From average parameters to statistical resolved resonances; Application to ^{135m}Xe

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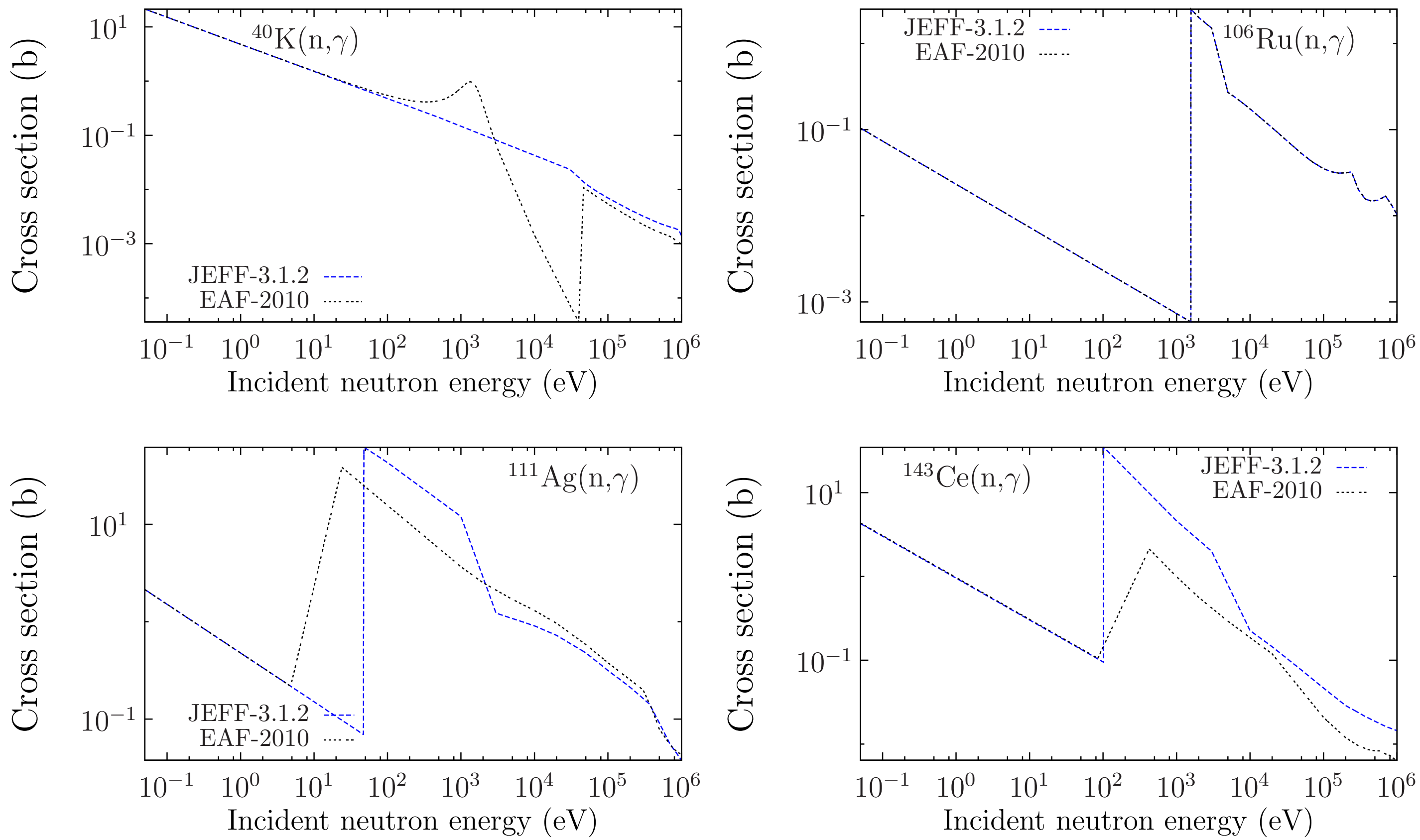
Motivation

① Improve the global calculations in the resonance range for short-lived nuclides with the TALYS system

② Use CALENDF-2010 to *statistically* reconstruct the URR

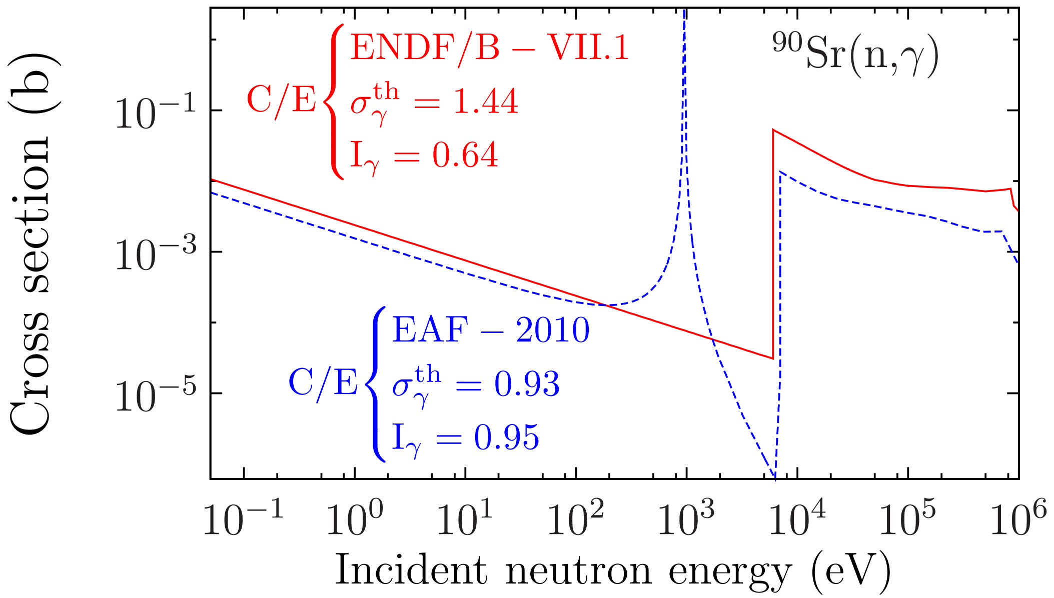
③ Apply the methodology to TENDL libraries and proposed isotopes for JEFF-3.2

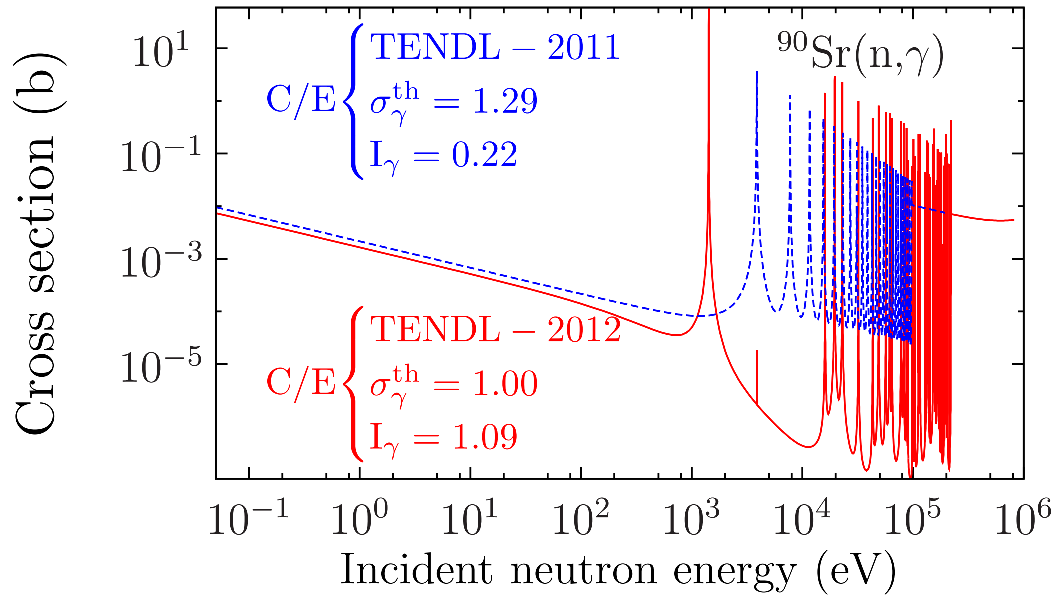
④ Detailed application for ^{135m}Xe



Motivation

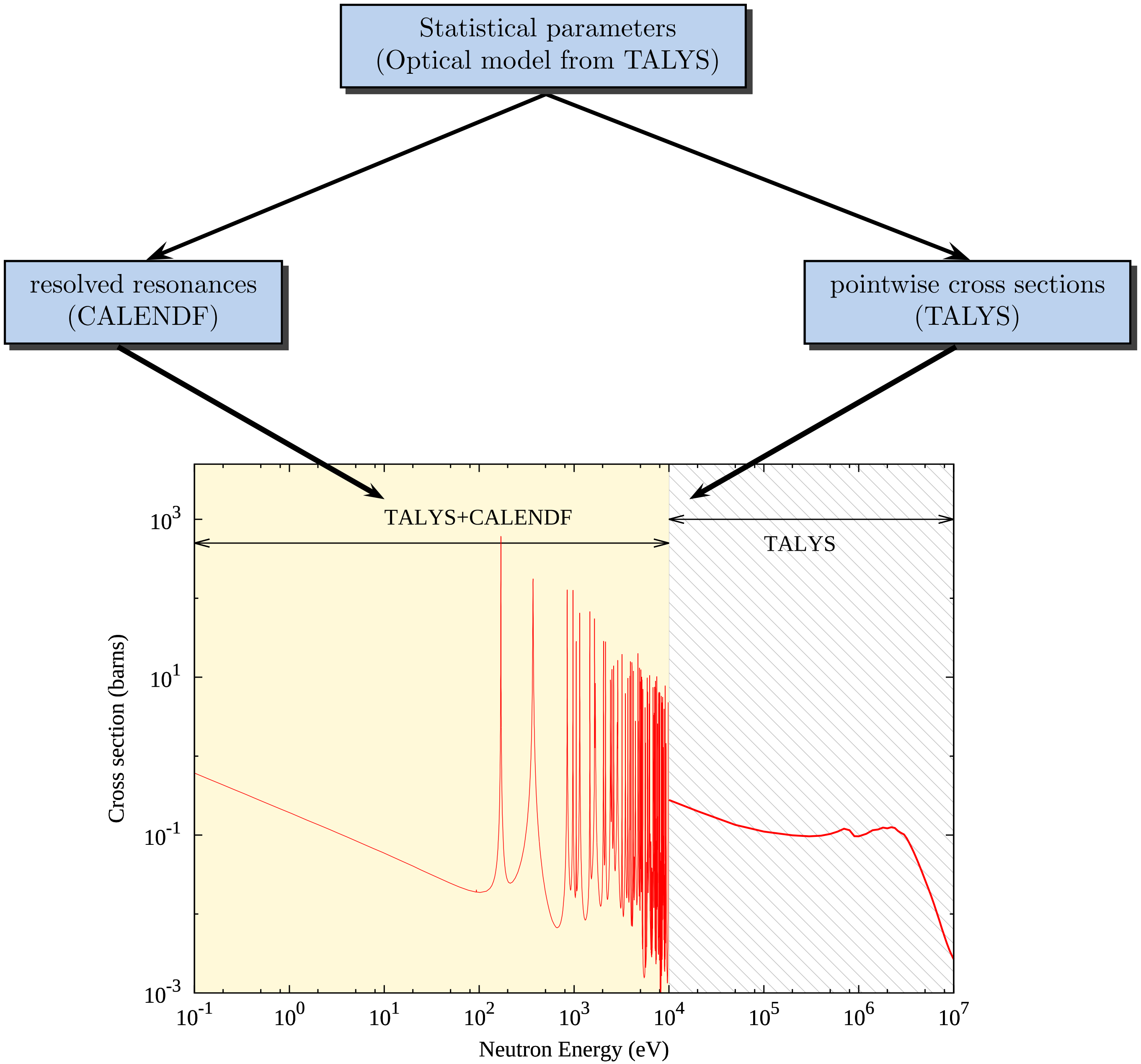
Examples of different approaches for ^{90}Sr ($h_{1/2} = 28$ sec) in the low energy region.





Left: basic optical model calculation for ENDF/B-VII.1 and Single Resonance Approximation (SRA) for EAF-2010. Right: multi-SRA for TENDL-2011 and the present methodology from TENDL-2012 to TENDL-2014.

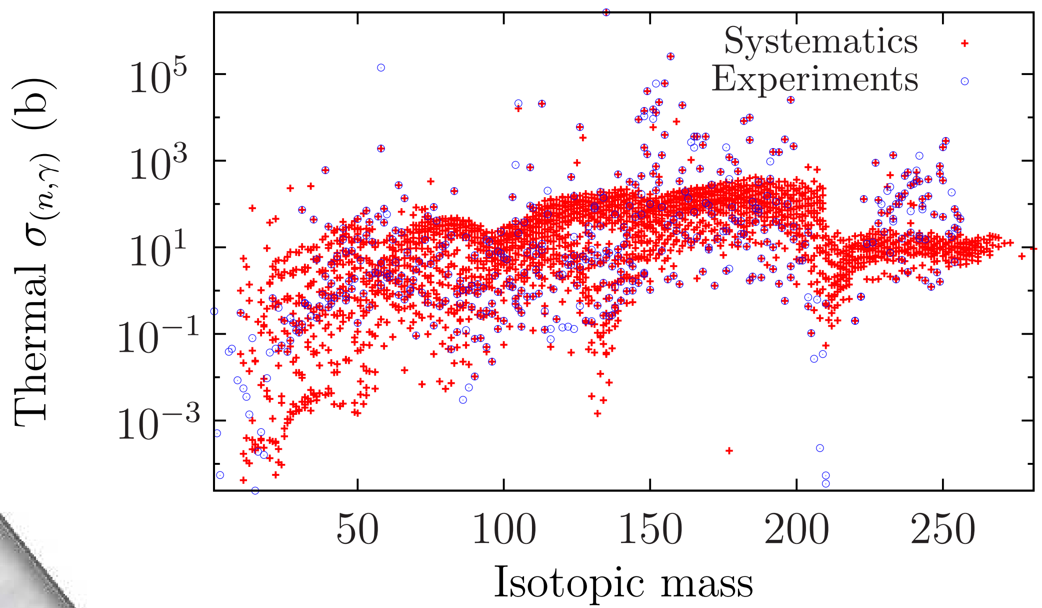
Schematic approach to use in combination TALYS and CALENDF-2010

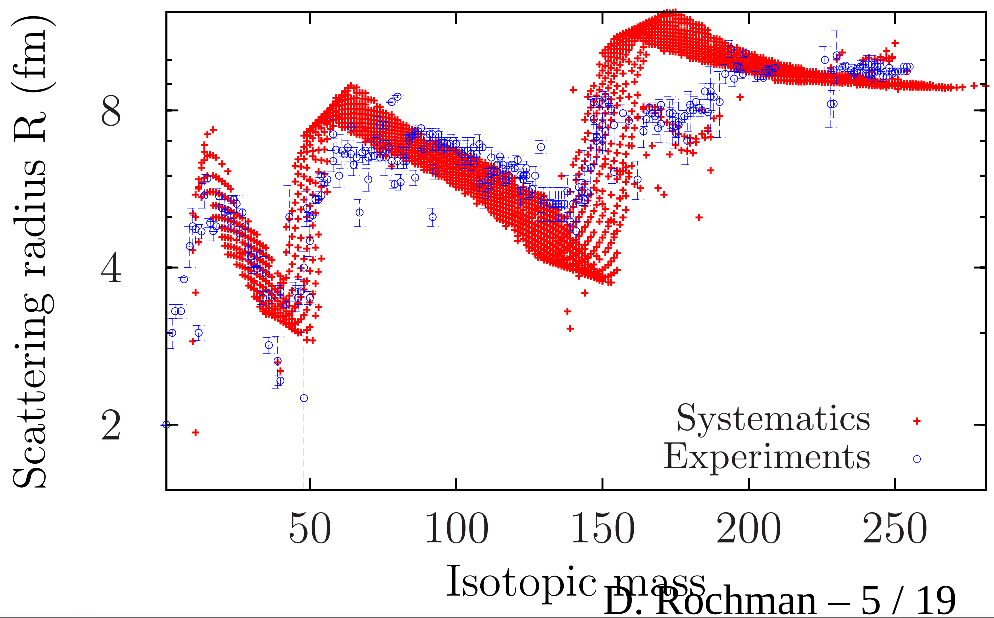


Necessary parameters

As a starting point energy-dependent statistical parameters as well as specific cross sections are needed in the whole energy range. These parameters are for each orbital angular momentum l and spin of the resonance state j:

- the scattering radius r,
- the average level spacing D_0,
- the average reduced neutron width Γ_n^0,
- the average radiation width Γ_γ,
- and if relevant the average fission width Γ_f.





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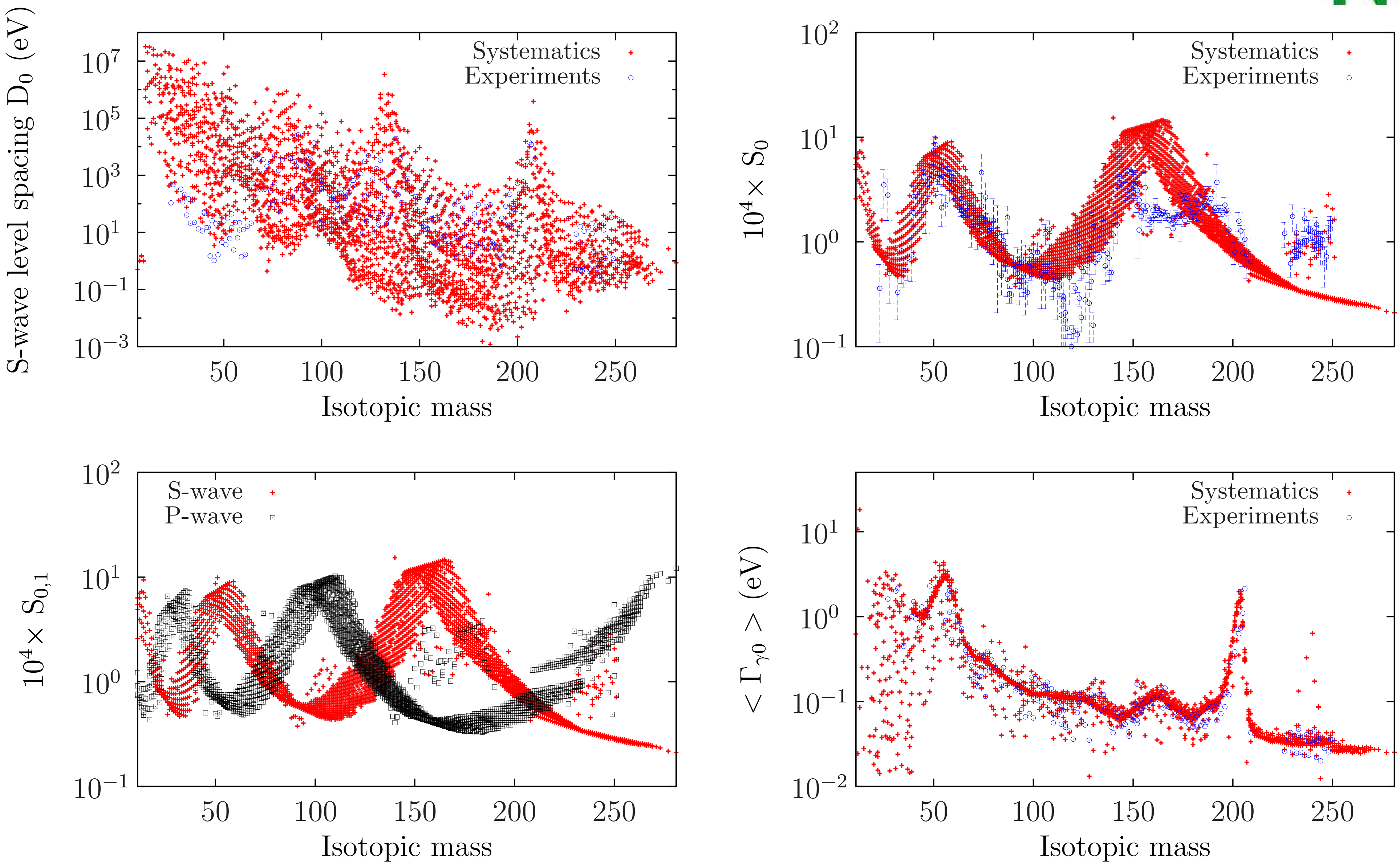


3 groups of isotopes ($t_{1/2} > 1$ sec.)

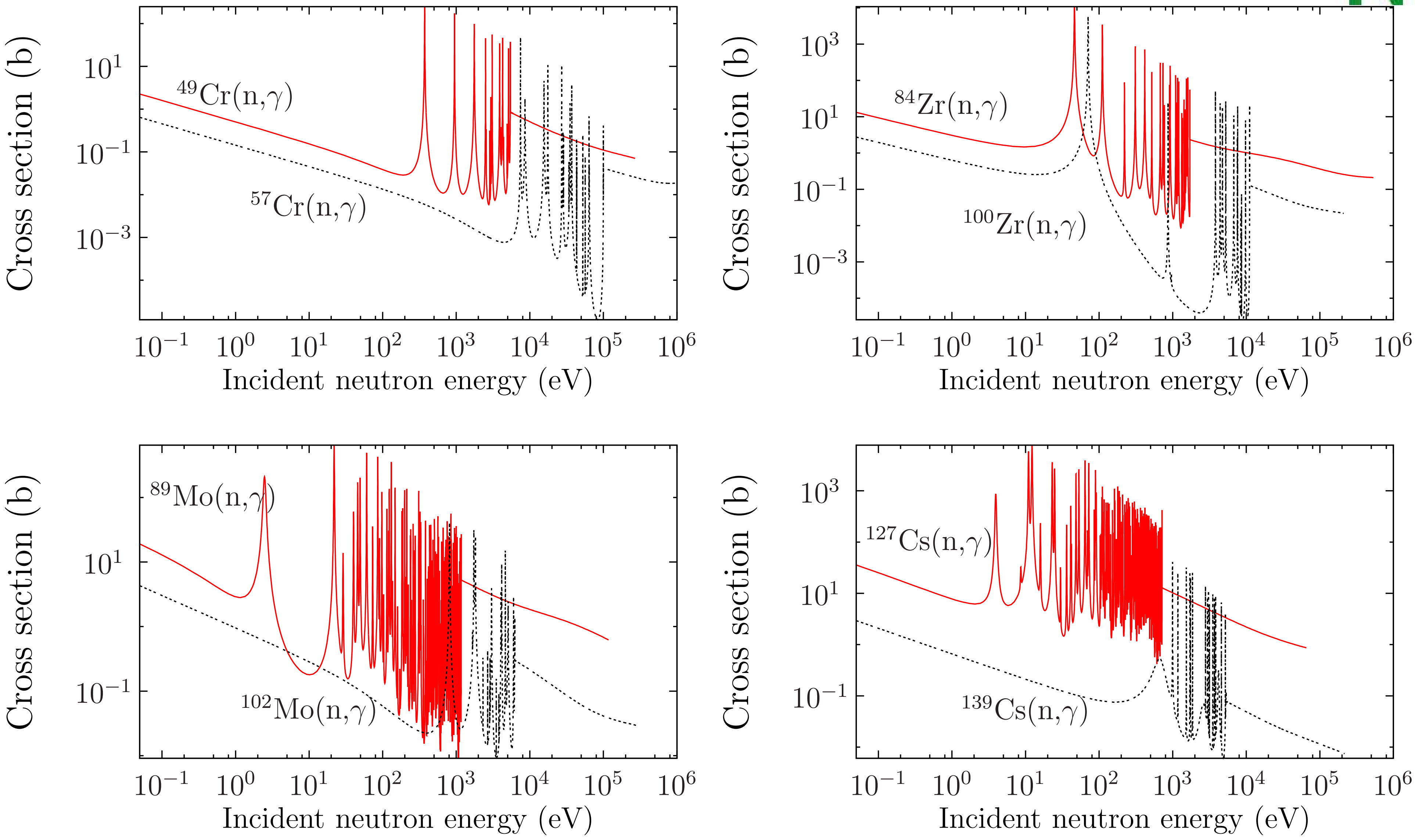
- isotopes without any experimental reaction information (about 1600 isotopes). In this case, as no specific information can be used to adjust calculations, we fully rely on systematics, as defined in TALYS.
- isotopes with scarce experimental data, such as thermal cross sections, resonance integrals, average cross sections at high energy (about 400 isotopes). Such isotopes are for instance ^{40}K, ^{54}Mn, ^{60}Co, ^{90}Sr, ^{105}Rh, ^{106}Ru, ^{109}Cd, ^{111}Ag, ^{138,143}Ce or ^{204}Hg.
- isotopes with measured pointwise cross sections, resonances, integral measurements, and resolved resonance parameters (about 400 isotopes).

Converting average parameters to statistical resonances

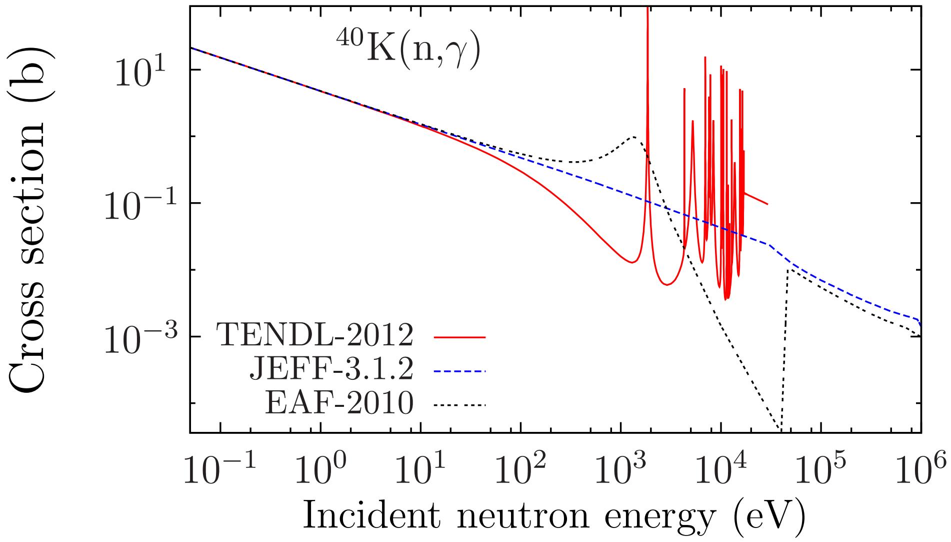
The idea is to generate random ladders of resonances using the statistical properties (as in the unresolved resonance range):

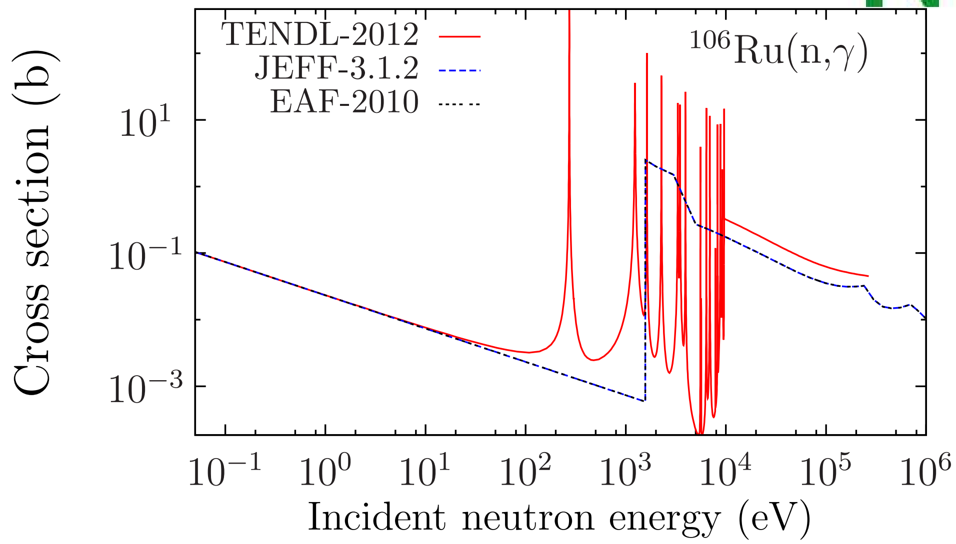
- one ladder can be generated for an energy E by randomly selecting a starting resonance energy for one (l, j) sequence, and also randomly selecting a set of widths for that resonance using the appropriate average widths and χ^2 distribution functions.
- We can then select the next higher resonance energy by sampling from the Wigner distribution for resonance spacings, and a new set of widths for that resonance can be chosen.
- The process is continued until a long ladder of resonances for that (l, j) is obtained.
- The process for the other (l, j) sequences is then repeated, each such sequence being uncorrelated in positions from the others.
- for each (l, j) couples, 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).

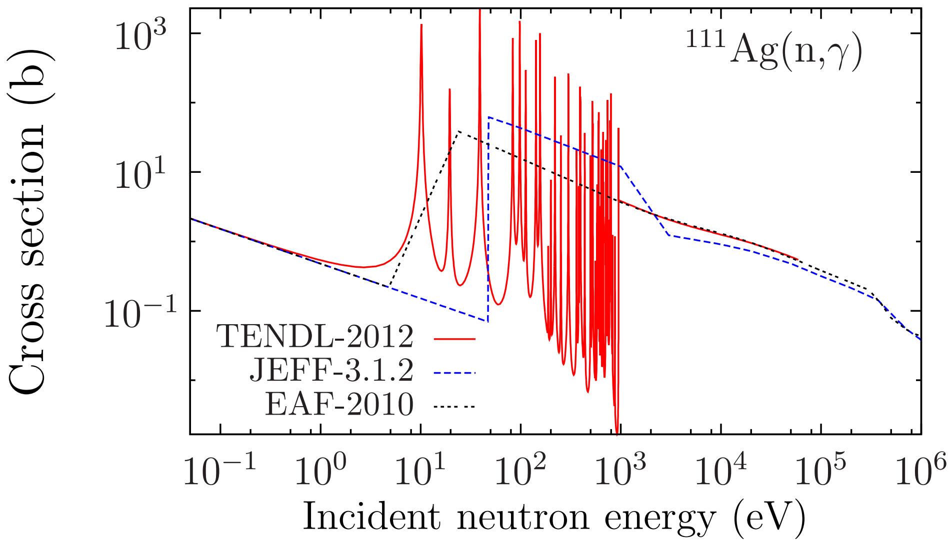
Example 1: short lived isotopes

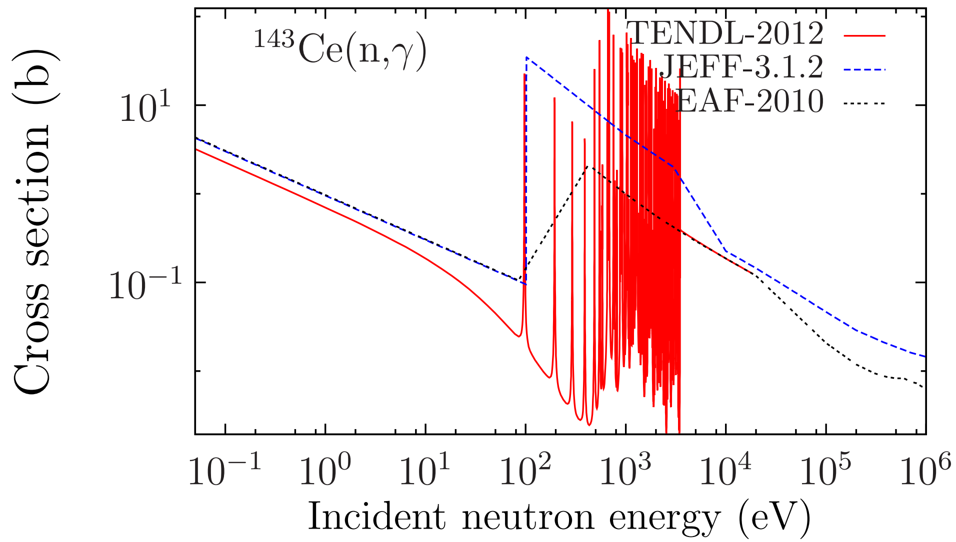


Example 2: isotopes with known thermal cross sections

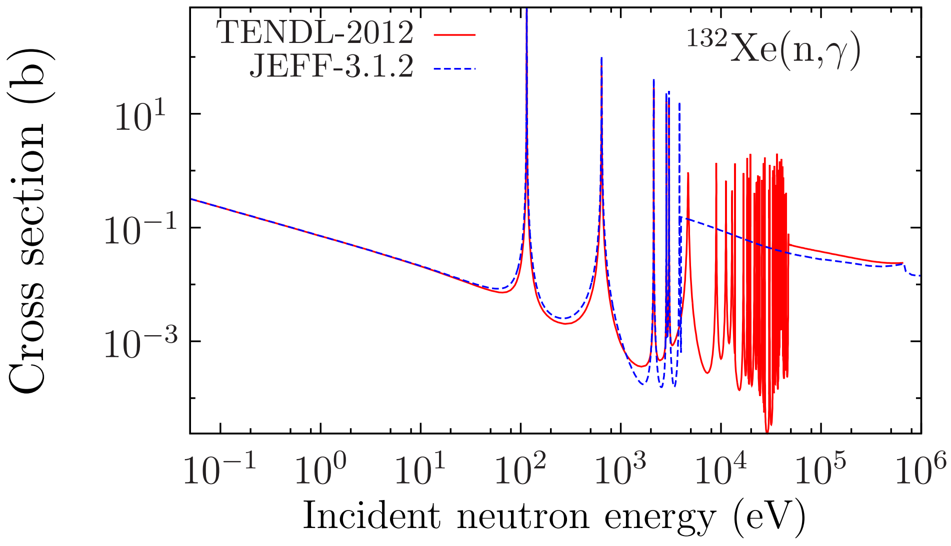


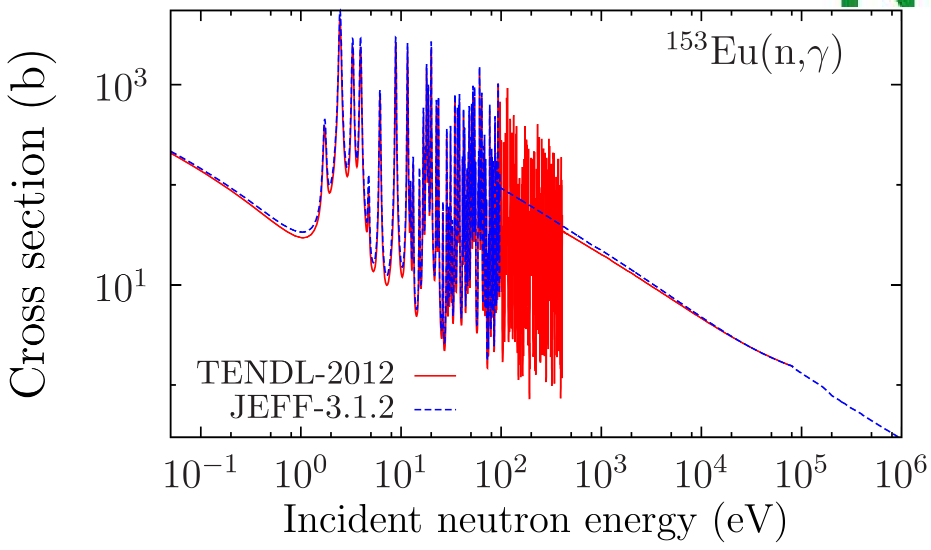


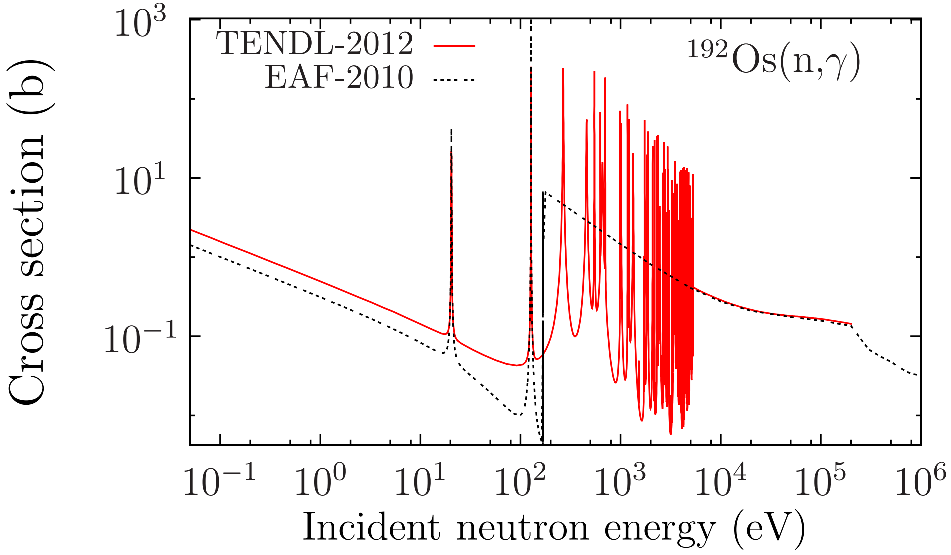


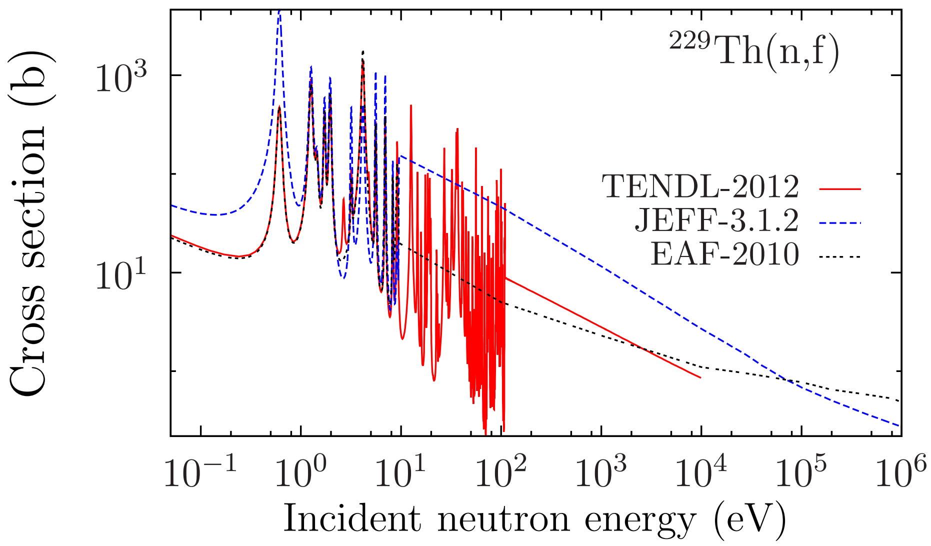


Example 3: isotopes with known resonances









Example 4: Thermal cross sections and resonance integrals

Table 1: Comparison of C/E for the thermal capture cross section σ_{th} (n,γ) and for the capture integral I_γ for a selection of isotopes.

Isotope	C/E σ_{th} (n,γ)		C/E I_γ	
	TENDL-2012	JEFF-3.1.2	TENDL-2012	JEFF-3.1.2
^{40}K	1.00	1.00	1.02	1.03
^{54}Mn	1.00	1.02	0.94	1.22
^{60}Co	1.00	1.00	0.95	1.19
^{105}Rh	0.99	0.76	0.84	0.72
^{106}Ru	1.00	1.00	1.43	1.01
^{109}Cd	0.99	1.05	0.83	0.28
^{111}Ag	1.00	1.00	1.03	0.98
^{138}Ce	1.00	0.86	1.07	2.48
^{143}Ce	1.00	1.33	1.73	15.3
^{192}Os	1.00	1.00	1.46	2.75
^{204}Hg	1.00	1.00	0.92	3.14

Cross sections for isomer (new feature in 2013)

For the cross sections of isomers, we are using the following approximations:

- ☞ cross sections can be represented by the Breit Wigner formalism,
- ☞ resonances are located far from the the thermal energy ($E_0 >> E_{\mathrm{th}}$),
- ☞ and the total width Γ of a resonance is smaller than its energy E_0 ($E_0 >> \Gamma$).

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In this case, the capture cross section at 0.0253 eV is:

$$\sigma_\gamma = 4.1 \times 10^6 \left(\frac{A+1}{A}\right)^2 \sum_j \frac{g\Gamma^0_{nj}\Gamma_{\gamma j}}{E^2_{0j}} \tag{1}$$

Therefore:

$$\frac{\sigma_\gamma^{\mathrm{isomer}}}{\sigma_\gamma^{\mathrm{ground}}} = \frac{\sum_j \frac{g\Gamma^0_{nj}\Gamma_{\gamma j}}{E^2_{0j}}}{\sum_i \frac{g\Gamma^0_{ni}\Gamma_{\gamma i}}{E^2_{0i}}} \tag{2}$$

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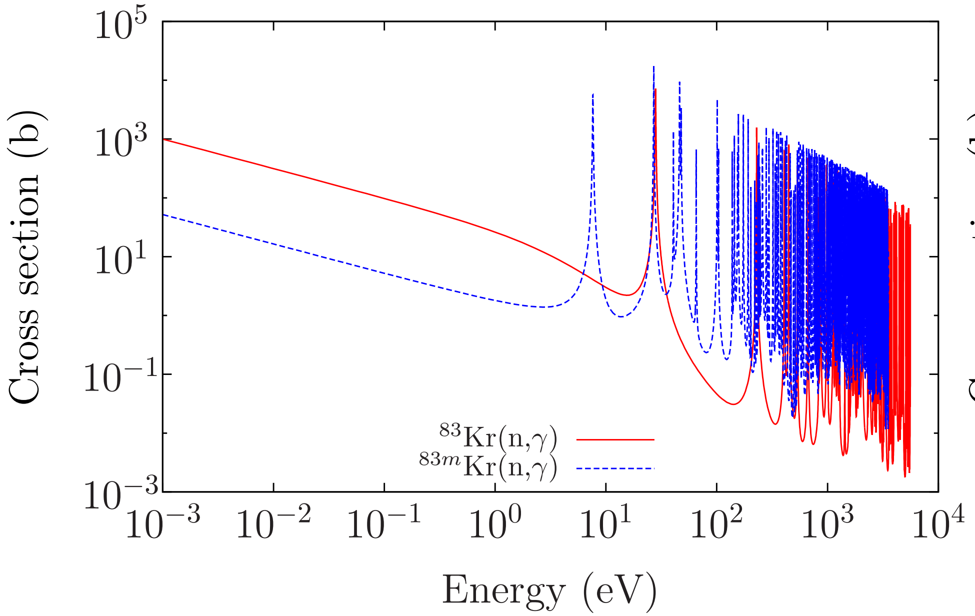
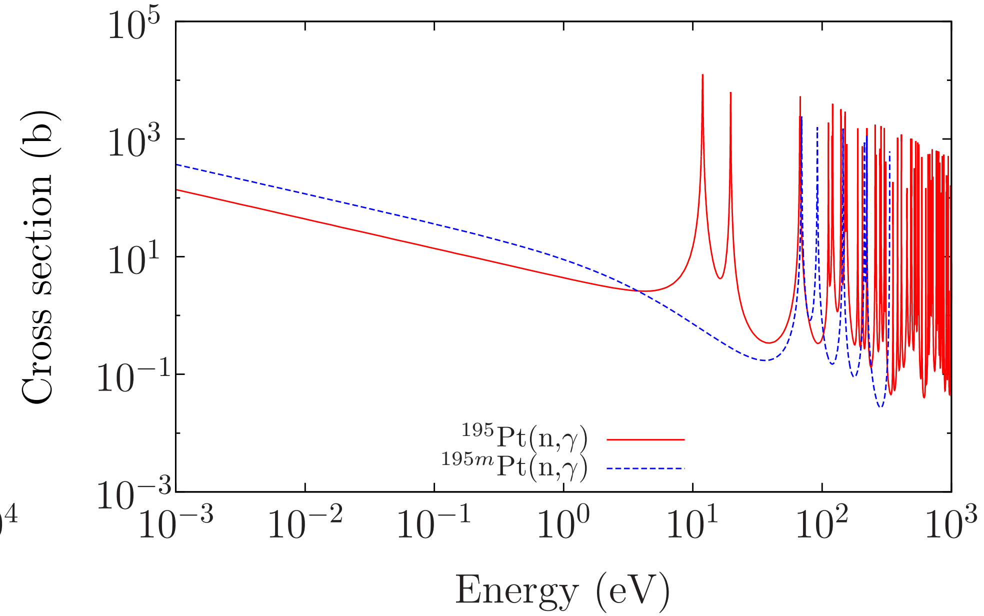
$\sigma_\gamma^{\text{ground}} \Longrightarrow$ known from measurements (or systematics)

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





What about ^{135m}Xe ?

- $t_{1/2}$ =15.3 m (9.10 h for ^{135g}Xe)
- no data in EXFOR, neither in JENDL, JEFF or ENDF/B-VII,
- ^{235}U cumulative thermal fission yield: 1.10 $\pm$ 0.01 % (6.54 $\pm$ 0.04 % for ^{135g}Xe)

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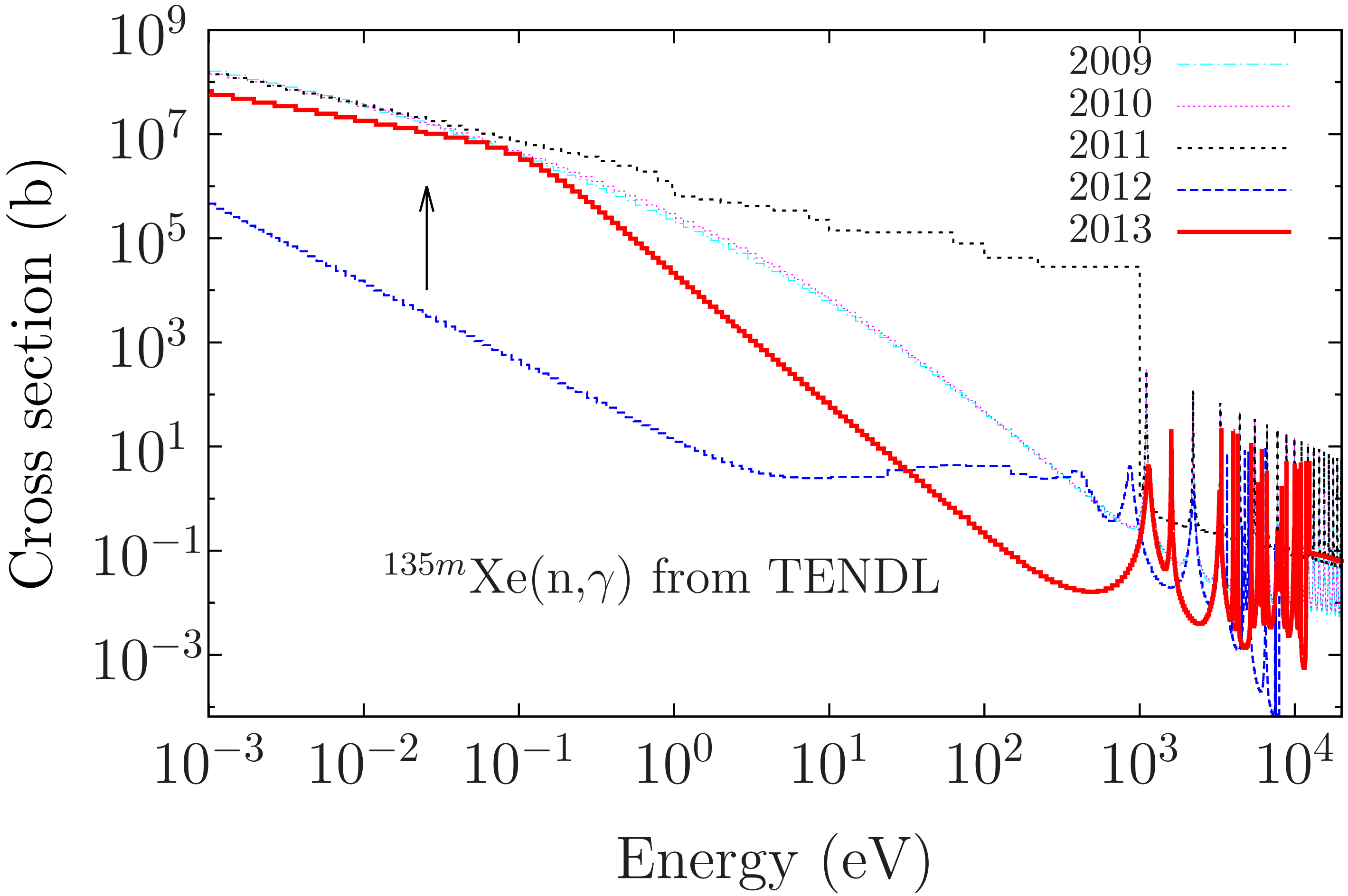
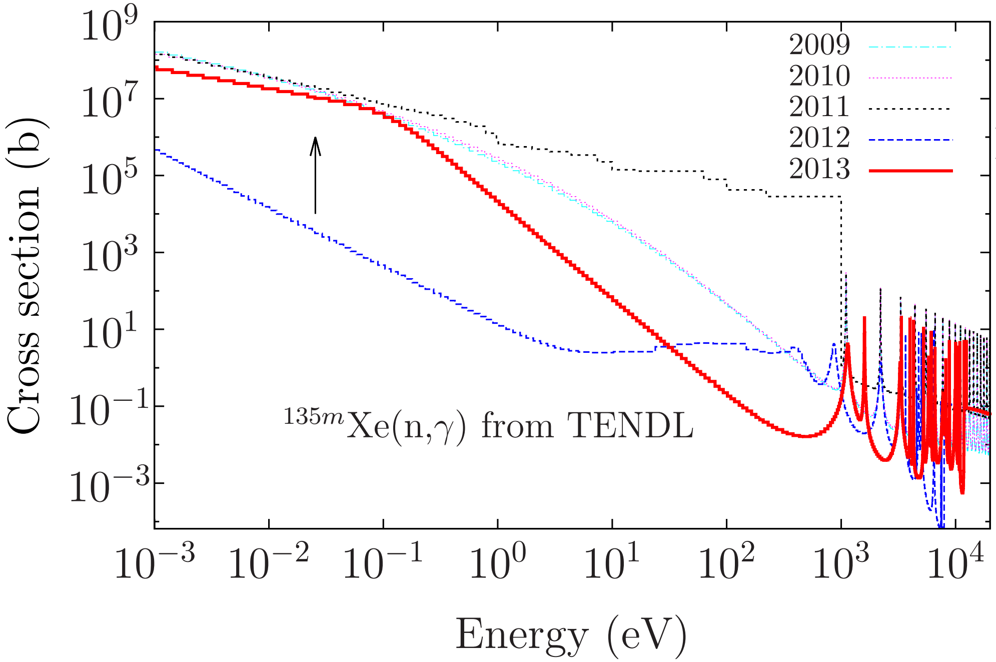
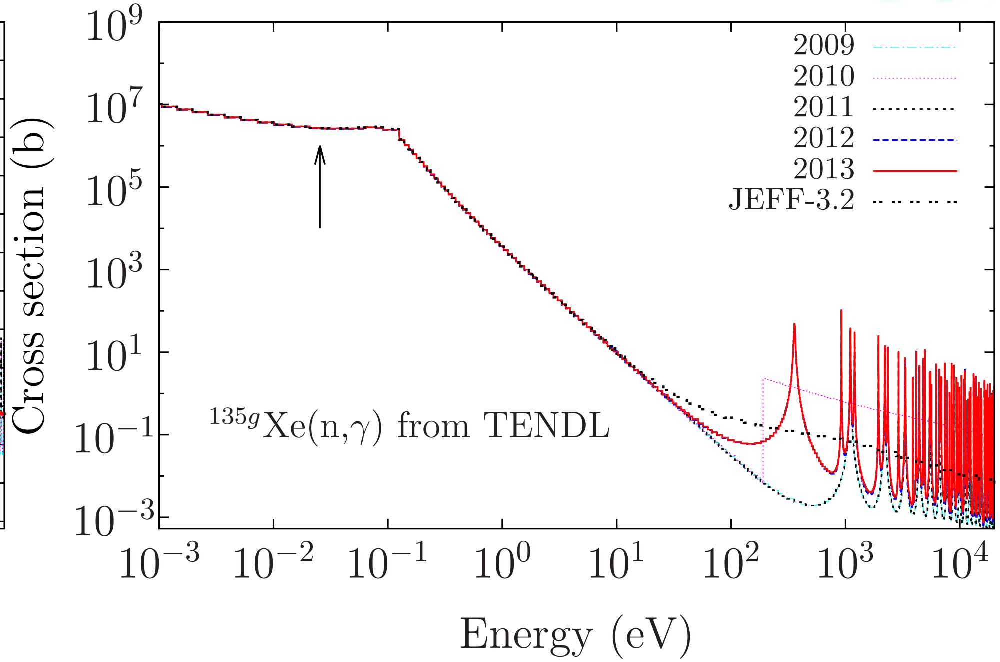


^{135m}Xe compared to ^{135g}Xe in TENDL





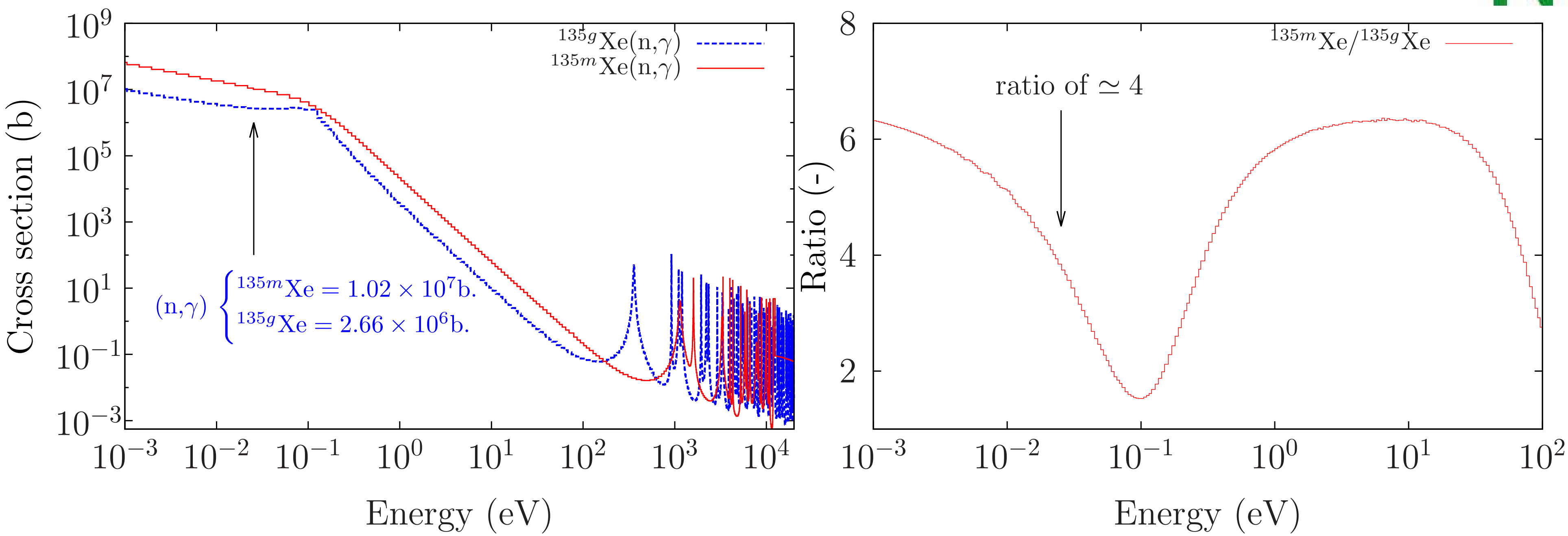
^{135m}Xe

- ☞ Thermal (n,γ) xs not known,
- ☞ No information in the RRR and above,

^{135g}Xe

- ☞ Thermal (n,γ) xs well known (5 %),
- ☞ No information in the RRR and above,

^{135m}Xe best estimate

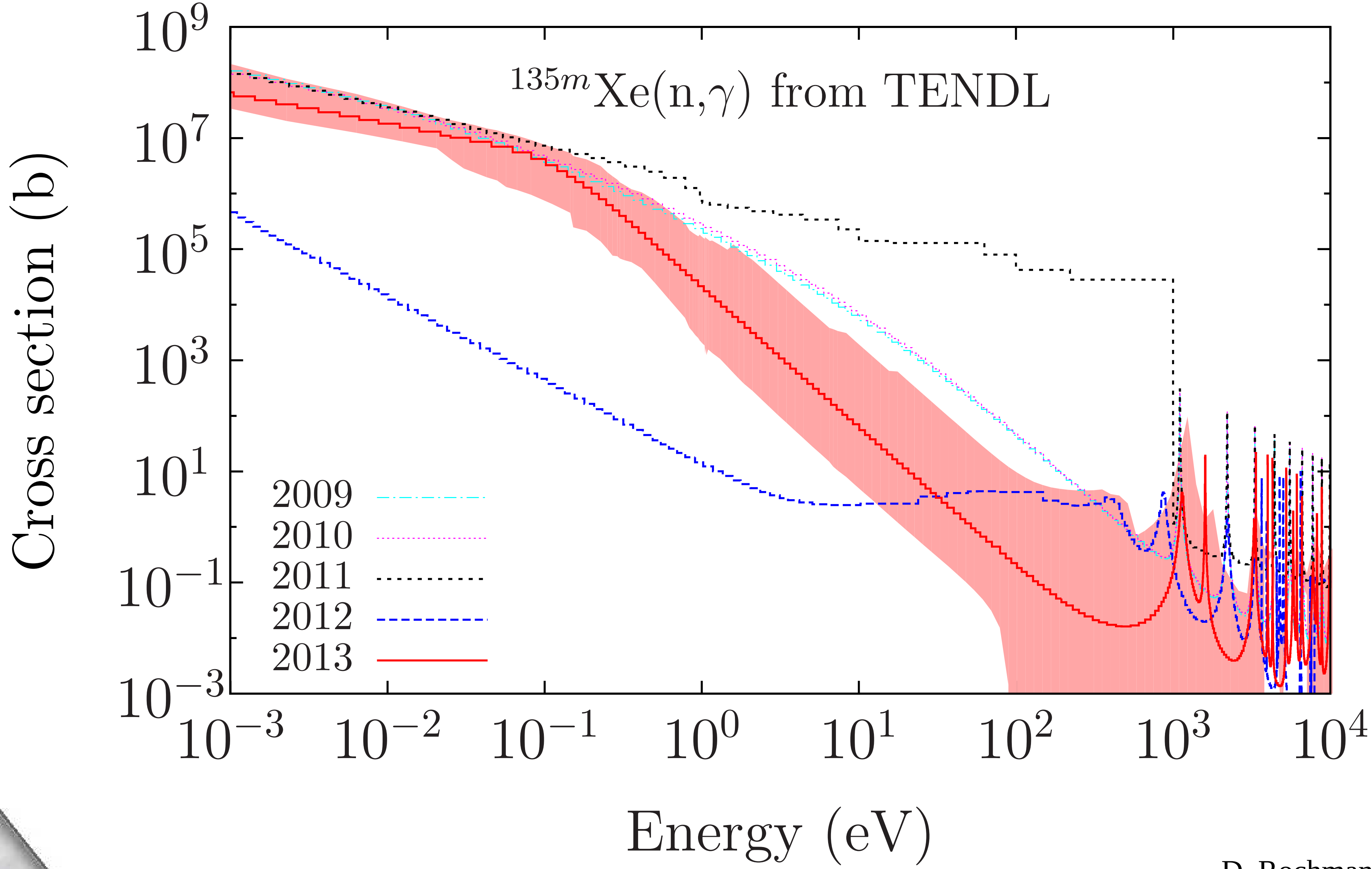


Some approximations are done:

- $E_0 >> \Gamma$ is not correct (can change xs by a factor 2),
- How well known are the OMP parameters for ^{135}Xe (can change xs by a factor ??) ?

^{135m}Xe uncertainties

For uncertainties, a detailed study is necessary (not performed yet).



Conclusion

☞ Combination of TALYS + CALENDF-2010:
consistent parameters from 0 to 20(0) MeV,

☞ Applied to 2400 isotopes for TENDL-2012 to TENDL-2014,

☞ Sensible improvements compared to other libraries for short-lived and low abundance isotopes,

☞ For ^{135m}Xe, additional studies would be necessary to gain more confidence in the recommended values.