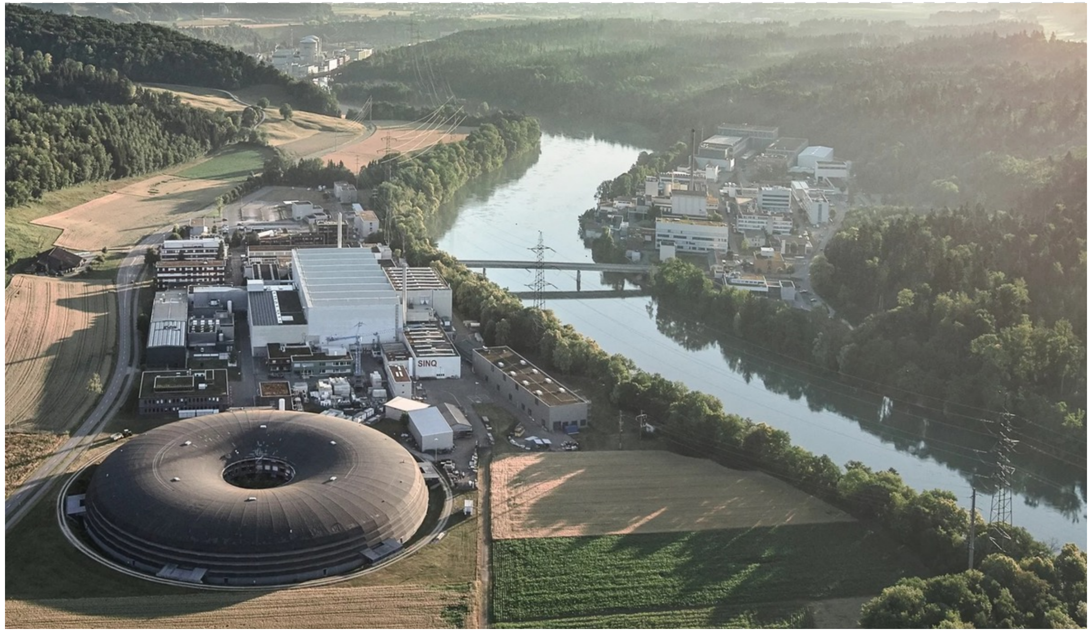
PSI Center for Nuclear Engineering and Sciences



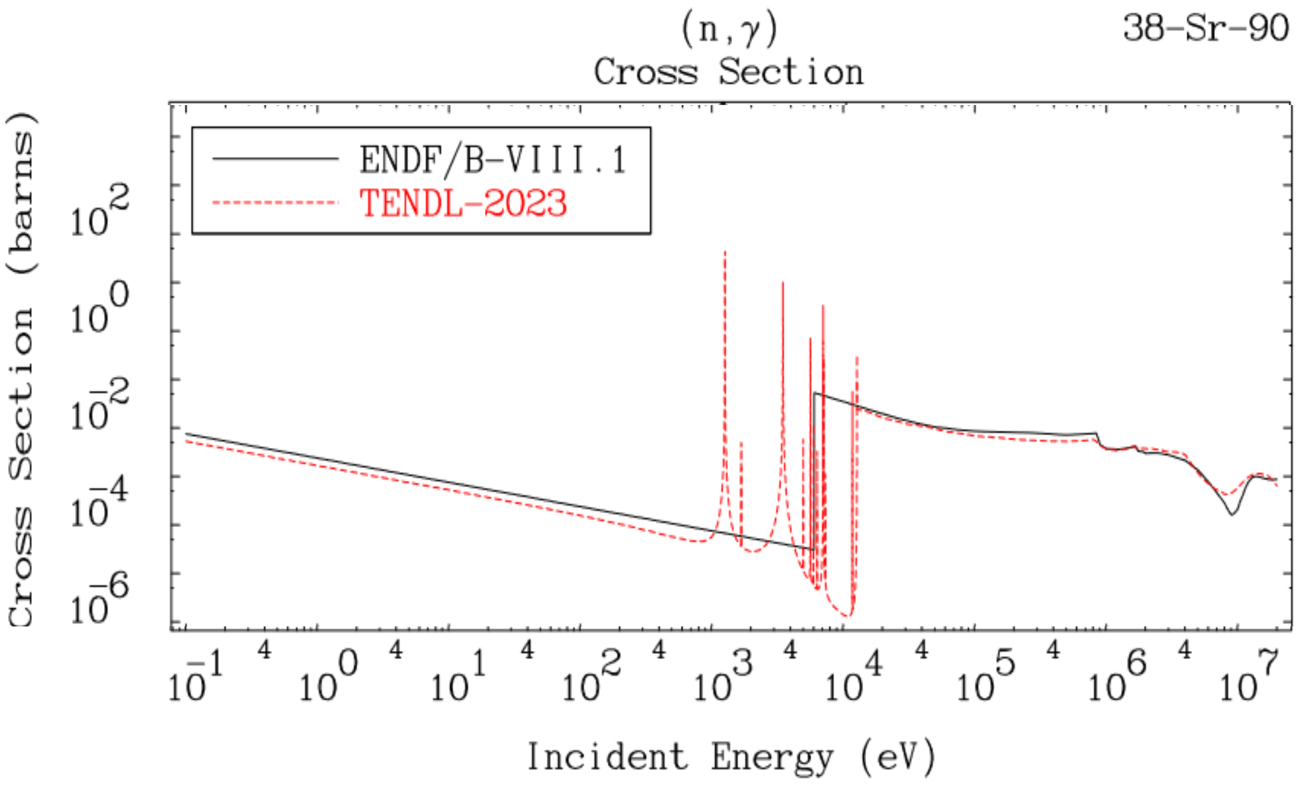
From HF to HFR: how to use compound nucleus information in the resonance range

D. Rochman

LLNL seminar, online, November 13, 2024

Summary

- Historical approach
- Modern tools and data
- Physics tests
- Examples
- MACS
- World dissemination
- Conclusion



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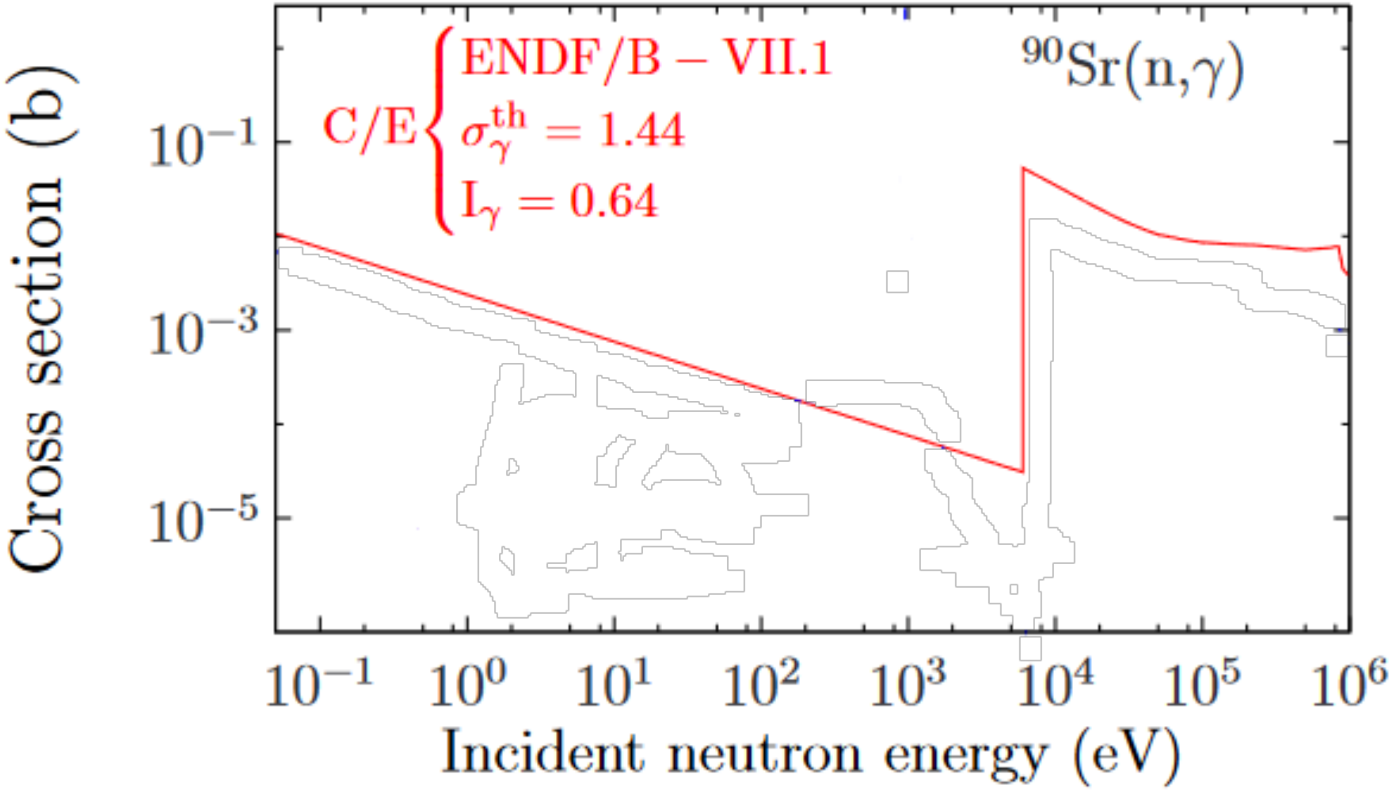
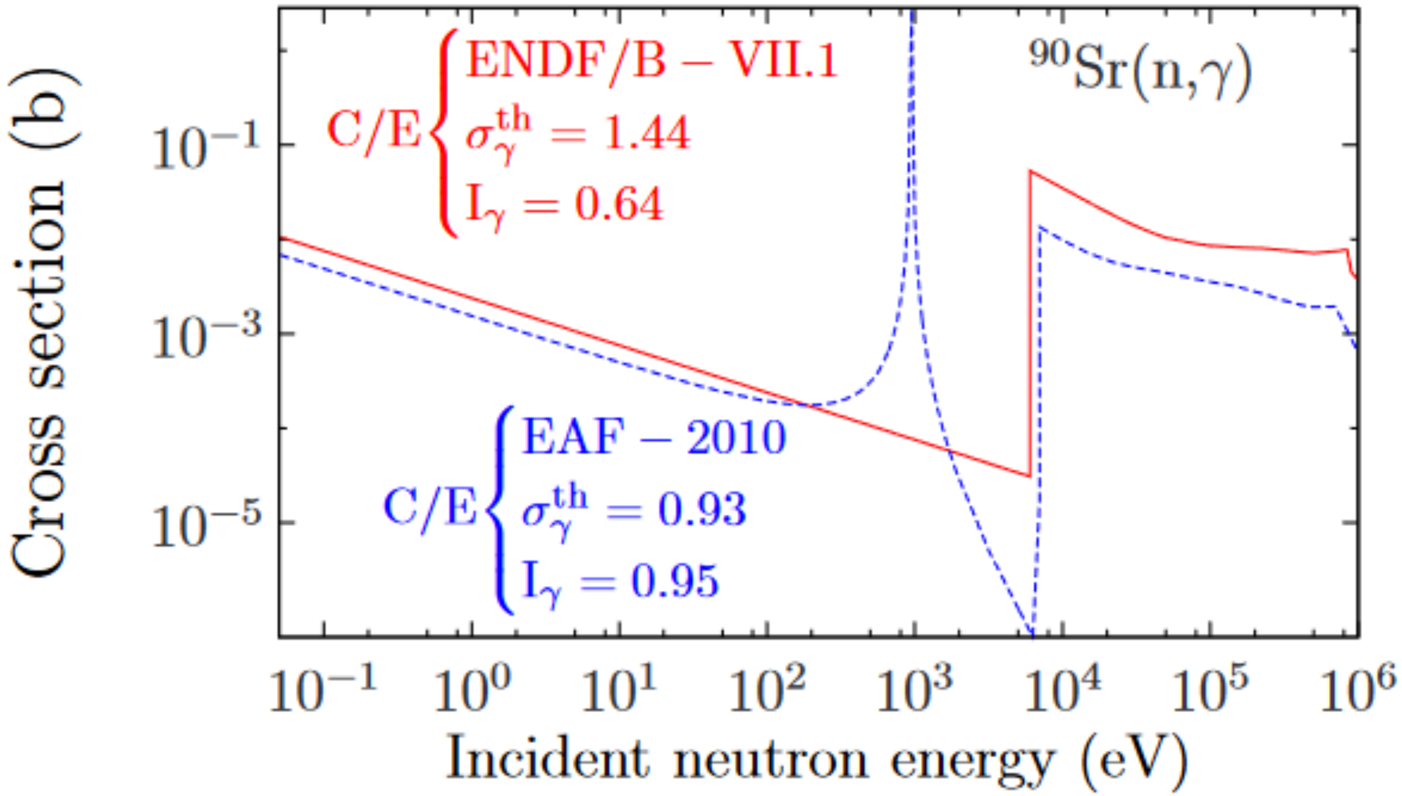
Historical approach

- Only ≈ 400 isotopes have resonance parameters (not systematically complete)
- Only ≈ 400-500 isotopes have integral resonance information ($\sigma_{thermal}$, I_γ. MACS)
- The vast majority has no experimental information (≈ 8000 for astrophysics)



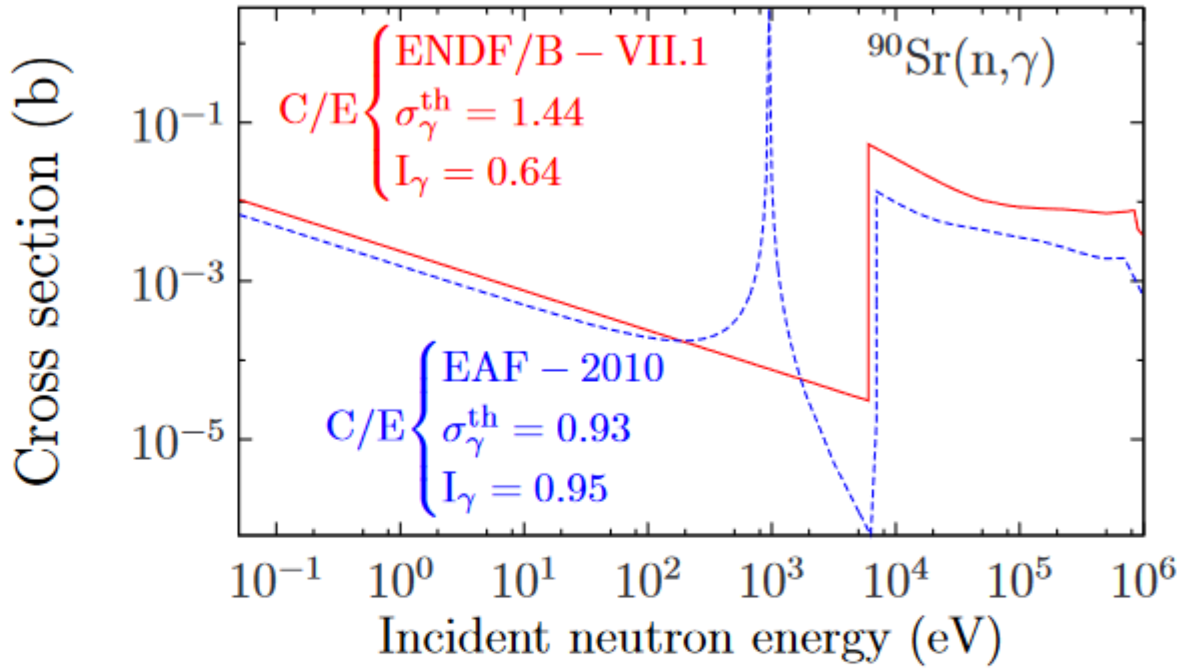
Historical approach

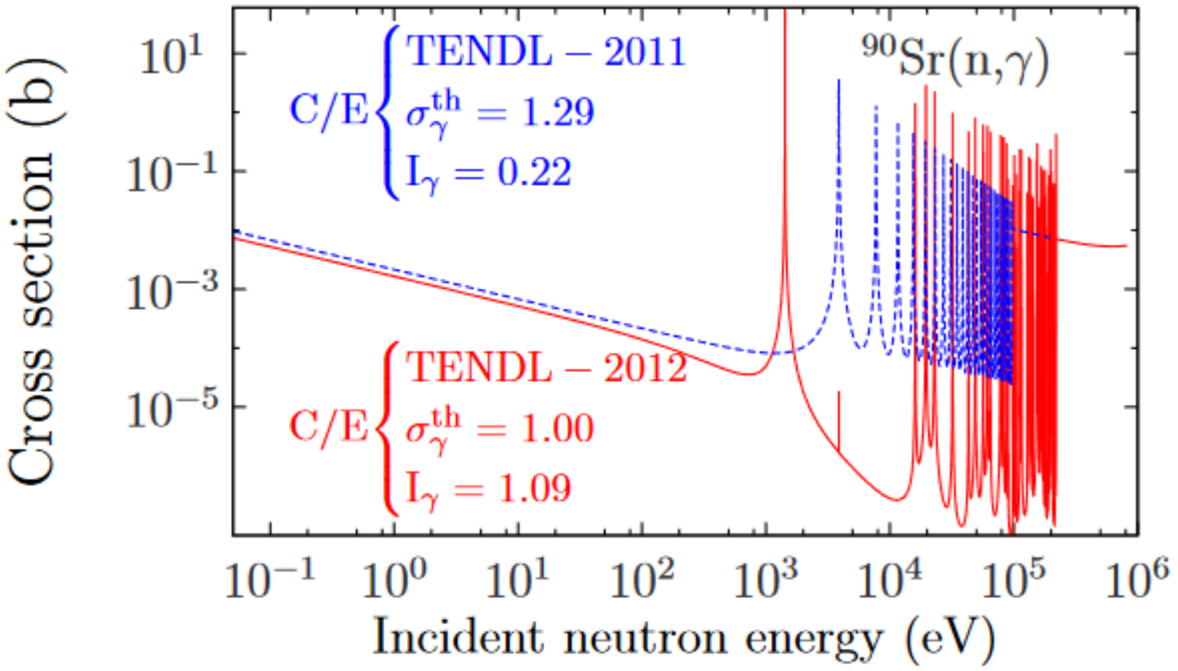
- First solution found in the EAF libraries: SRA (Single Resonance Approximation)
- Used for activation-relevant isotopes (up to year 2010)



Historical approach

- After 2010, transition to the HFR approach (“Hauser-Feshbach Resonance”) in TENDL...
- Based on TALYS average parameters, CALENDF processing and generation of statistical resonances





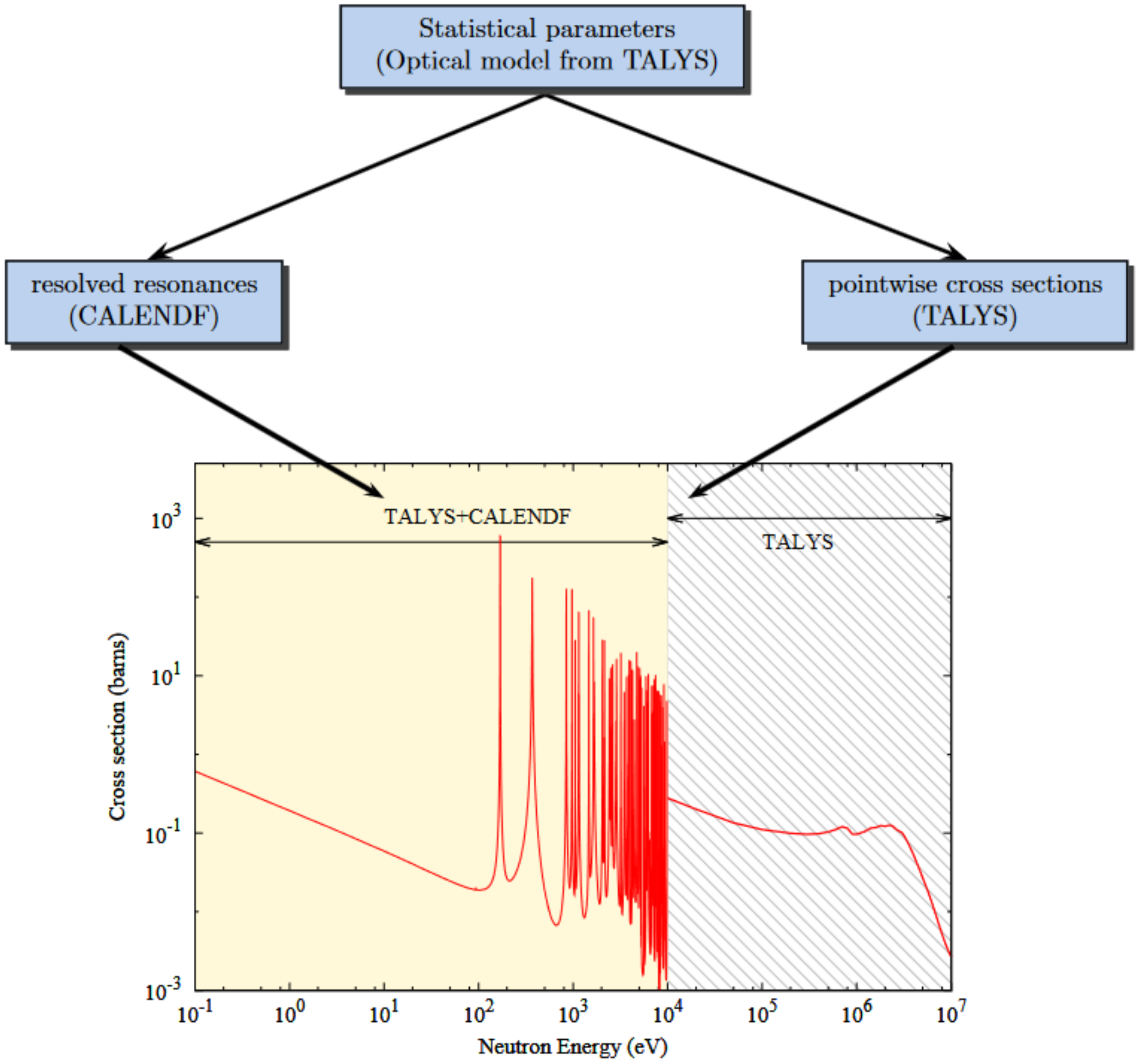
Modern tools and data

Presented in ANE 50 (2013) 60

- Combine 3 model types:
  - Level density,
  - Optical model potential and
  - γ-strength function)
- to produce statistical resonances

Uses the following scheme:

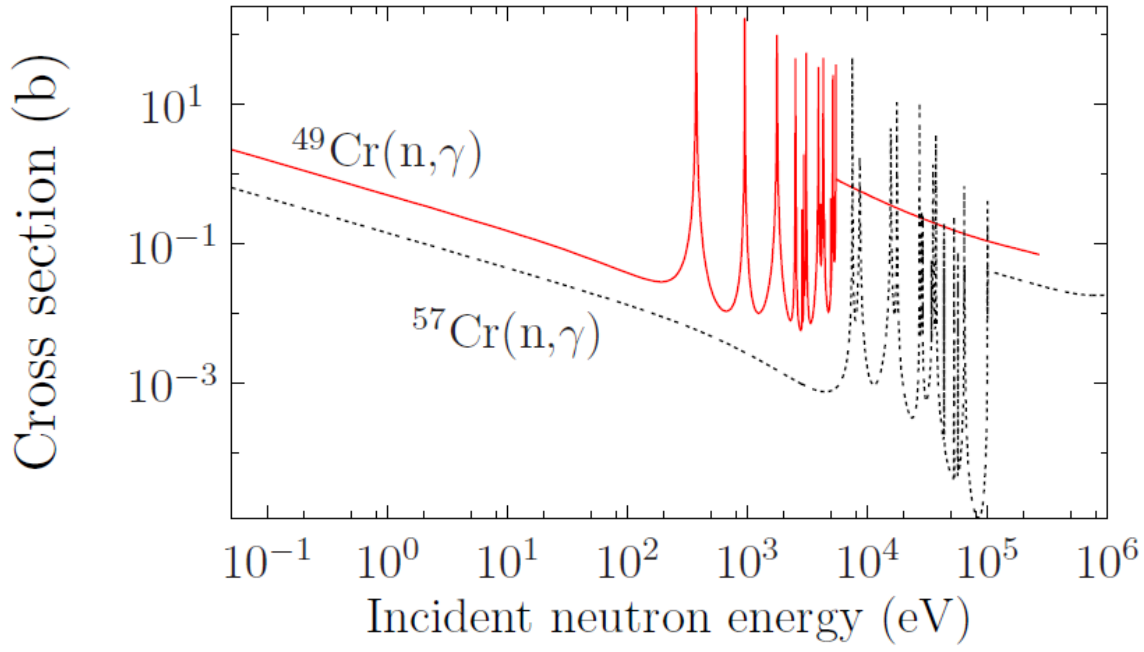
- TALYS (input: ld + omp + γ-str)
- CALENDF (input: TALYS output)
- Output: statistical resonances



Modern tools and data

HFR calculations:

1. TALYS + specific ld + specific omp + specific γ-str
2. TALYS output: average D_0, Γ_γ, Γ_n, Γ_f... as a function of E_n
3. CALENDF + TALYS output in the form of an ENDF-6 file
   - generate random ladders of resonances using the statistical properties
   - Just like in the unresolved resonance range,
   - But this time from 0 to a few 10 or 100 keV.



Modern tools and data

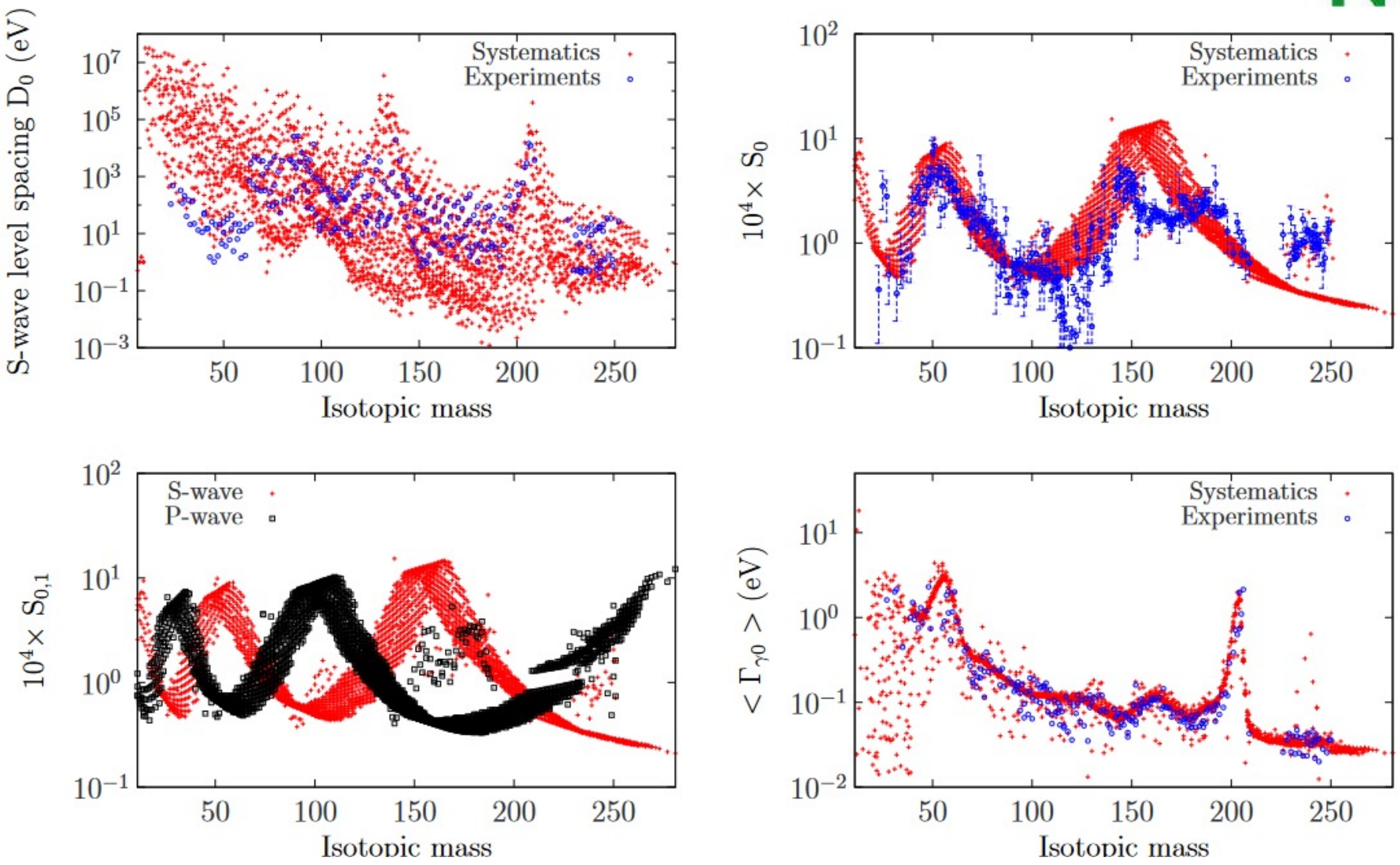
The idea is to generate random ladders of resonances using the statistical properties (as in the unresolved resonance range):

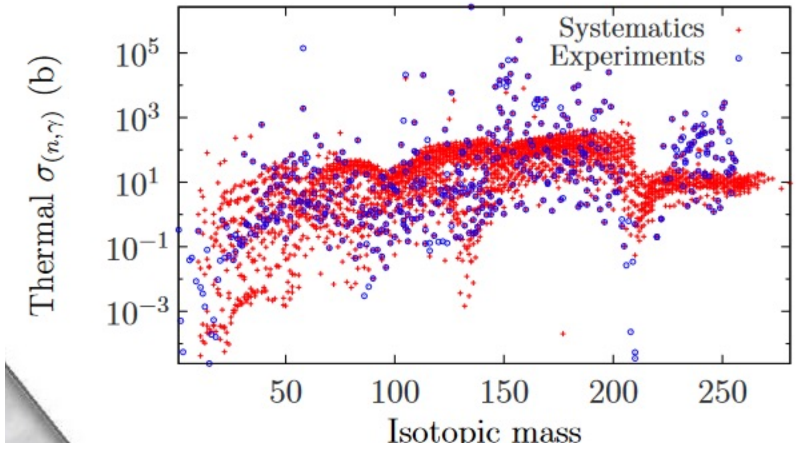
1. one ladder can be generated for an energy E by randomly selecting a starting resonance energy for one (l, j) sequence, and also randomly selecting a set of widths for that resonance using the appropriate average widths and χ^2 distribution functions.
2. We can then select the next higher resonance energy by sampling from the Wigner distribution for resonance spacings, and a new set of widths for that resonance can be chosen.
3. The process is continued until a long ladder of resonances for that (l, j) is obtained.
4. The process for the other (l, j) sequences is then repeated, each such sequence being uncorrelated in positions from the others.
5. for each (l, j) couple , a GOE random matrix (Gaussian Orthogonal Ensemble) is used to generate resonance energies (allowing to follow the Wigner law and to include correlations between two successive resonances).

Modern tools and data

Different possibilities exist for the 3 models in TALYS

- Level density models: 6 (from 1 to 6)
- Gamma-strength function: 8 (from 1 to 8)
- Optical model: 2 (Koning-Delaroche or Semi-microscopic optical model (JLM): y or n)





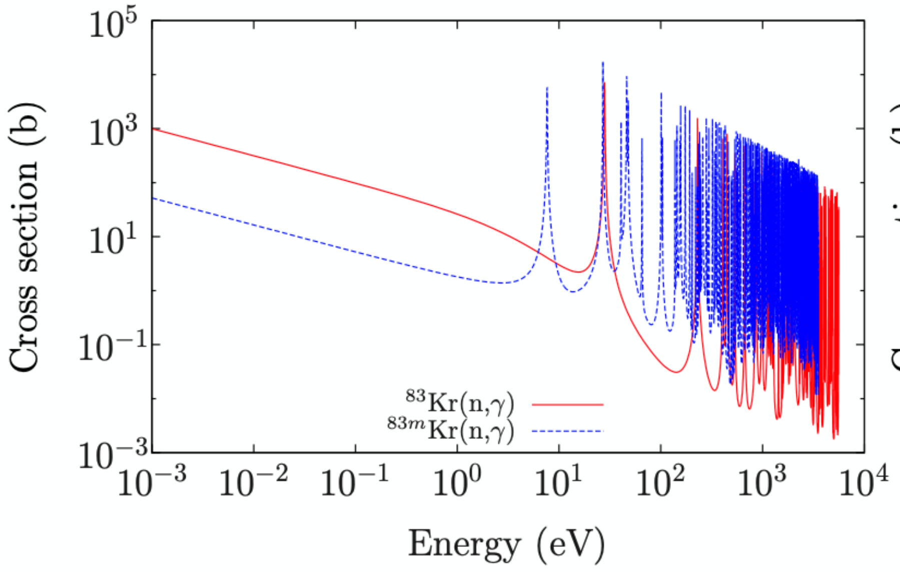
Modern tools and data

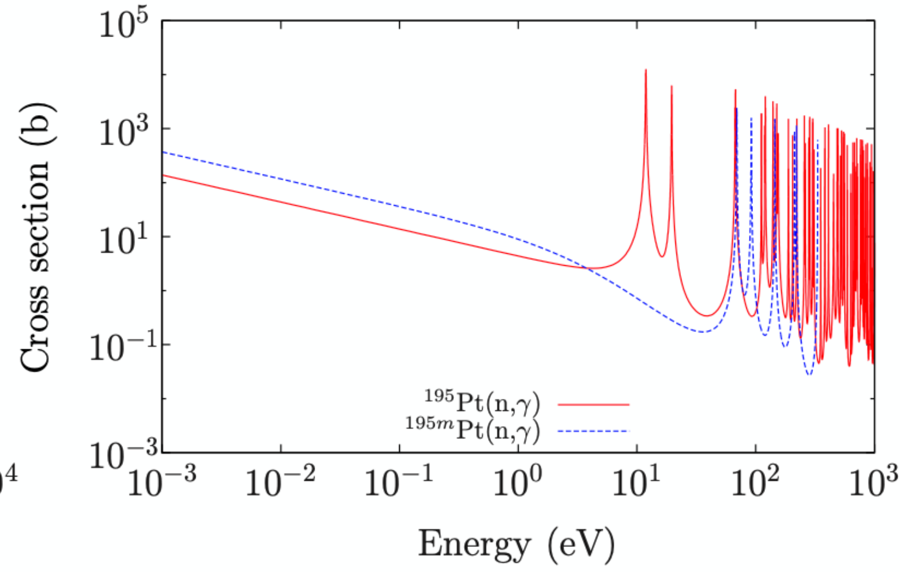
Thermal cross sections for isomers: HFR applied for ground state and isomeric states

$$\sigma_\gamma^{\text{isomer}} = \sigma_\gamma^{\text{ground}} \frac{\sum_j \frac{g\Gamma_{nj}^0 \Gamma_{\gamma j}}{E_{0j}^2}}{\sum_i \frac{g\Gamma_{ni}^0 \Gamma_{\gamma i}}{E_{0i}^2}}$$

$\sigma_\gamma^{\text{ground}} \Longrightarrow$ known from measurements (or systematics)

$\sum_j$ and $\sum_i \Longrightarrow$ taken (as before) from the global OMP of TALYS.





Physics tests

Spacing distribution, Wigner distribution, Porter-Thomas distribution

Cumulative level distribution

Average total capture width

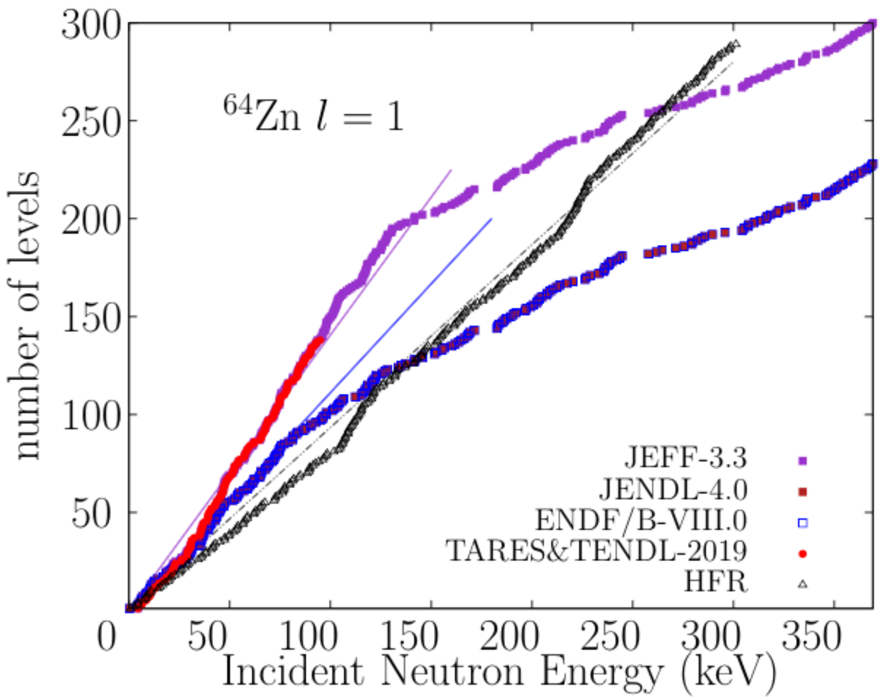
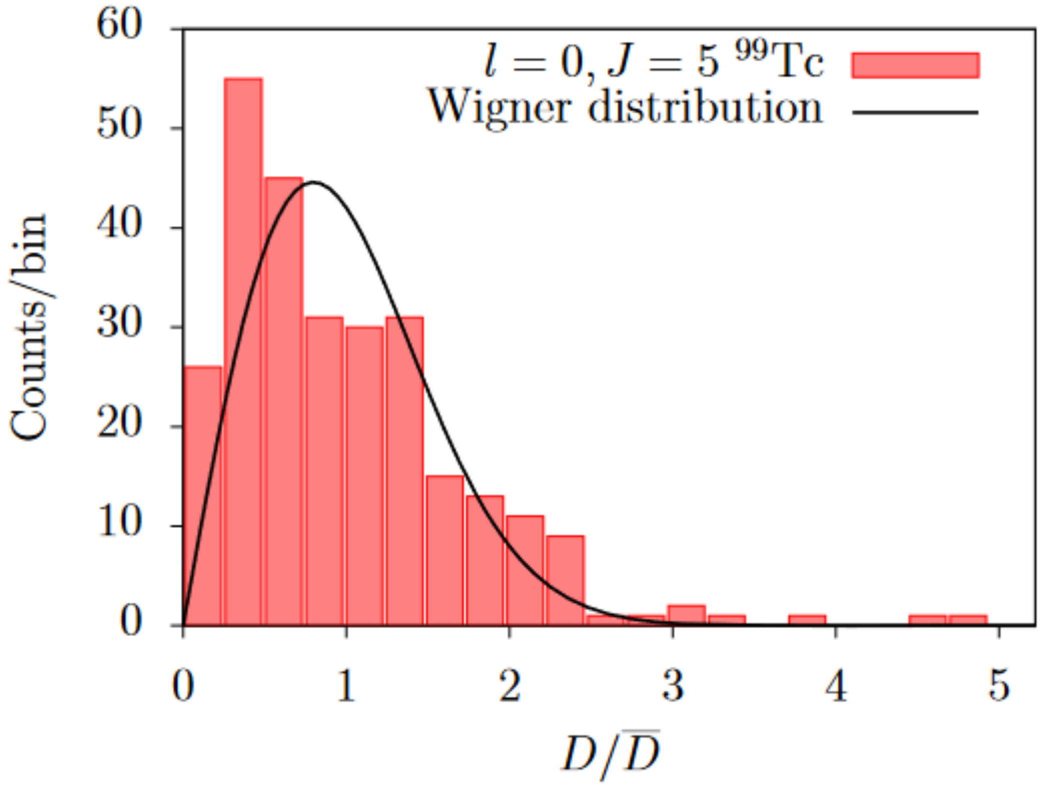
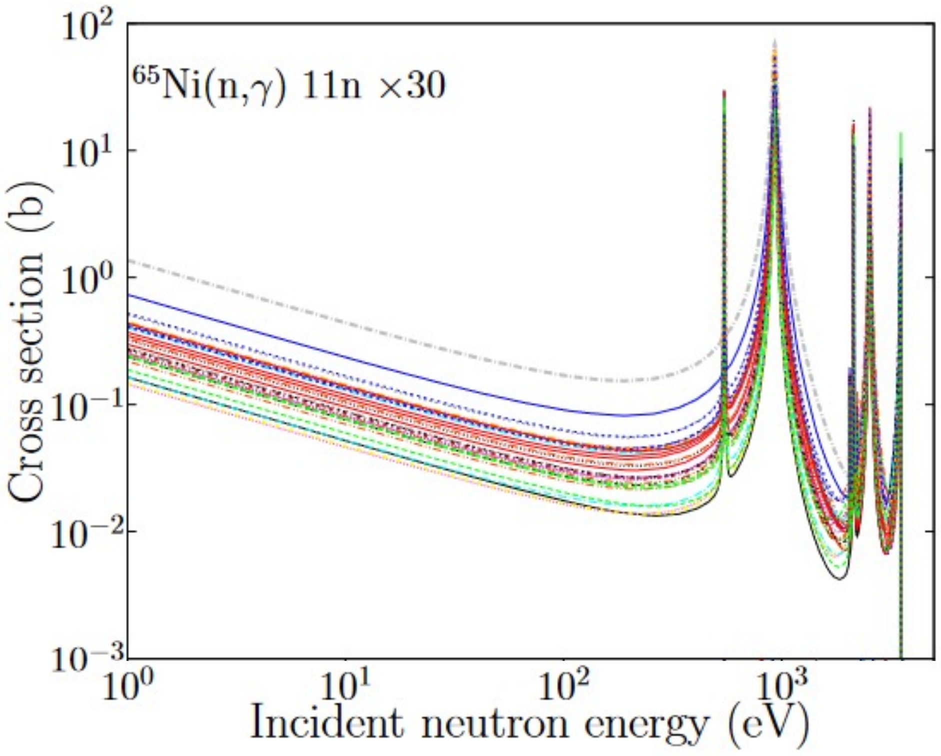


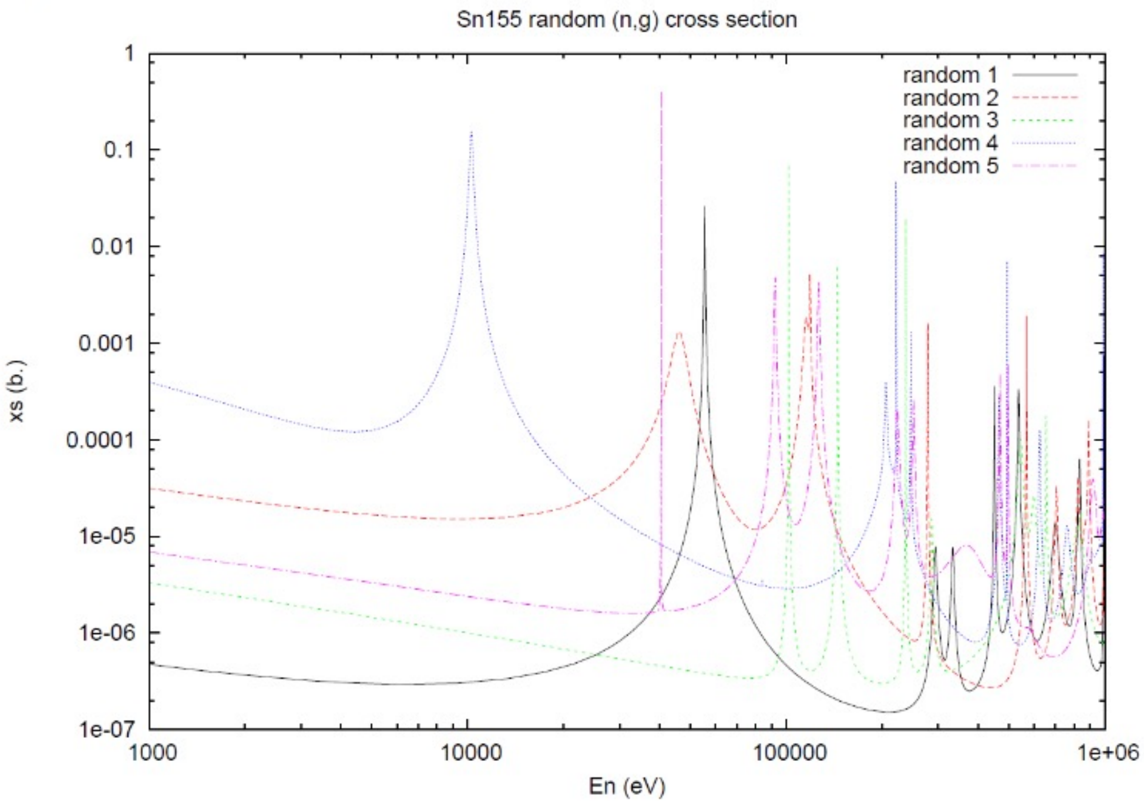
FIG. 16. (Color online) Top: cumulative level distribution for ^{120}Sn and $l = 0$; Bottom: same for ^{64}Zn and $l = 1$.



Examples

Given a specific selection of TALYS models (one level density model, one gamma-strength function, one optical model), one can generate sets of HFR



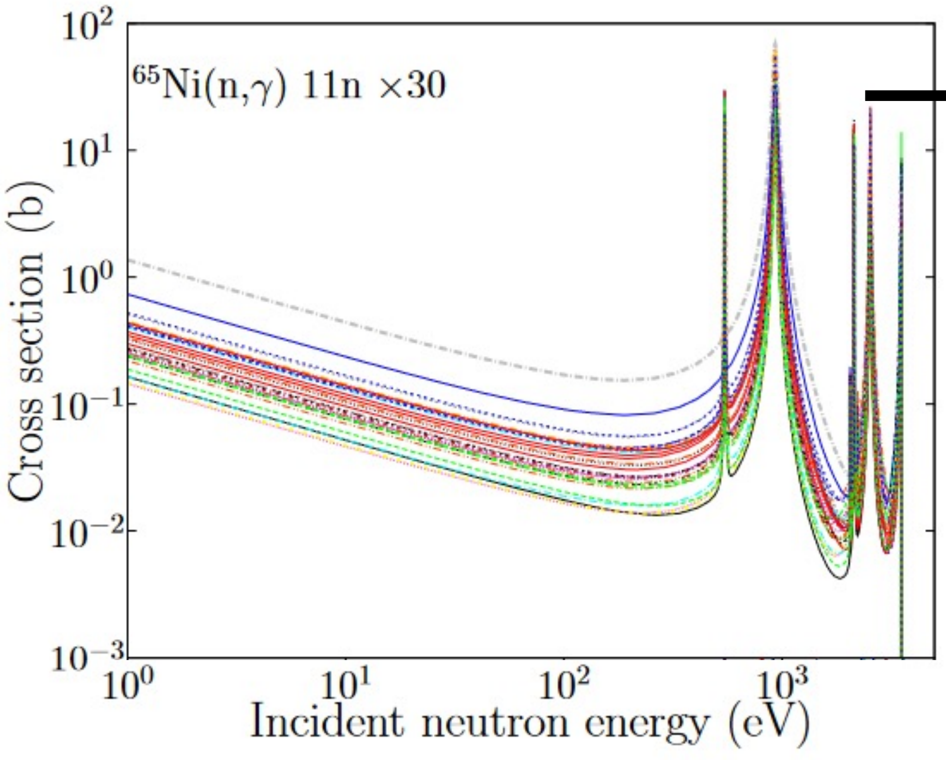


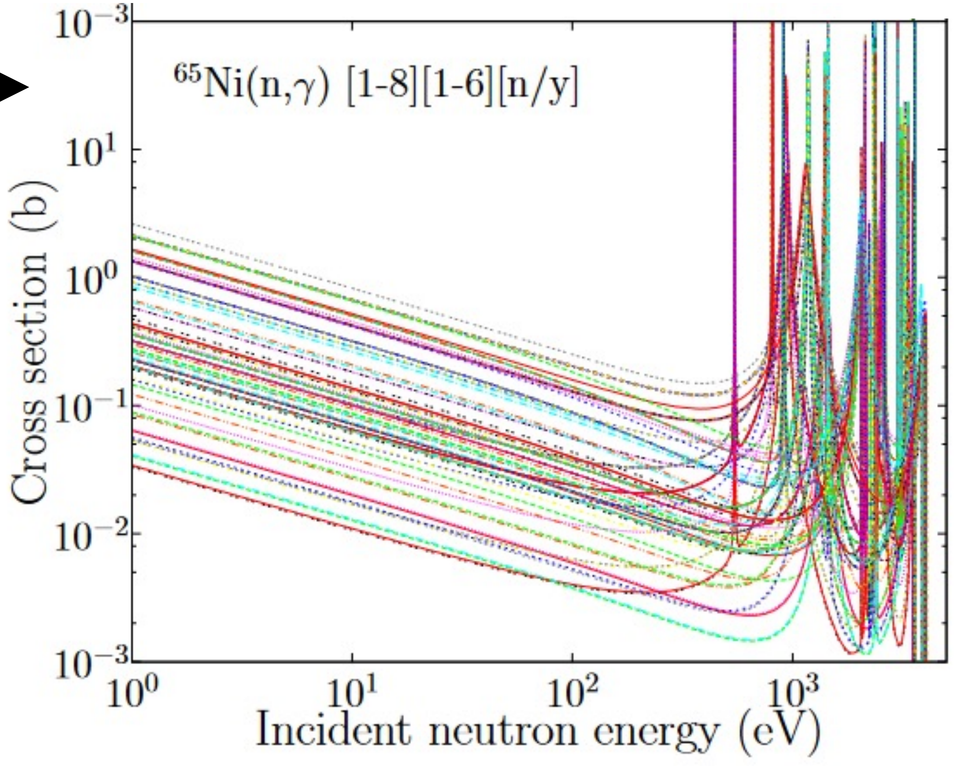
Resonance energies as fixed parameters

Resonance energies as free parameters

Examples

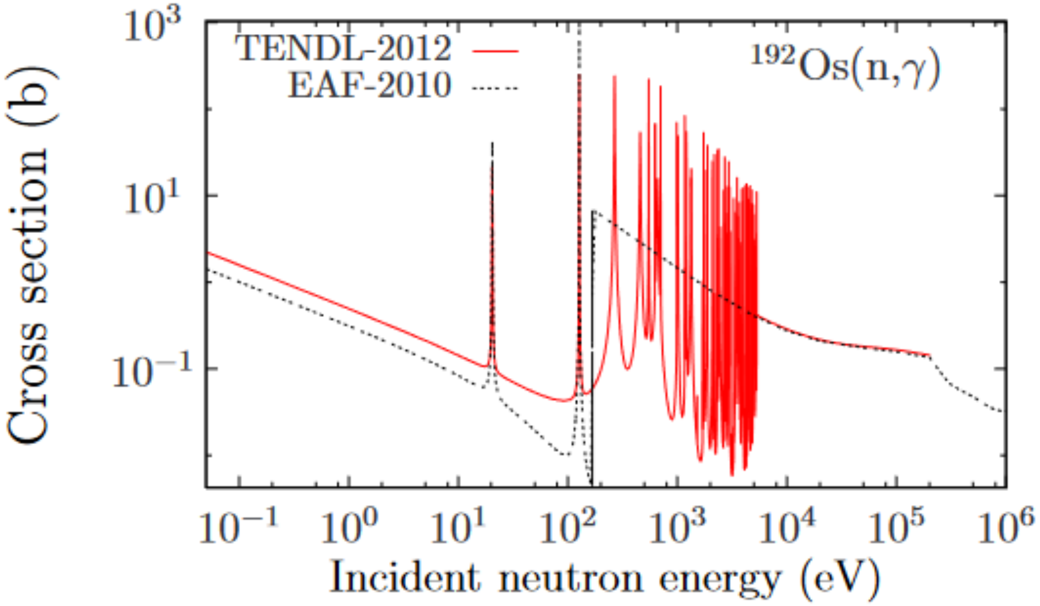
Given many TALYS models (one level density model, one gamma-strength function, one optical model), one can generate sets of HFR

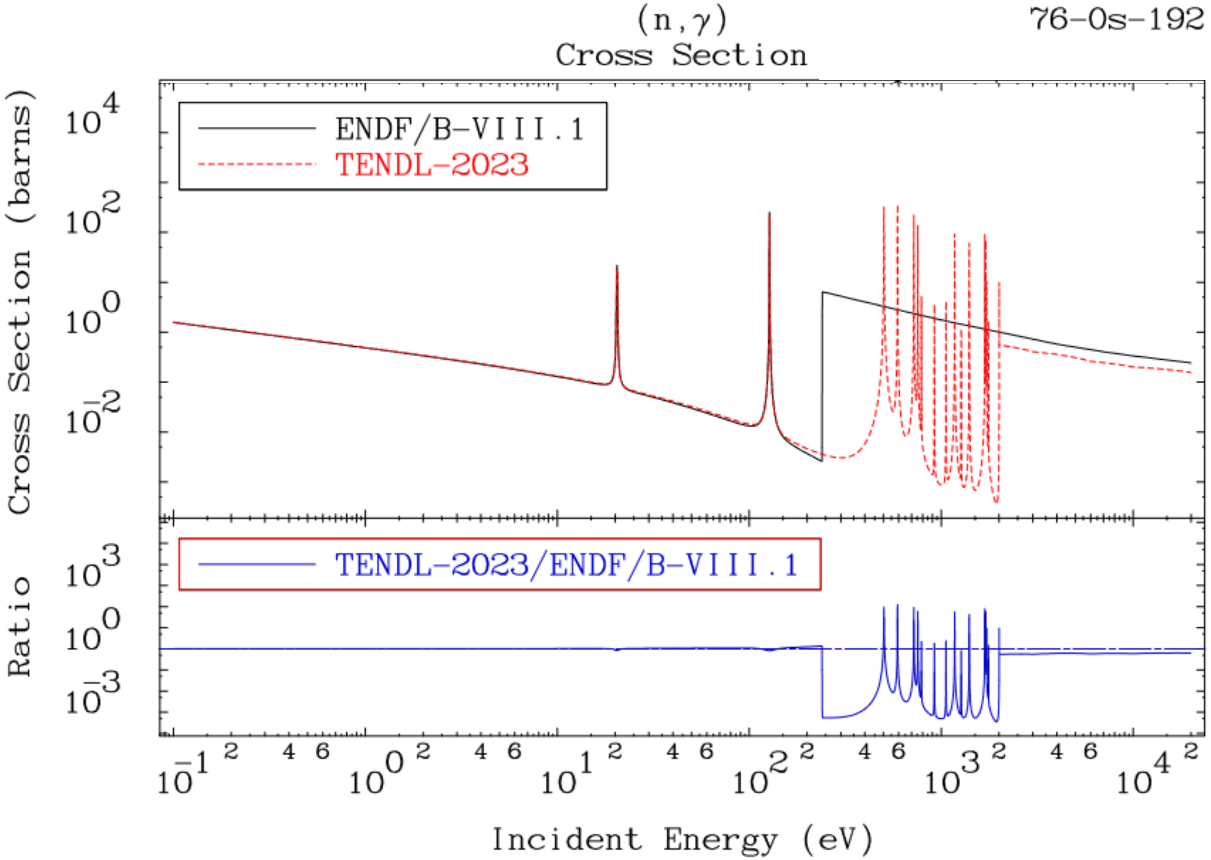




Examples

Combination with "real" resonances





MACS: Maxwellian Averaged Cross Section

σ_γ: capture cross section, obtained from measurements or calculations,

kT: from 5 to 120 keV, with 30 keV commonly used as a reference,

kT=30 keV: see the Kadonis database with experimental data.

$$\sigma_{Maxw} = \left(\frac{8}{\pi\mu(kT)^3}\right)^{1/2} \int_0^\infty dE\ \sigma_\gamma(E) E e^{-E/kT},$$

The capture cross section for MACS is usually calculated with the Hauser-Feshbach approximation (HF)

Statistical model & Continuous capture cross sections

Valid if

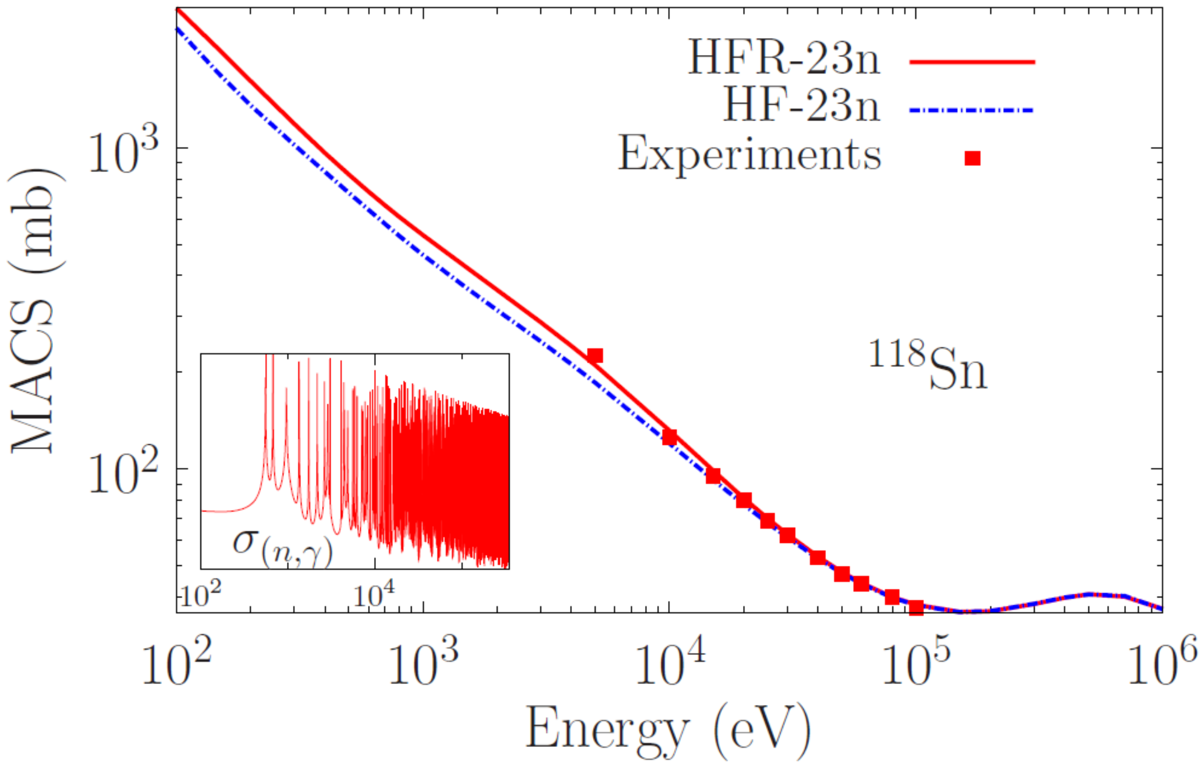
- The compound framework is applicable (compound nucleus fully equilibrated before breaking)
- The level density must be sufficiently large for individual resonances to overlap

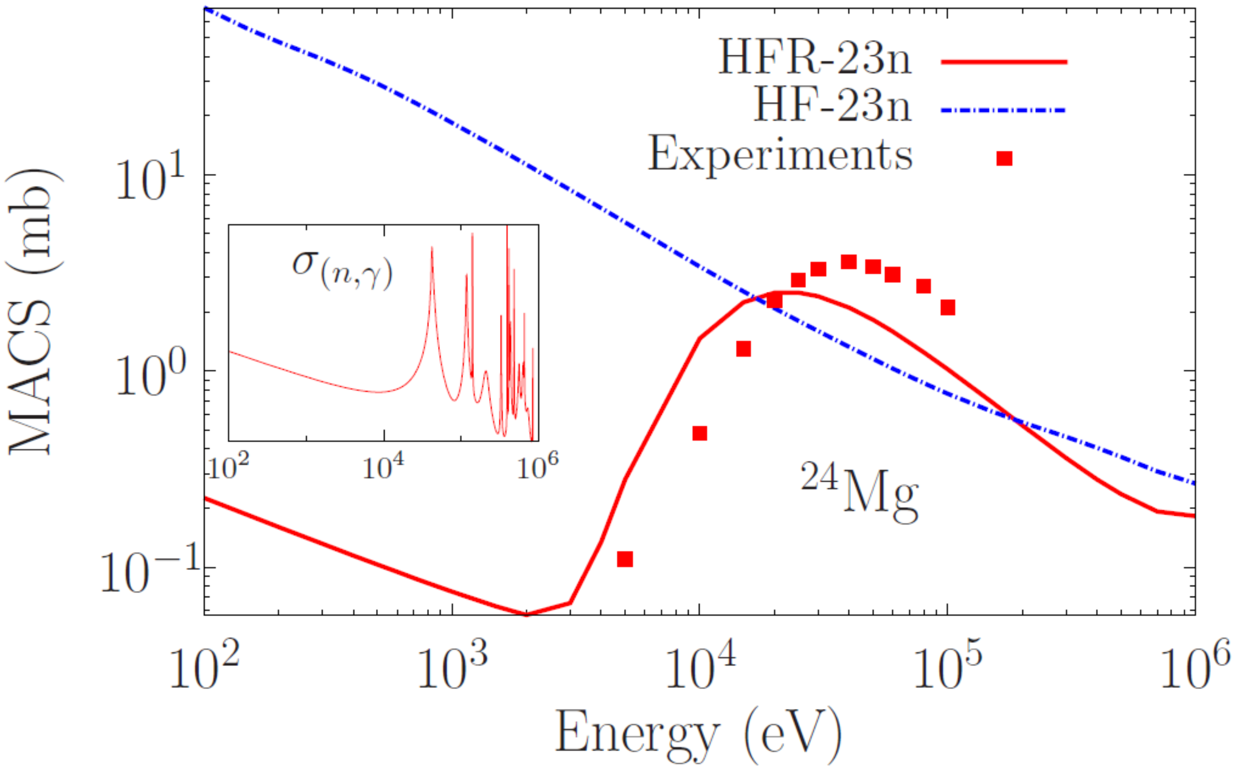
Different possibilities exist for the 3 models in TALYS,

- Level density models: 6 (from 1 to 6)
- Gamma-strength function: 8 (from 1 to 8)
- Optical model: 2 (Koning-Delaroche or Semi-microscopic optical model (JLM): y or n)
- noted as “ijn” (11n, 23n…)

MACS: Maxwellian Averaged Cross Section

- The HF is not applicable for the light isotopes and far from the stability line, but still used...



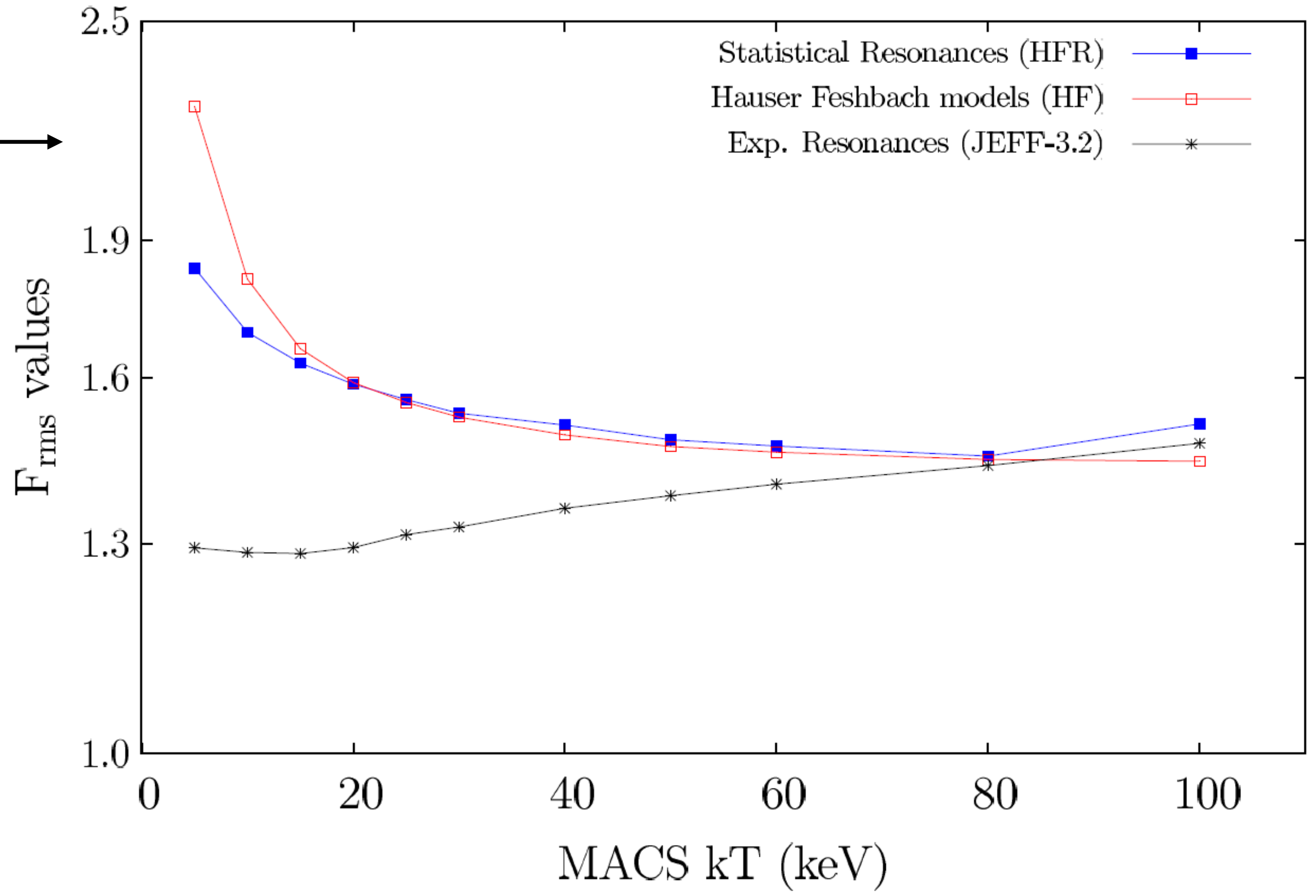


MACS: Maxwellian Averaged Cross Section

- To perform a validation, a comparison to Kadonis is performed with the f_{rms} factor for 215 measured isotopes
- In total 96 possibilities: 6x8x2 (96 for HF and 96 for HFR)
  - Level density models: 6 (from 1 to 6)
  - Gamma-strength function: 8 (from 1 to 8)
  - Optical model: 2 (Koning-Delaroche or Semi-microscopic optical model (JLM): y or n)

$$f_{rms} = \exp\left[\frac{1}{N_{tot}}\sum_{Z,A}\ln^2\frac{\langle\sigma_{th}\rangle}{\langle\sigma_{exp}\rangle}\right]^{1/2}$$

Case 23n
(Level density 2: Back-shifted Fermi gas Model
+
Gamma-strength function 3: Hartree-Fock BCS tables
+
KD OMP)



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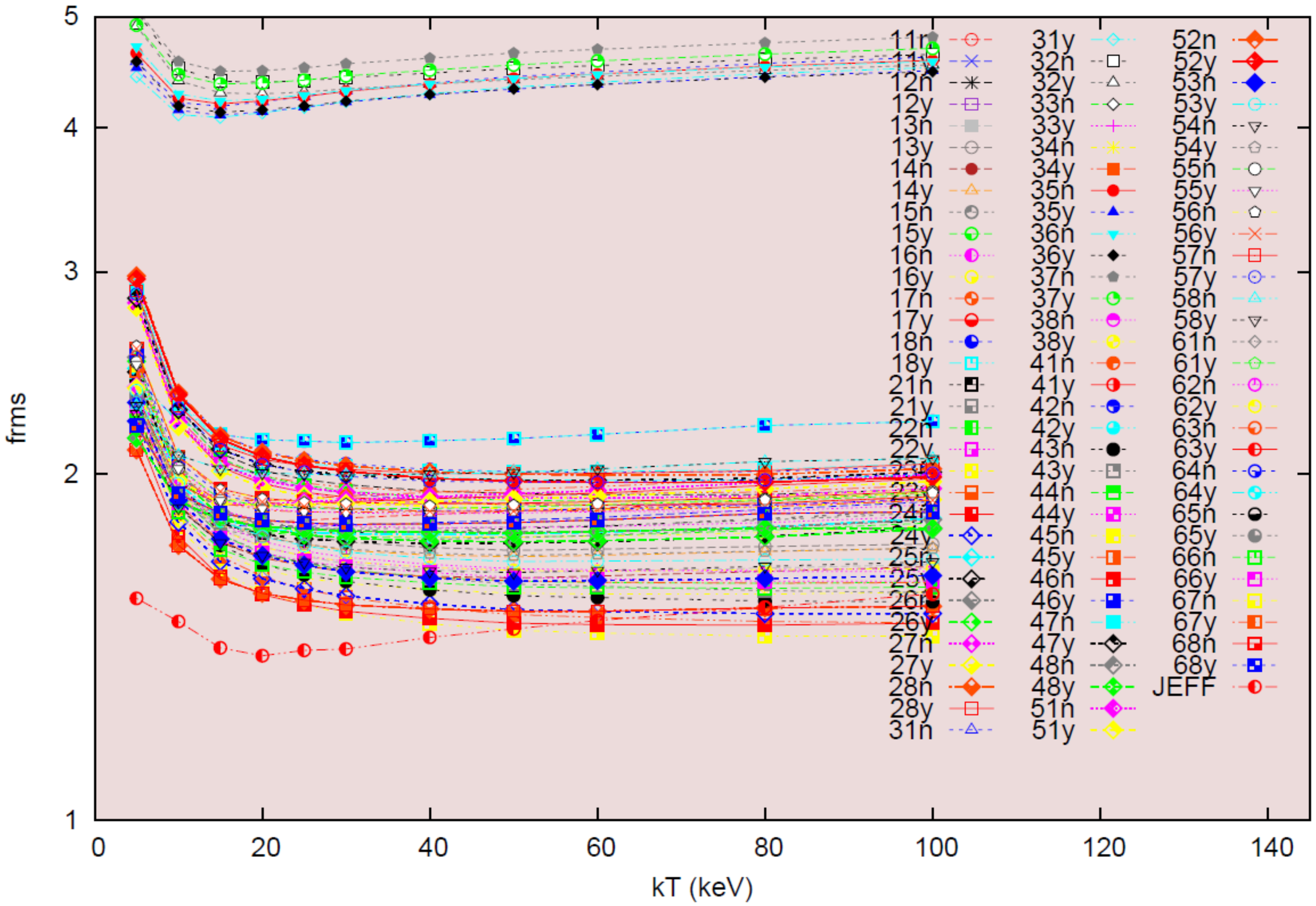
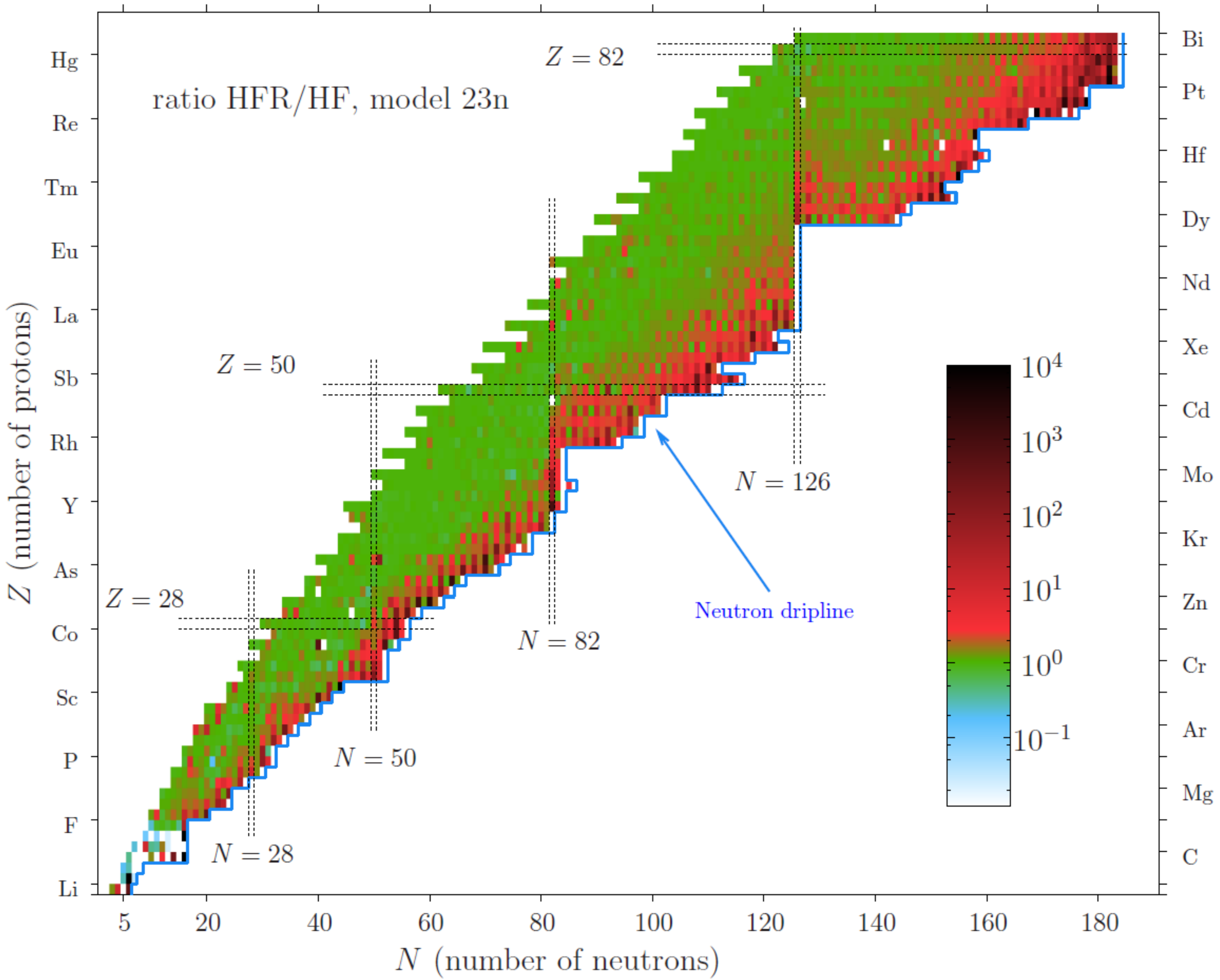


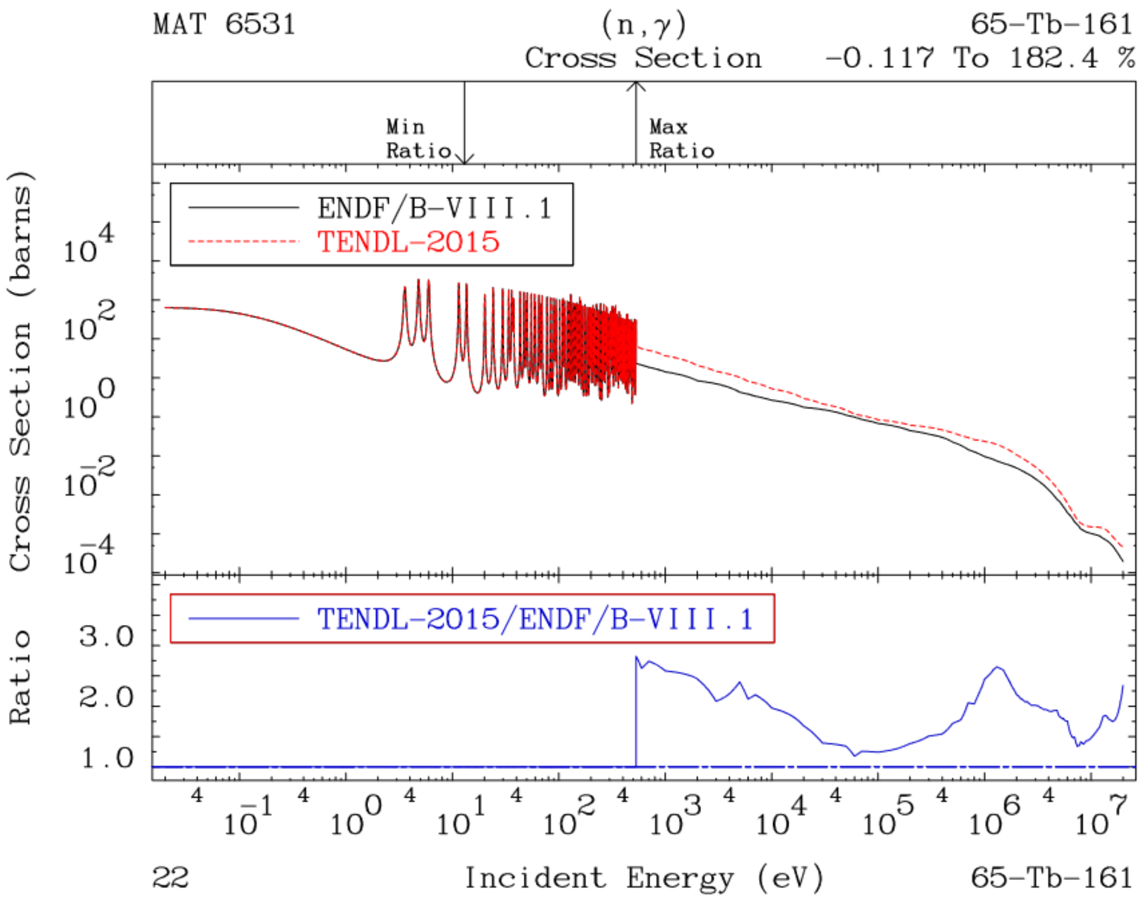
$$f_{rms} = \exp\left[\frac{1}{N_{tot}}\sum_{Z,A}\ln^2\frac{\langle\sigma_{th}\rangle}{\langle\sigma_{exp}\rangle}\right]^{1/2}$$

MACS: 23n, to the drip line



World dissemination

- The HFR method is used in the TENDL libraries (unless measured resonances exist)
- It is now in JEFF-3.3 and JEFF-4.0 (soon to be)
- ENDF/B-VIII.1 is also importing ENDF-6 MF2 (resonances) with the HFR (22 MF2)
- Similar approach is used for astrophysics (MACS), see TENDL-2023 webpage



Conclusion

- HFR: outcome of a long-term evolution
- Link the fast neutron range to the thermal and resonance range
- Today applied to thousands of nuclides
- Based on TALYS models
- MACS: see TENDL-Astro
- Advantages: provide an answer
- Drawback: provide an answer

- Future: better TALYS, better TENDL, more model variations

Different reaction "model sets" were used: "a model set" represents a combination of 9 TALYS models:

1. Gamma strength function (values 8 or 9): either E1 photon strength function: Gogny D1M Hartree-Fock-Bogoluybov (HFB) plus QRPA [1], or SMLO
2. Level density (values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Skyrme-Hartree-Fock-Bogoluybov plus combinatorial level densities [2]
3. JLM microscopic optical model potential or KD henomenological Koning-Delaroche optical model potentia [3] (values y or n)
4. Gamma strength function for M1 (values 3 or 8): Hartree-Fock BCS tables or Gogny D1M HFB+QRPA [4]
5. Collective enhancement (values y or n): yes or no
6. Width fluctuation (values 0, 1 or 2): Moldauer model, or Hofmann-Richert-Tepel-Weidenmueller model
7. Mass model (values 0, 1, 2 or 3): Duflo-Zuker formula, Moeller table, Goriely HFB-Skyrme table (HFB-24), or HFB-Gogny D1M table (except for known masses, where the experimental value is used)
8. Alpha optical model (values 5 or 6): Demetriou/Goriely, or Avrigeanu
9. Fission model (values 1 or 5): "experimental" fission barriers, or Skyrme-HFB fission barriers [5].

Many thanks

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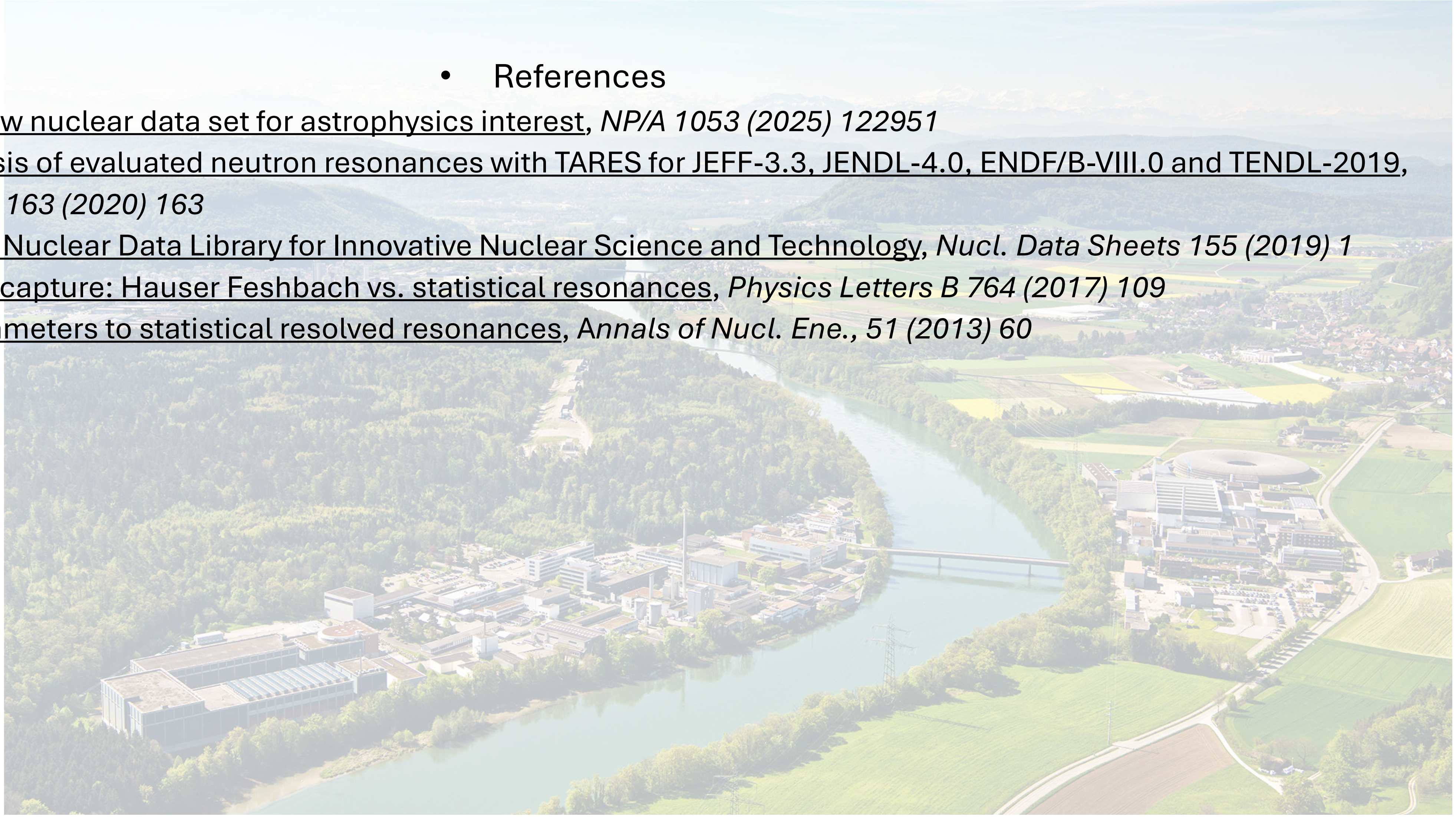

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