 3 : Simplified Modified Lorentzian for M1, with spin-flip and scissors mode
strengthM1 4 : RIPL-2 M1 + Kawano Scissors model
strengthM1 8 : Gogny-D1M HFB tables
strengthM1 10: Skyrme-HFB tables
strengthM1 11: D1M-Intra-M1 tables
strengthM1 12: Shellmodel-M1 tables

Range

1, 2, 3, 4, 8, 10, 11, 12

Default

strengthM1=strength for **strength 8, 10, 11 or 12**, **strengthM1 2** for **strength 1 or 2**, and **strengthM1 3** otherwise.

Essential for (n,γ) and all other channels: Level densities

ldmodel

Model for level densities. There are 3 phenomenological level density models and 5 options for microscopic level densities, all described in Chapter 9. It is also possible to choose a level density model per nuclide considered in the reaction.

Examples

ldmodel 1: Constant Temperature + Fermi gas model (CTM)
ldmodel 2: Back-shifted Fermi gas Model (BFM)
ldmodel 3: Generalised Superfluid Model (GSM)
ldmodel 4: Skyrme-Hartree-Fock-Bogolyubov level densities from numerical tables
ldmodel 5: Skyrme-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 6: Temperature-dependent Gogny-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 7: BSKG3 - Skyrme-Hartree-Fock-Bogolyubov triaxial combinatorial level densities from numerical tables ← Candidate for default
ldmodel 8: QRPA level densities from numerical tables
ldmodel 2 41 93: Back-shifted Fermi gas Model just for this particular nucleus

Range

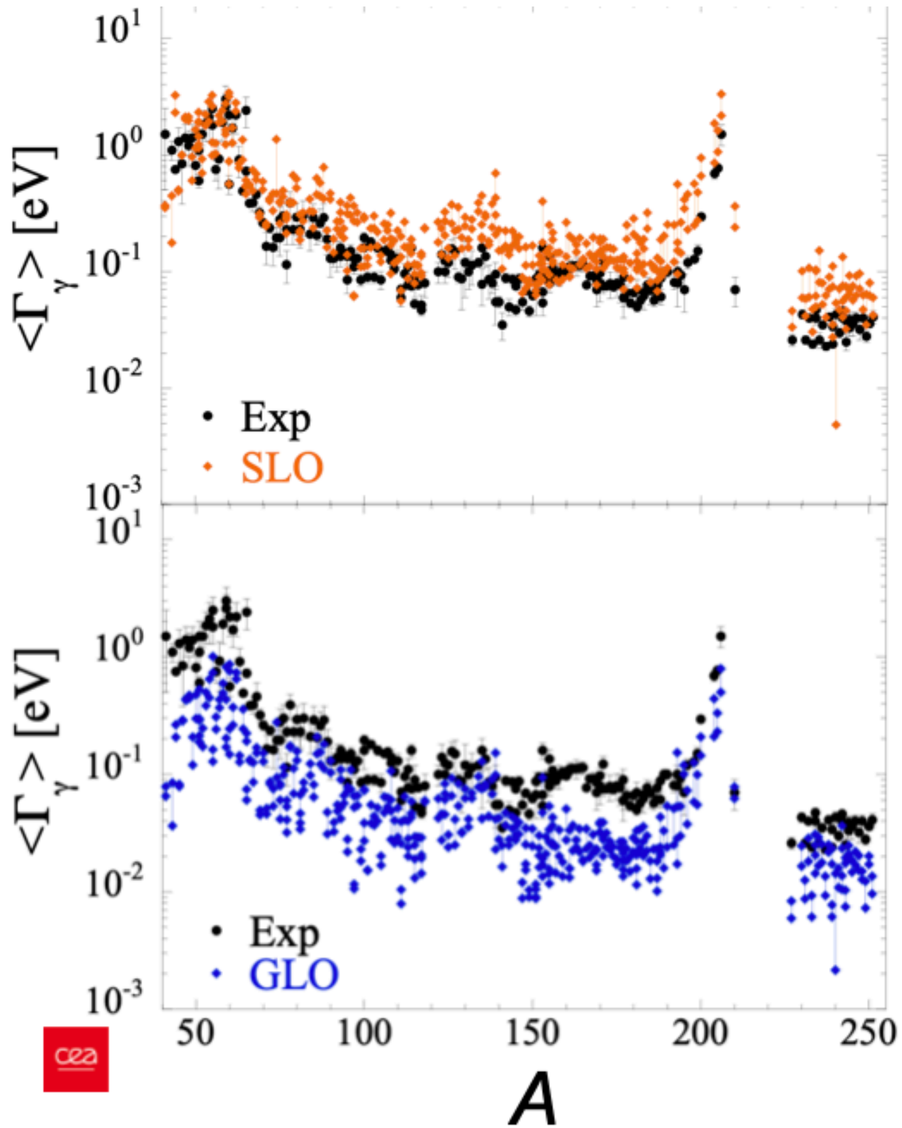
1 $\leq$ **ldmodel** $\leq$ **8**

Default

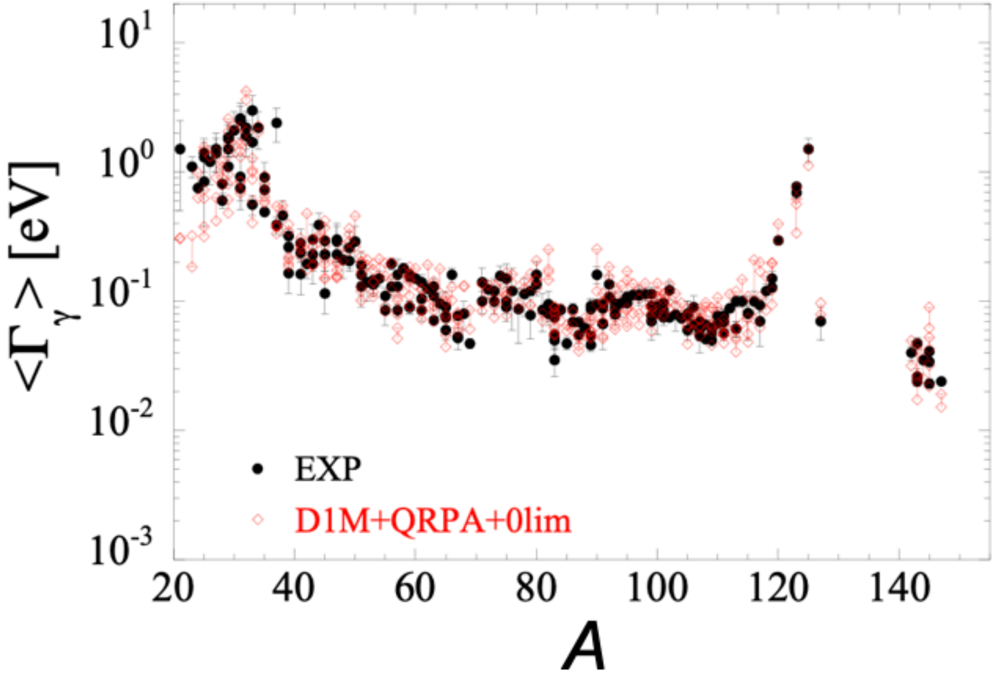
ldmodel 1

2015-2025: Significant improvement of photon strength functions

Older, analytical models



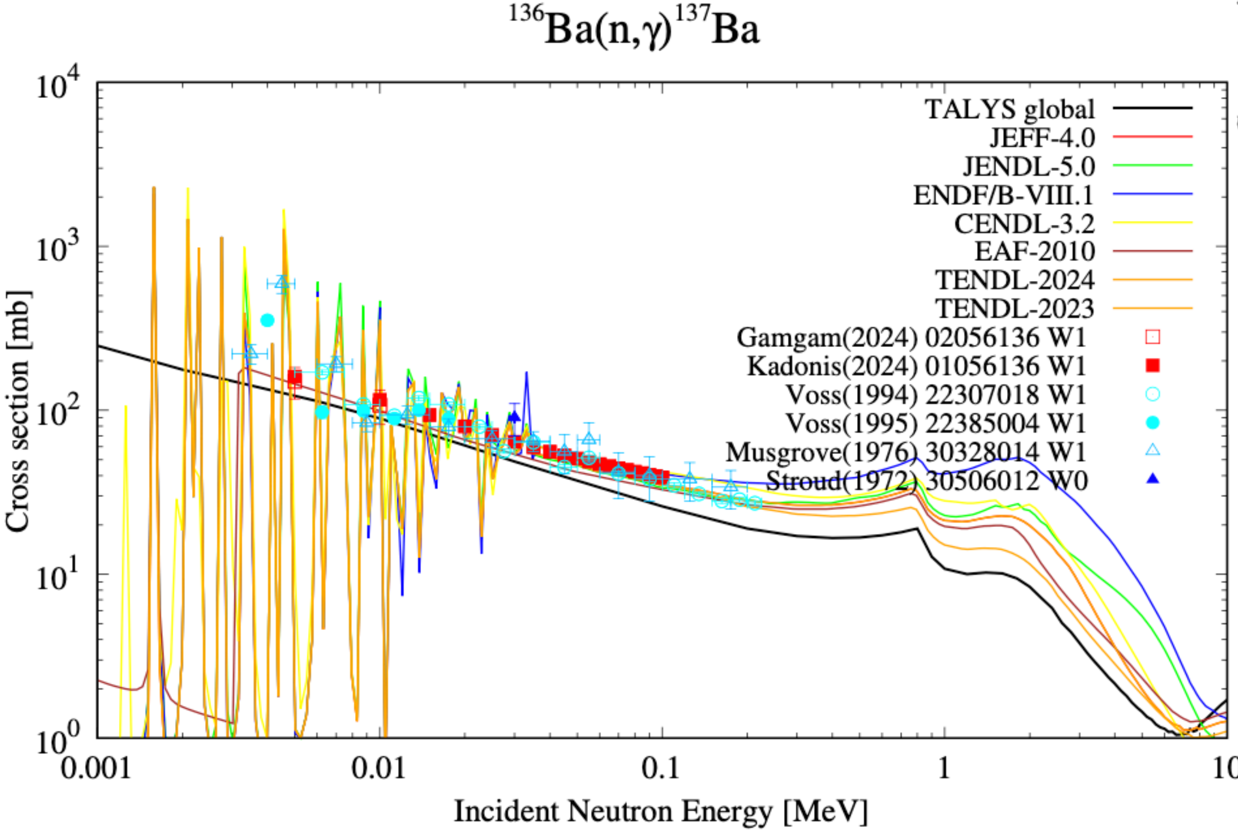
QRPA + M1 upbend

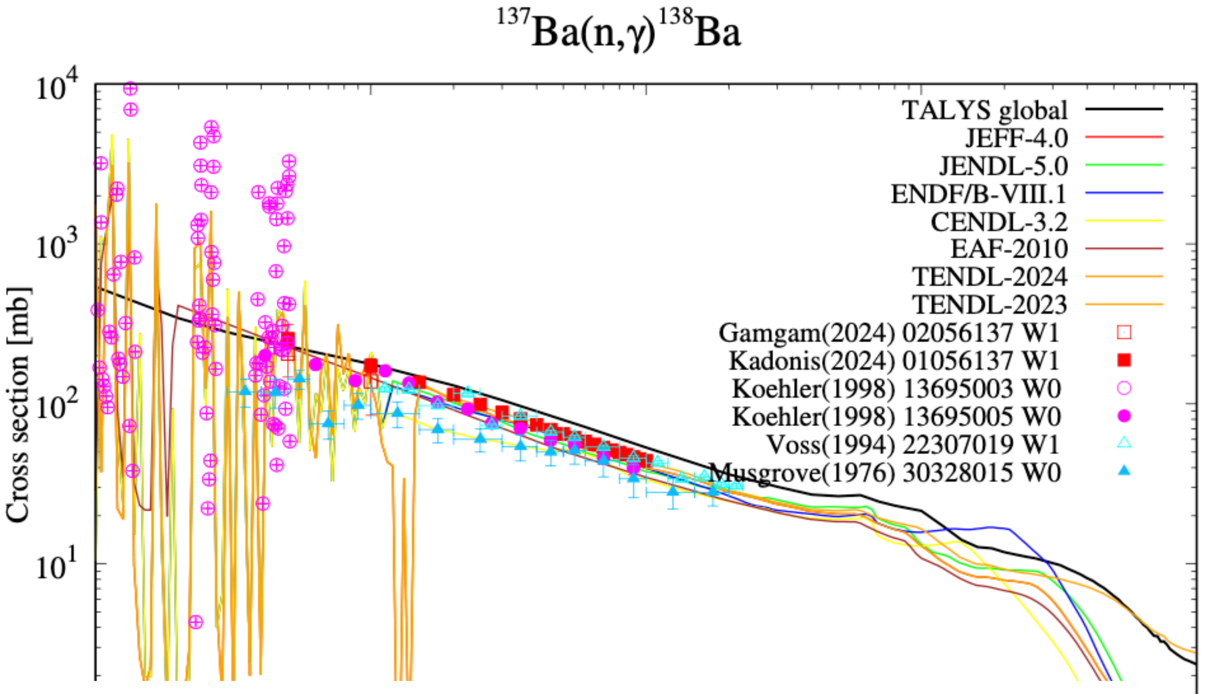


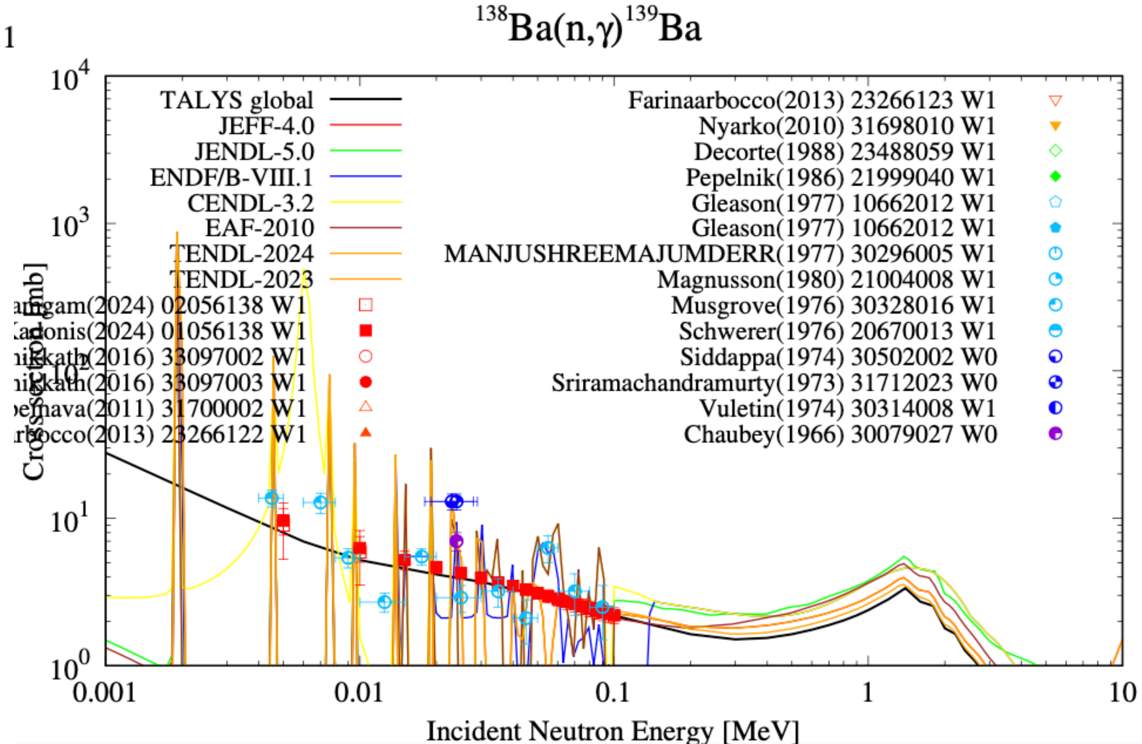
$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$

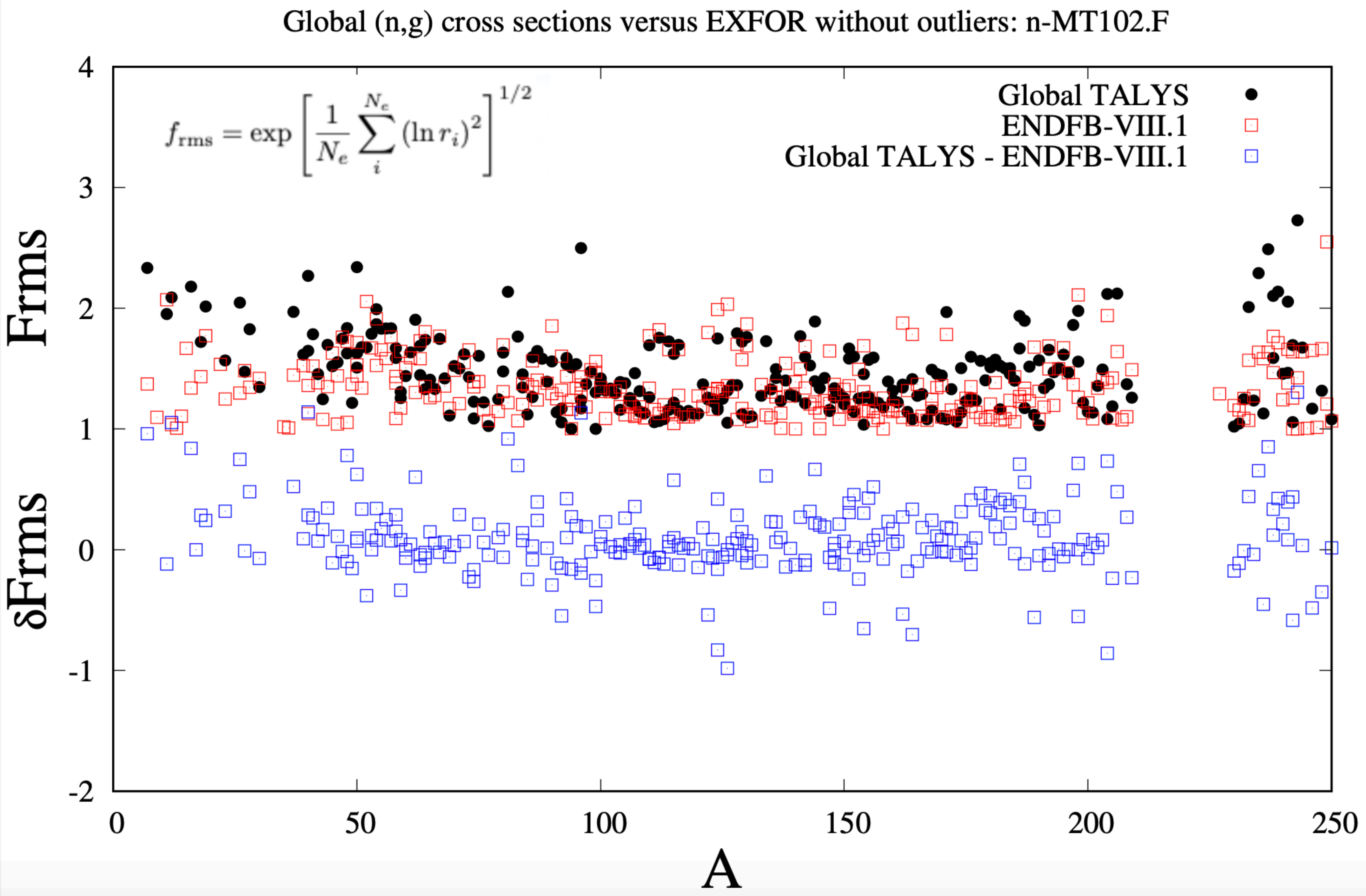
From Goriely et al

Global (n,γ) : Ba isotopes



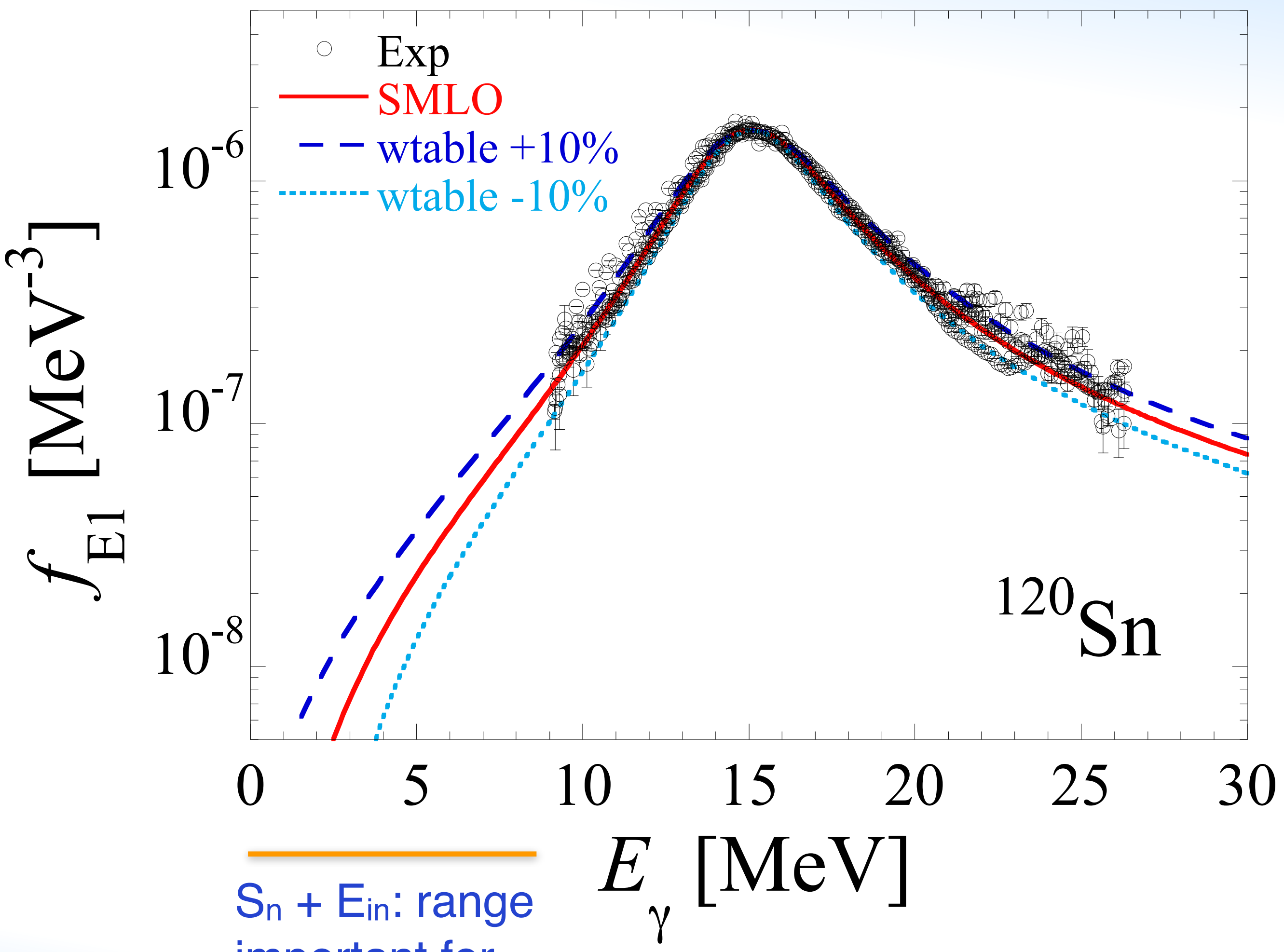






Global (n,g) cross sections versus EXFOR without outliers: n-MT102.F
$f_{\mathrm{rms}} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2}$
Global TALYS
ENDFB-VIII.1
Global TALYS - ENDFB-VIII.1
Frms
δFrms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250

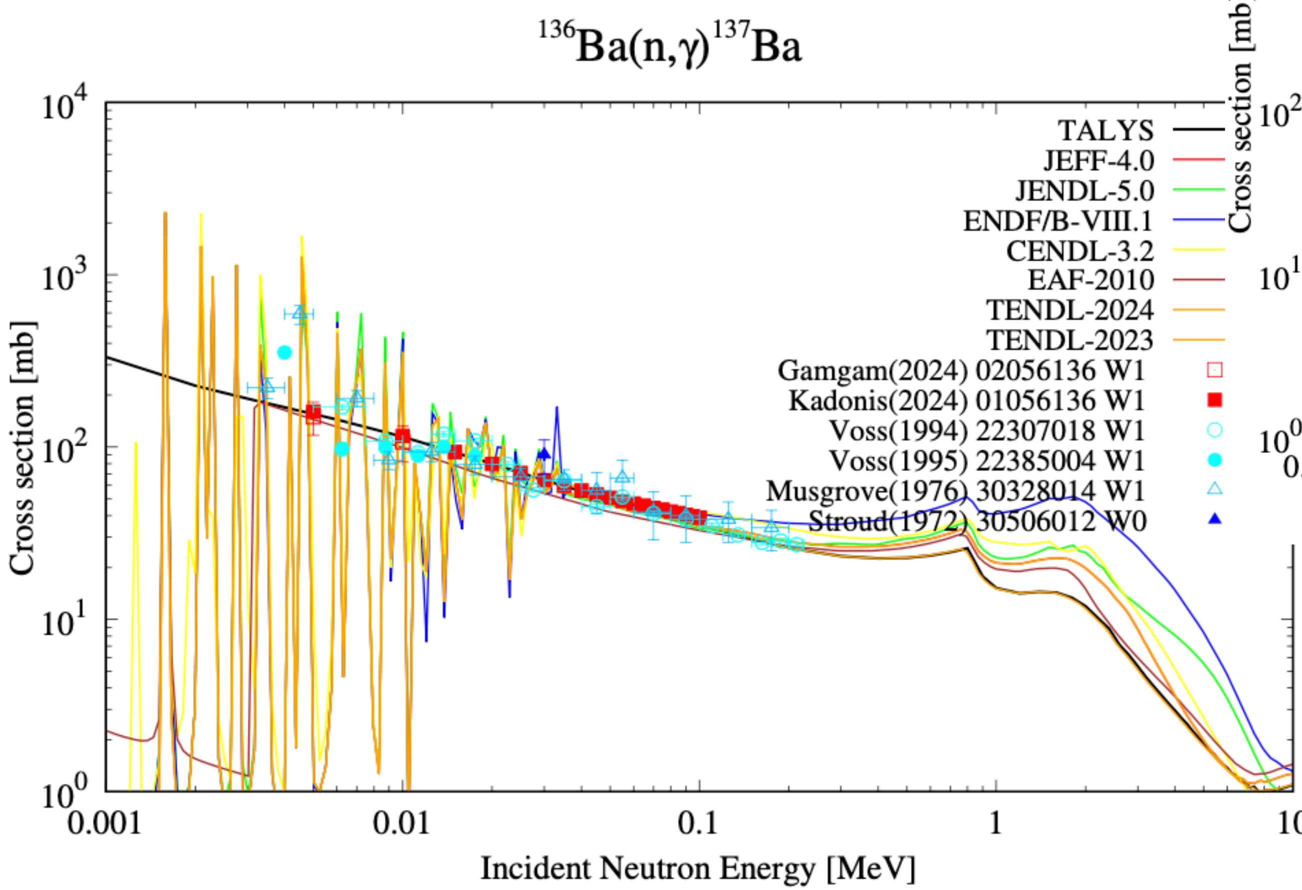
Adjusting (n,γ) cross sections with PSF width parameter

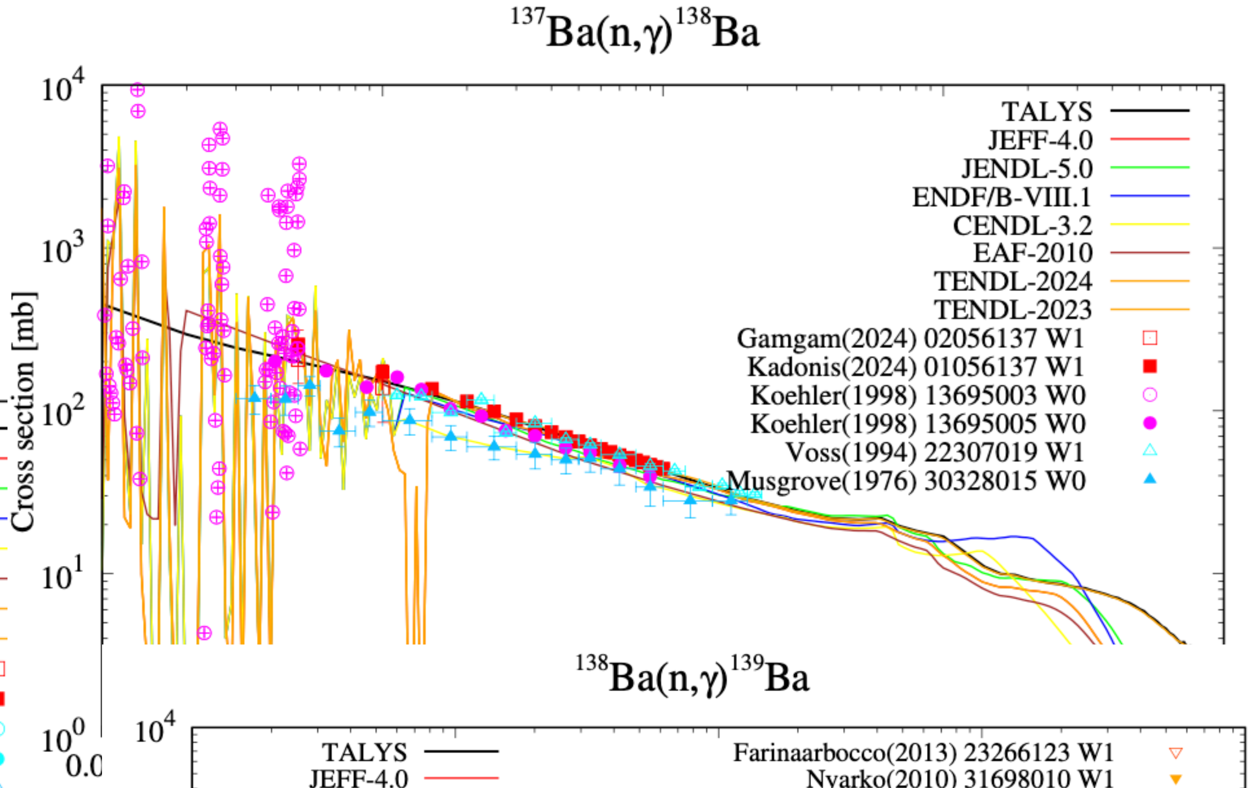


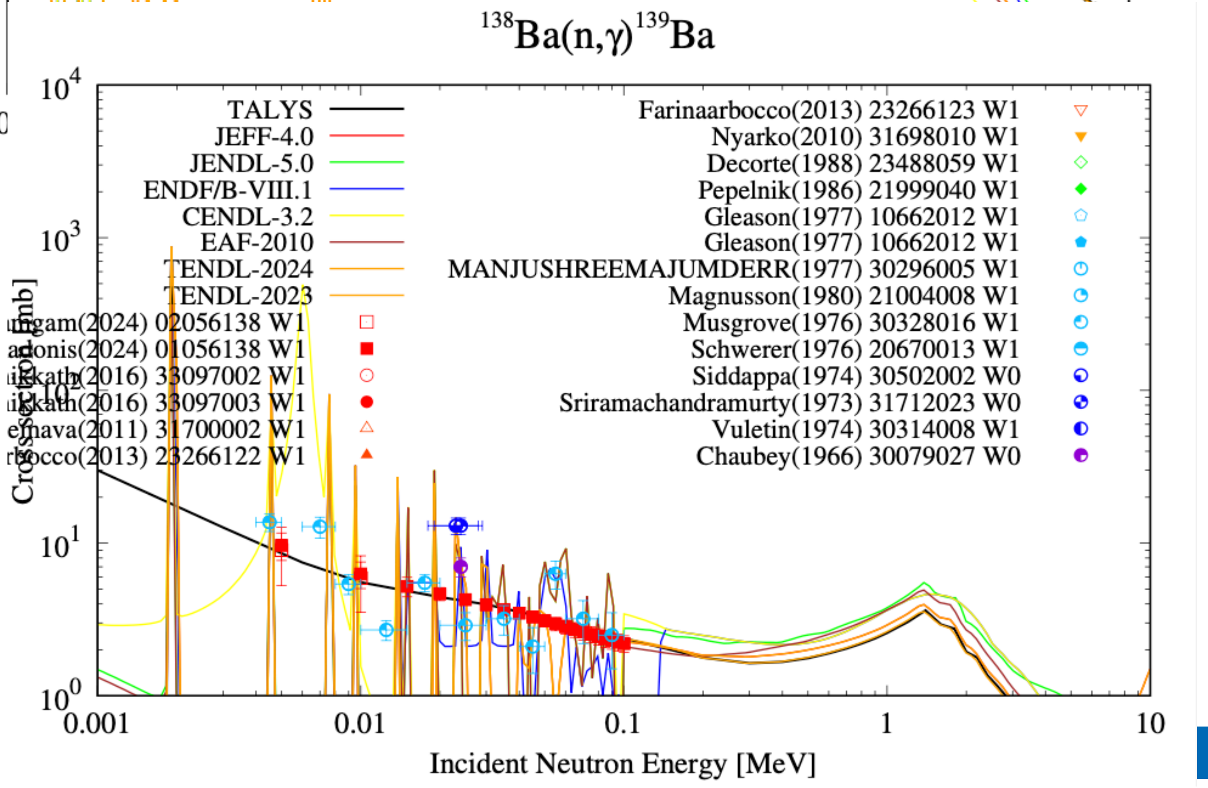
$S_n + E_{in}$: range important for (n,γ)

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

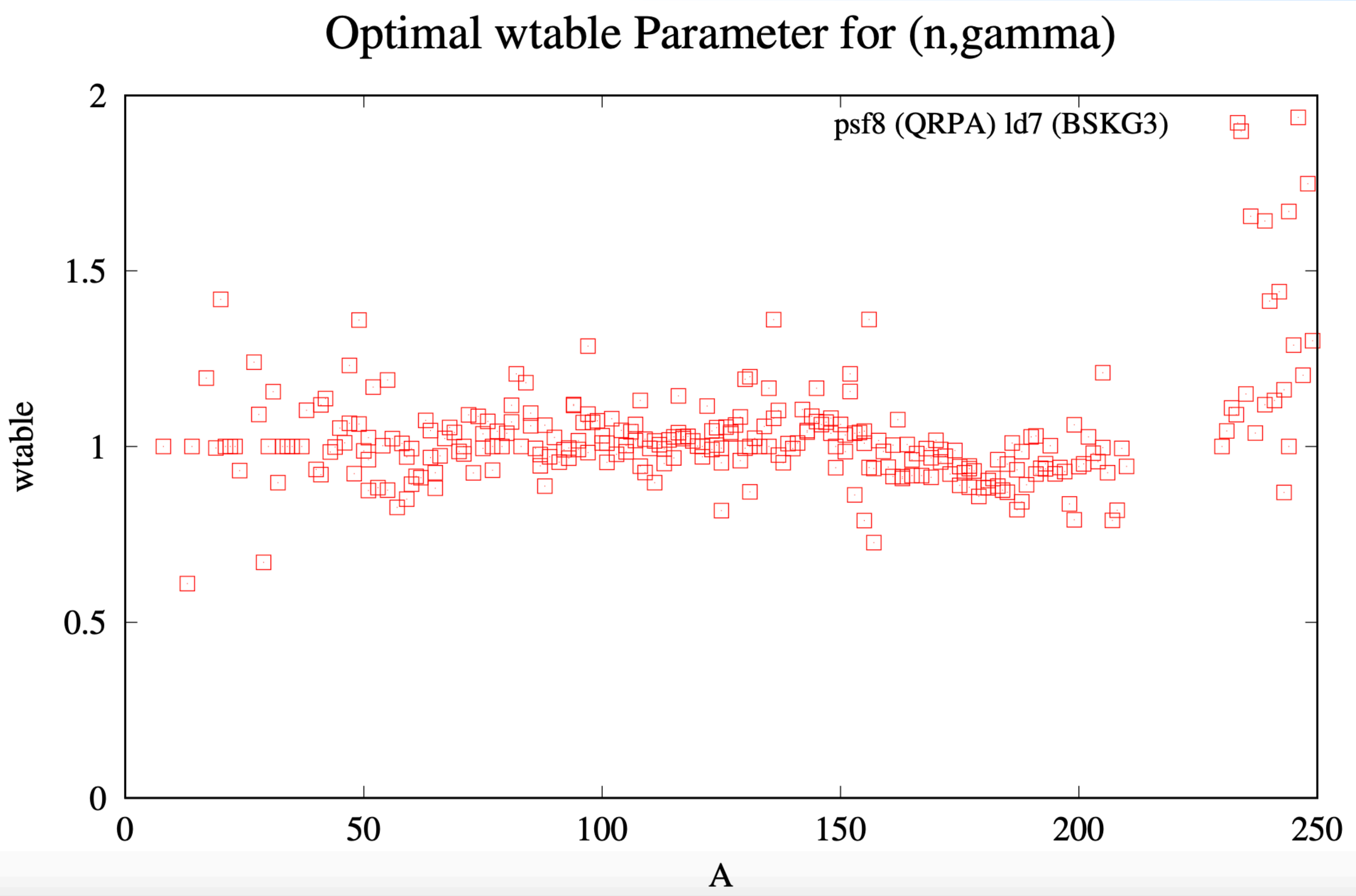
Optimised (n,γ) : Ba isotopes

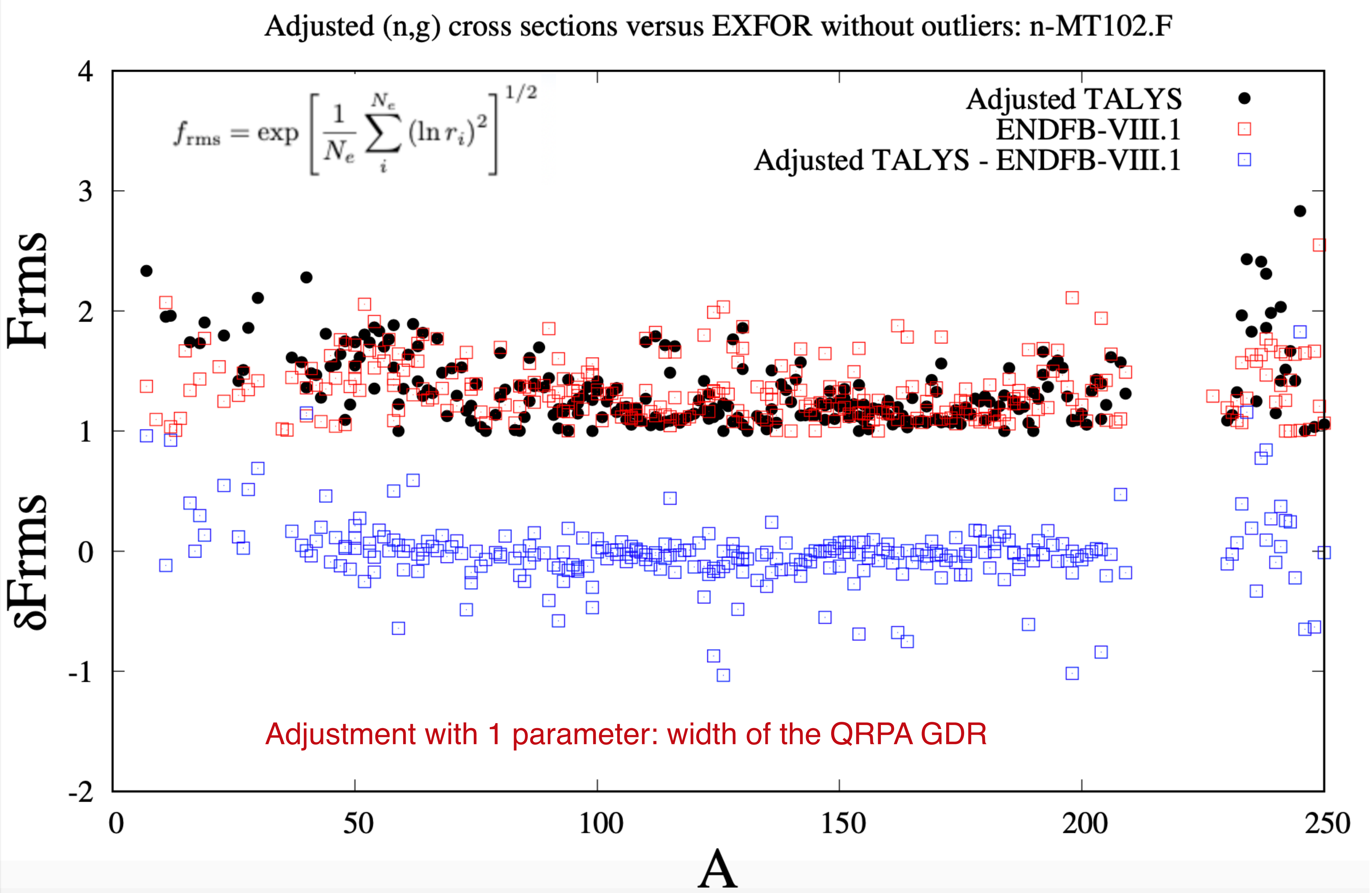


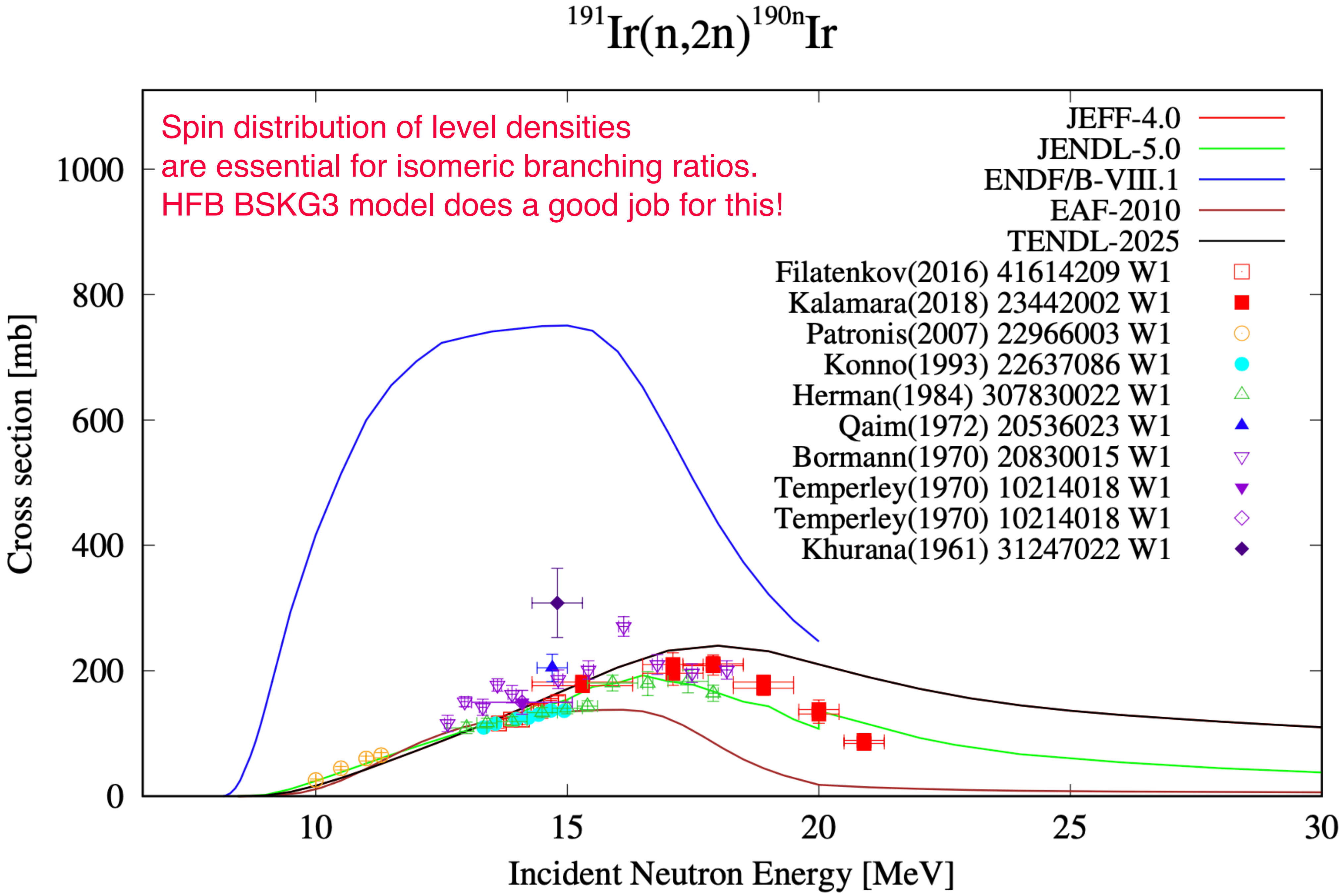




Simultaneous adjustment to MACS, <Γγ> and (n,γ) cross sections



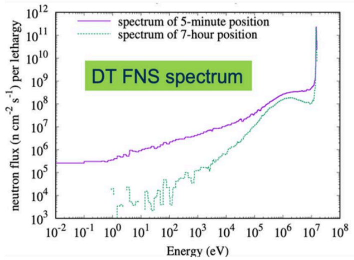

Adjusted (n,g) cross sections versus EXFOR without outliers: n-MT102.F
$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2}$$
Adjusted TALYS
ENDFB-VIII.1
Adjusted TALYS - ENDFB-VIII.1
Frms
δFrms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250
Adjustment with 1 parameter: width of the QRPA GDR

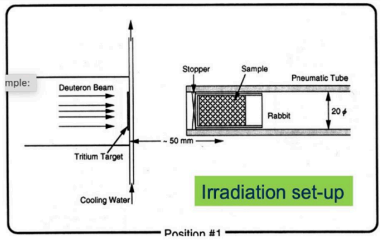


$^{191}Ir(n,2n)^{190n}Ir$
Spin distribution of level densities
are essential for isomeric branching ratios.
HFB BSKG3 model does a good job for this!
JEFF-4.0
JENDL-5.0
ENDF/B-VIII.1
EAF-2010
TENDL-2025
Filatenkov(2016) 41614209 W1
Kalamara(2018) 23442002 W1
Patronis(2007) 22966003 W1
Konno(1993) 22637086 W1
Herman(1984) 307830022 W1
Qaim(1972) 20536023 W1
Bormann(1970) 20830015 W1
Temperley(1970) 10214018 W1
Temperley(1970) 10214018 W1
Khurana(1961) 31247022 W1
Cross section [mb]
0
200
400
600
800
1000
10
15
20
25
30
Incident Neutron Energy [MeV]

Fusion Neutron Source Experiment

UK Atomic Energy Authority





- The Japan Atomic Energy Agency (JAEA) used their Fusion Neutron Source (FNS) to irradiate several materials
- 2 mA deuteron beam onto a tritium target producing a fusion neutron flux (14MeV peak) ~10^10 n/cm2/s
- Samples were irradiated for 5 minutes or 7 hours and the resulting decay heat generated measured for cooling times between a few seconds up to a year or more
- Two major campaigns in 1996 and 2000

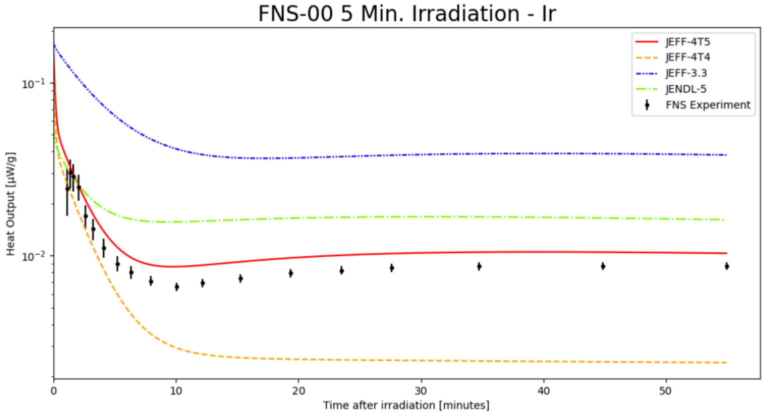
HFB-based nuclear structure —>
Microscopic level densities —>
TALYS nuclear model code —>
Better description of isomer/g.s. ratio —>
TENDL and JEFF nuclear data libraries —>
Improved prediction of decay heat for future fusion reactors

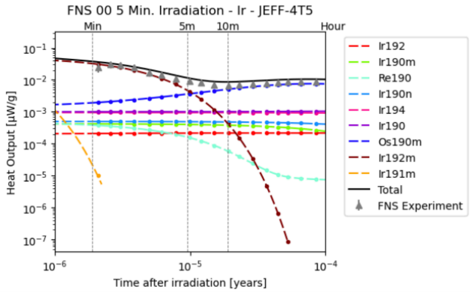
From: Jessica Hollis, UKAEA

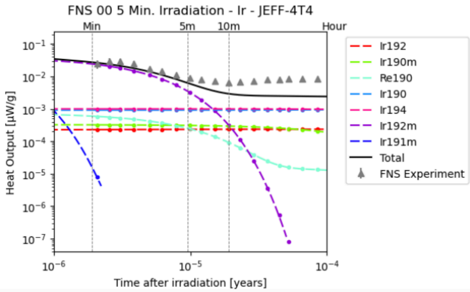
Iridium

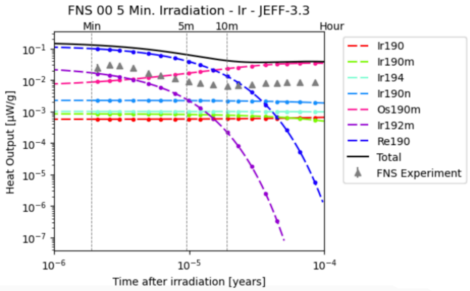
UK Atomic Energy Authority

- JEFF-4T5 the best performing library tested against experiment
- Includes Ir191(n,2n)Ir190n(β+)Os190m production pathway which T4 missed
- Re190 heat output significantly reduced from 3.3









Conclusion

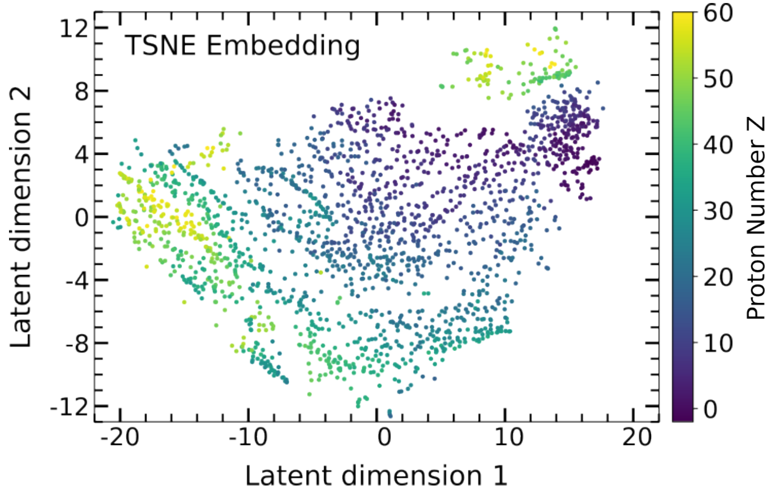
- Nuclear data for applications uses a variety of sources:
  - Compiled experimental databases for nuclear structure and reactions
  - Evaluated experimental databases for nuclear structure and reactions
  - Nuclear model codes
  - Fortunately, all these topics are continuously revisited by the IAEA!
- Fundamental nuclear physics has an impact on nuclear energy and other applications:
  - Fundamental nuclear structure and reaction measurements lead to improved photon strength functions and level densities
  - Powerful nuclear model codes predict nuclear data, and interpolate between experimental data.
  - TALYS model code now more combined with DL techniques, reaction code simulators

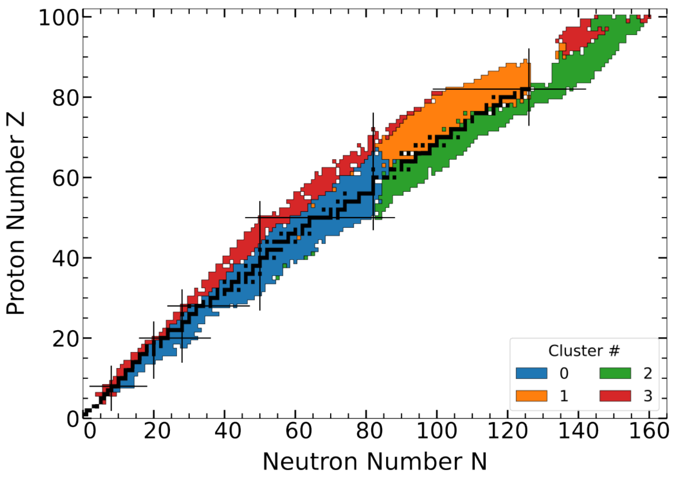
Thank you for your attention!

Implicit neural representations are an extremely powerful tool to encode complex signals

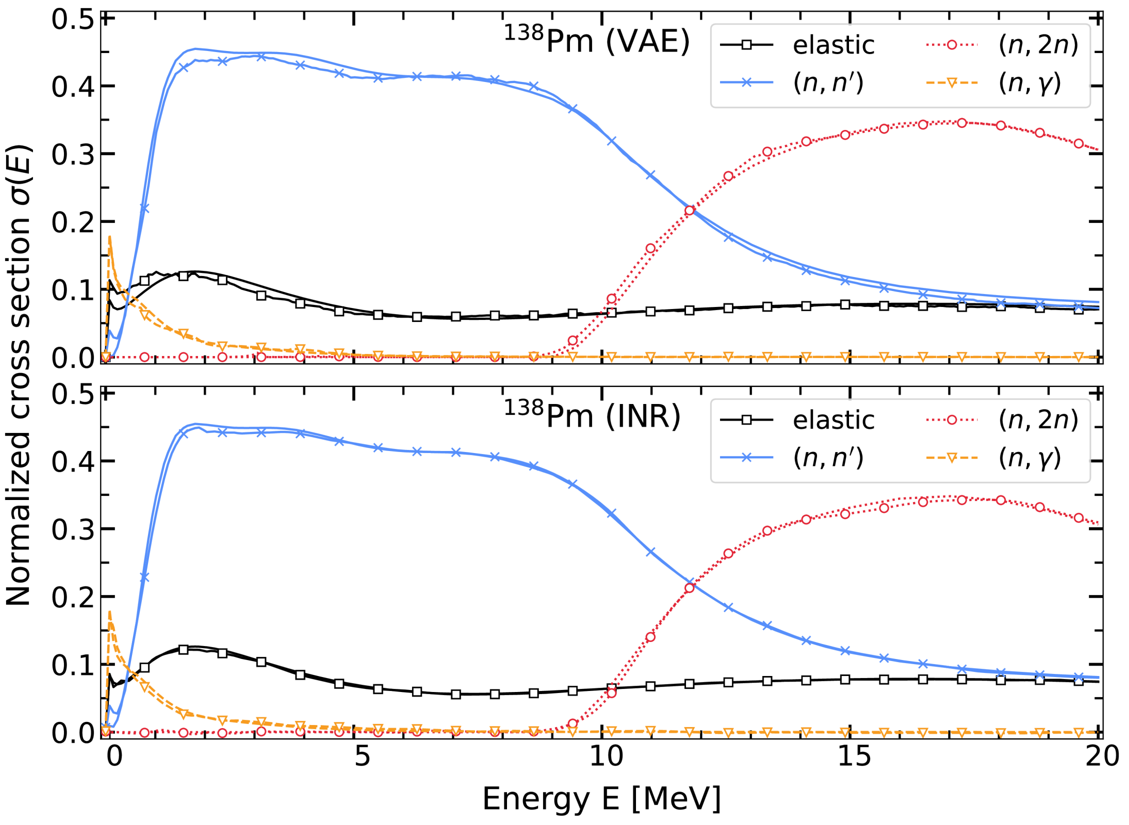
- Simultaneous encoding of 4 different channels with factor ~30x compression
- AI/ML can learn physical properties from encoding alone!

Mitra, Choi, Liu, Glatt, Wendt and Schunck, arXiv:2404.02332 - Lawrence Livermore + Arizona state Univ.





Deep Learning versus TALYS/TENDL



Precision of reconstruction is superior to typical experimental/model uncertainties