From nuclear structure to neutron-induced cross-section evaluations for reactor applications

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Nuclear model codes for fission product evaluation

From optical model parameters to total neutron cross section

From photon strength function to neutron capture cross section

Dissemination of the results

Conclusions

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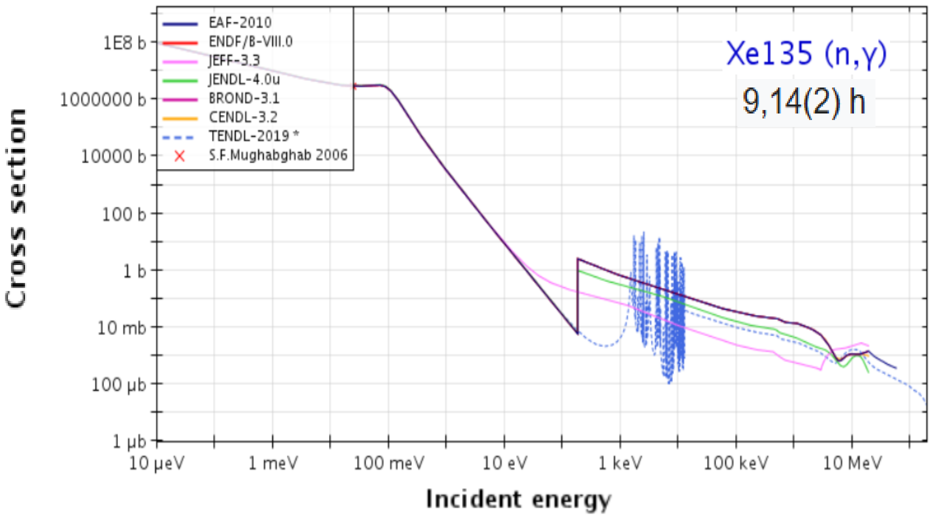
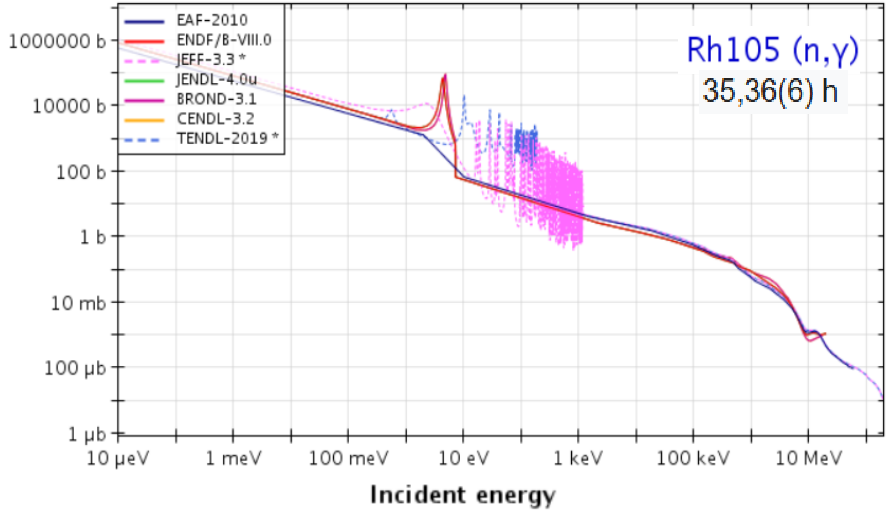
	PWR	SFR
1	**Xe-135**	Ru-101
2	Rh-103	Rh103
3	Nd-143	Tc-99
4	Xe-134	Cs-133
5	Cs-133	**Rh-105**
6	Sm-149	Pd-107
7	Tc-99	Cs-135
8	Sm-152	Sm-149
9	Pm-147	Mo-97
10	Sm-151	Nd-145
11	Eu-153	Ru-102
12	Nd-145	Nd-143
13	Eu-155	Sm-151
14	Eu-154	Pm-147
15	Ag-109	Mo-95
16		Xe-131
17		Pu-104
18		Ag-109
19		Mo-98
20		Mo-100
21		Pd-106
22		Pr-141
23		Sm-147
24		Eu-153
25		Pd-108
26		Xe-132
27		Sm-152

Context

→ Fission products that contribute to 80% of the poisoning effect in PWR and SFR

Among them, some short-lived nuclei are of interest for nuclear reactor applications but their neutron capture cross-section is poorly known





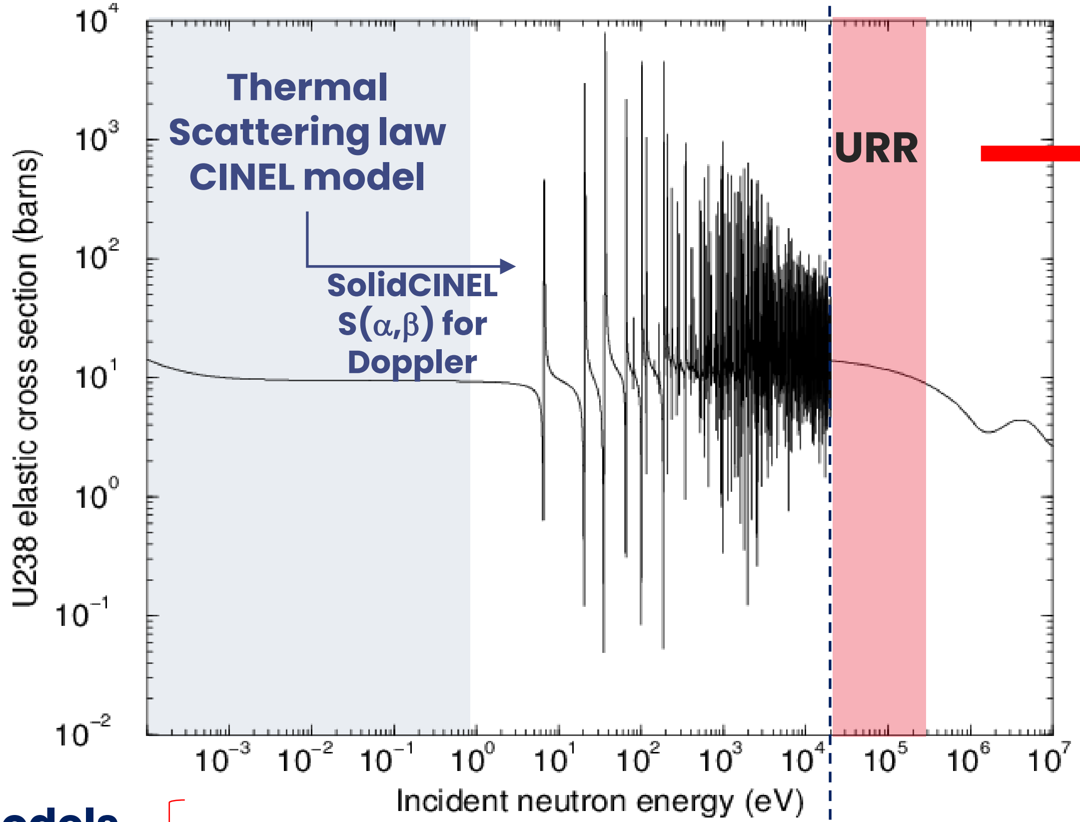
Microscopic models, which directly model the nucleus properties from interacting nucleons, provide useful observables that can be used for reinforcing the systematic and predictive power of the phenomenological models.

This topic is widely studied in the literature, the objective here is to revisit the nuclear data evaluation strategy thanks to “on the fly” HFB calculations.

Neutron cross section models

RRR

« Continuum »



Average parameters calculated with the urr option of TALYS

① **Optical model parameters from HFB results**

② **Photon strenght functions from QFAM results**

Standard models implemented in CONRAD

R-Matrix formalism

MLBW, RM, LRF7, Brune, (n,γf)
$P_f(E)$, R^∞ for direct capture

Optical model (HFBr+ECIS, CCCP)

Statistical model (panacea+TALYS, CONRAD)

ESTIMA method

SPRT method

Nuclear model code suite

Codes	Optical Model Parameters	Deformation parameters	Level density	Photon strength function	Average radiation width	Fission barrier parameters	Resonance parameters
TALYS A. Koning et al.	From OMP RIPL-3 library	From FRDM	From Gilbert-Cameron composite formula	From GDR models	From HF γ-decay formula	From Empirical Hill–Wheeler–type fission barriers	From URR option
HFBr code suite A. Pastore	From 160 Skyrme forces + 4 Gogny forces	From FRDM					
Panacea M. Frosini, P. Tamagno et al.	From 160 Skyrme forces + 4 Gogny forces Nearly ready …	Natural outcome of the code		From QFAM with D1S and D1M forces			
HFBaxial L. Robledo (in-house version of R. Bernard)		Natural outcome of the code				From TDGCM (not presented in this talk)	
FIFRELIN O. Litaize					From Monte-Carlo de-excitation		
CONRAD P. Tamagno C. de Saint Jean		From FRDM					From R-Matrix formalism

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Models routinely used for cross-section evaluations

Nuclear model code suite

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Models used in this work

Nuclear model codes for fission product evaluation

From optical model parameters to total neutron cross sections

From photon strength function to neutron capture cross section

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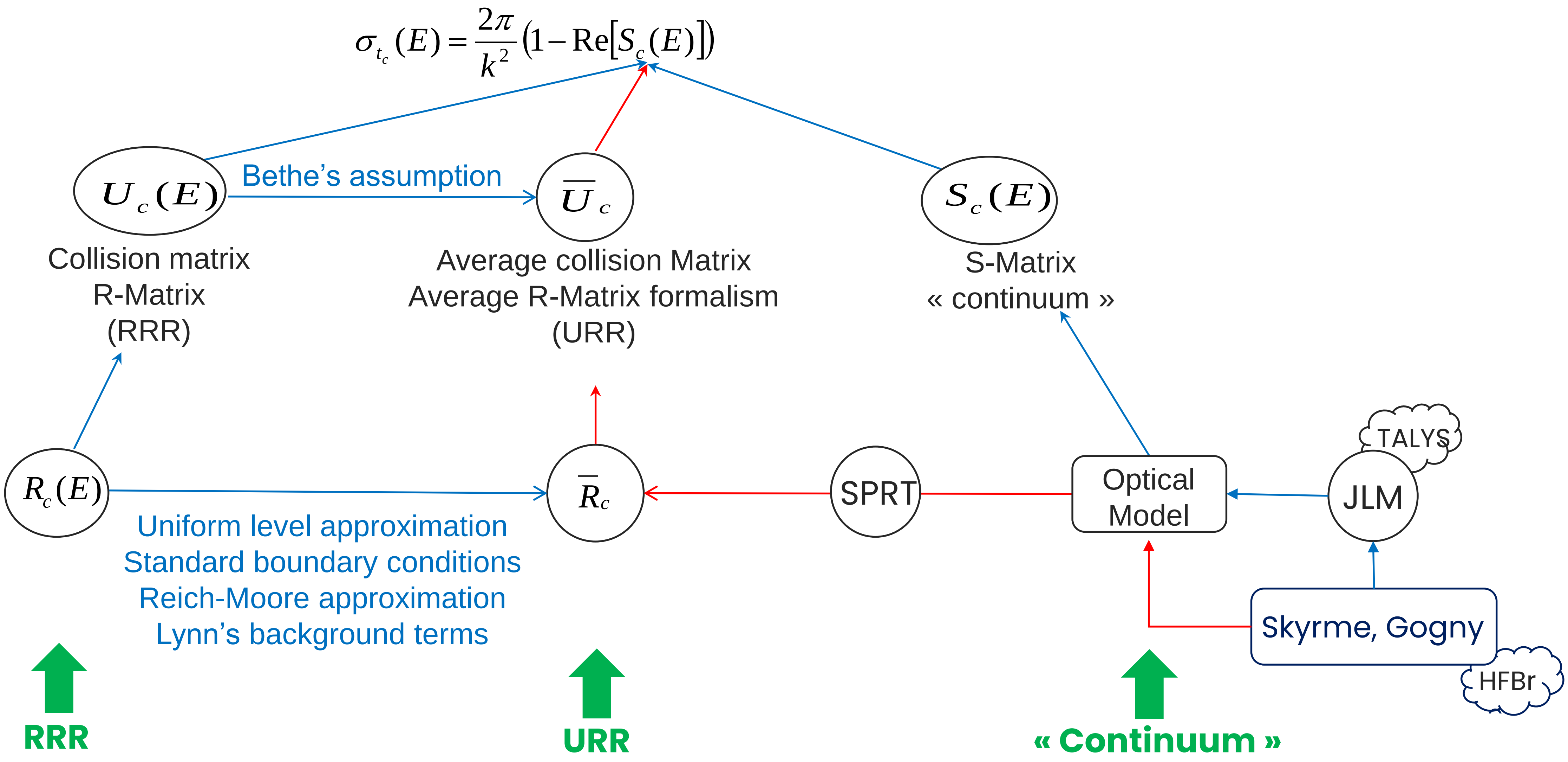
Total cross section formalism



Optical model potential

« Standard » formulation of the optical model potential with a Wood Saxon form factor

$$U(r,E) = [V_v(E) + iW_v(E)] f(r,R,a) - 4a\, [V_s(E) + iW_s(E)] \frac{df(r,R,a)}{dr} - 4\, [V_{so}(E) + iW_{so}(E)] \left(\frac{h}{m_\pi c}\right)^2 \frac{1}{r} \frac{df(r,R,a)}{dr} l.\sigma$$

Volume contribution Surface contribution spin-orbite contribution

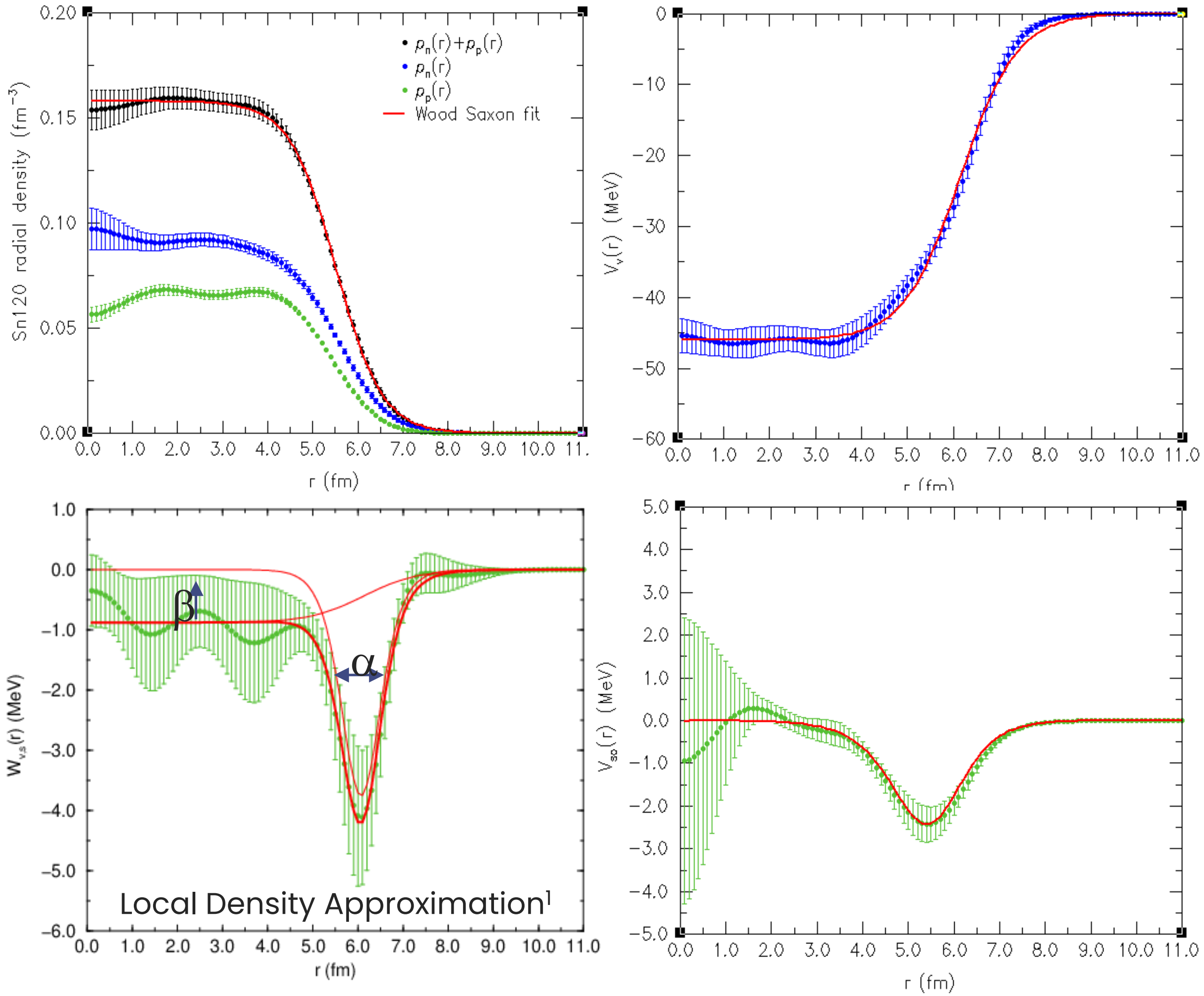
$$f(r,R,a) = \frac{1}{1 + \exp[(r-R)/a]}$$

Optical Model Parameters deduced from the radial densities, central potential, imaginary parts and spin-orbit contributions calculated with HFBr

*E. Rich et al., NSE 162, 76 (2009)

HFBr optical model

HFBr solves HFB equations in spherical symmetry using Gogny and Skyrme forces



\+ dispersive term[2]

$$\Delta V(E) = \frac{2}{\pi}(E - E_F) \int_{-\infty}^{E_F} \frac{W(E') - W(E)}{(E' - E_F)^2 - (E - E_F)^2} \, dE'.$$

Example of HFBr results at E = 1 keV from a selection of 130 Skyrme forces

Force selection based on the neutron strength function S_0

Limit of LDA:

- Diffuseness of the imaginary part of the surface contribution has to be increased by a factor 2
- Strength of the imaginary part of the volume contribution has to be decreased by at least a factor of 0.1

[1] J.L. Morana, X. Vinas, J. Phys. G. Nucl. Part. Phys. 50 (2023) 045108
[2] J.M. Quesada et al., Computer Physics Communications 153 (2003) 97–105

Energy dependence of the HFBr optical model

Distant level parameter correction

Partial wave decomposition of the average collision matrix to improve the energy depence of the optical model via a shift correction R^{∞}_{shift}

Phase shift that depends of the channel radius a_c

Neutron strenght function

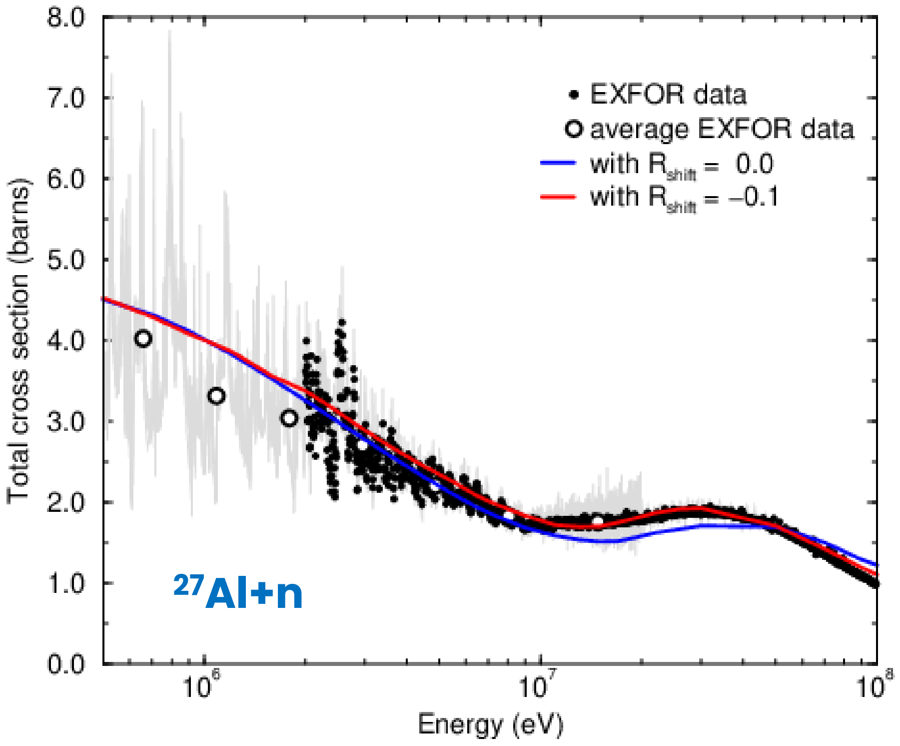
$$\overline{U}_c = e^{2i\phi_c}\,\frac{1 + iP_L\overline{R}^{\infty}_c - \dfrac{\pi S_c\sqrt{E}P_L}{2P_0} - \pi P_L s_c^{loc}}{1 - iP_L\overline{R}^{\infty}_c + \dfrac{\pi S_c\sqrt{E}P_L}{2P_0} + \pi P_L s_c^{loc}}$$

Penetration factor that depends of the channel radius a_c

Distant level parameter (scattering)

$R^{\infty}_c + R^{\infty}_{shift}$

Direct reaction contribution (absorption)



⇒ mainly used for light elements

Energy dependence of the HFBr optical model

Time-delay correction

Energy-dependent discrepancies observed in neutron cross sections calculated using static HFB+LDA optical model can be also corrected by introducing a finite time shift

$$T(E_{\text{eff}}) = T(E) + \Delta t$$

The effective energy is defined as

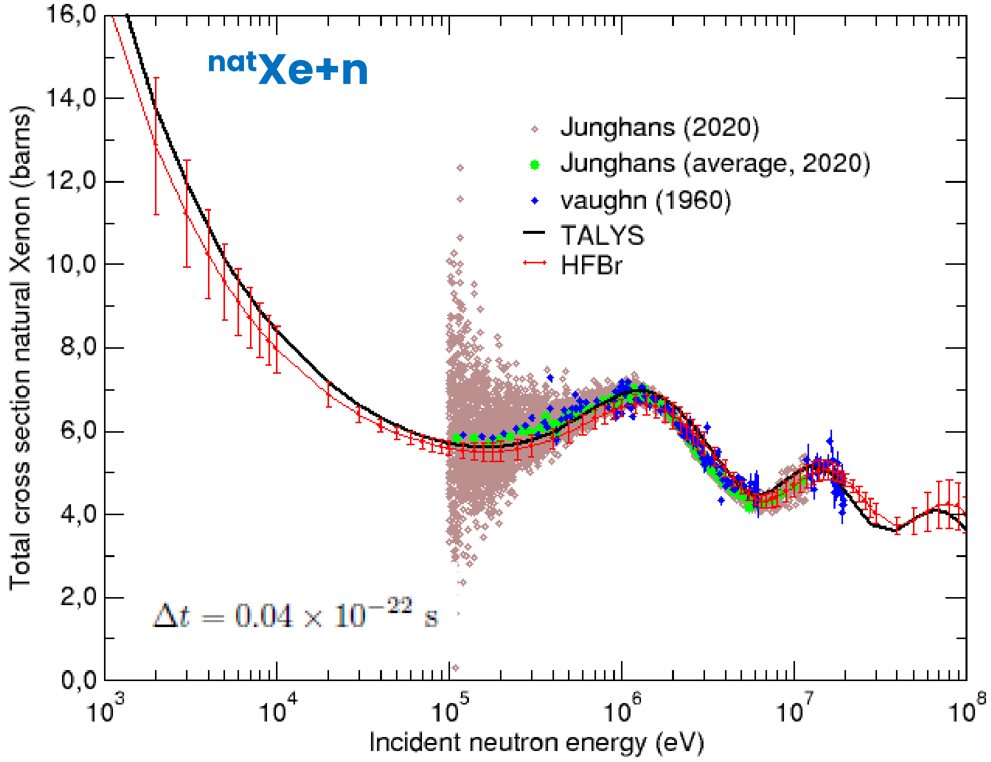
$$E_{\text{eff}} = m_n c^2 \left[\frac{1}{\sqrt{1 - \frac{1}{\left(\frac{1}{\beta}+\tau\right)^2}}} - 1 \right], \quad \beta = \sqrt{1 - \frac{1}{\left(1 + \frac{E}{m_n c^2}\right)^2}}, \quad \tau = \frac{c\,\Delta t}{R}$$

The momentum shift induced by the time shift is

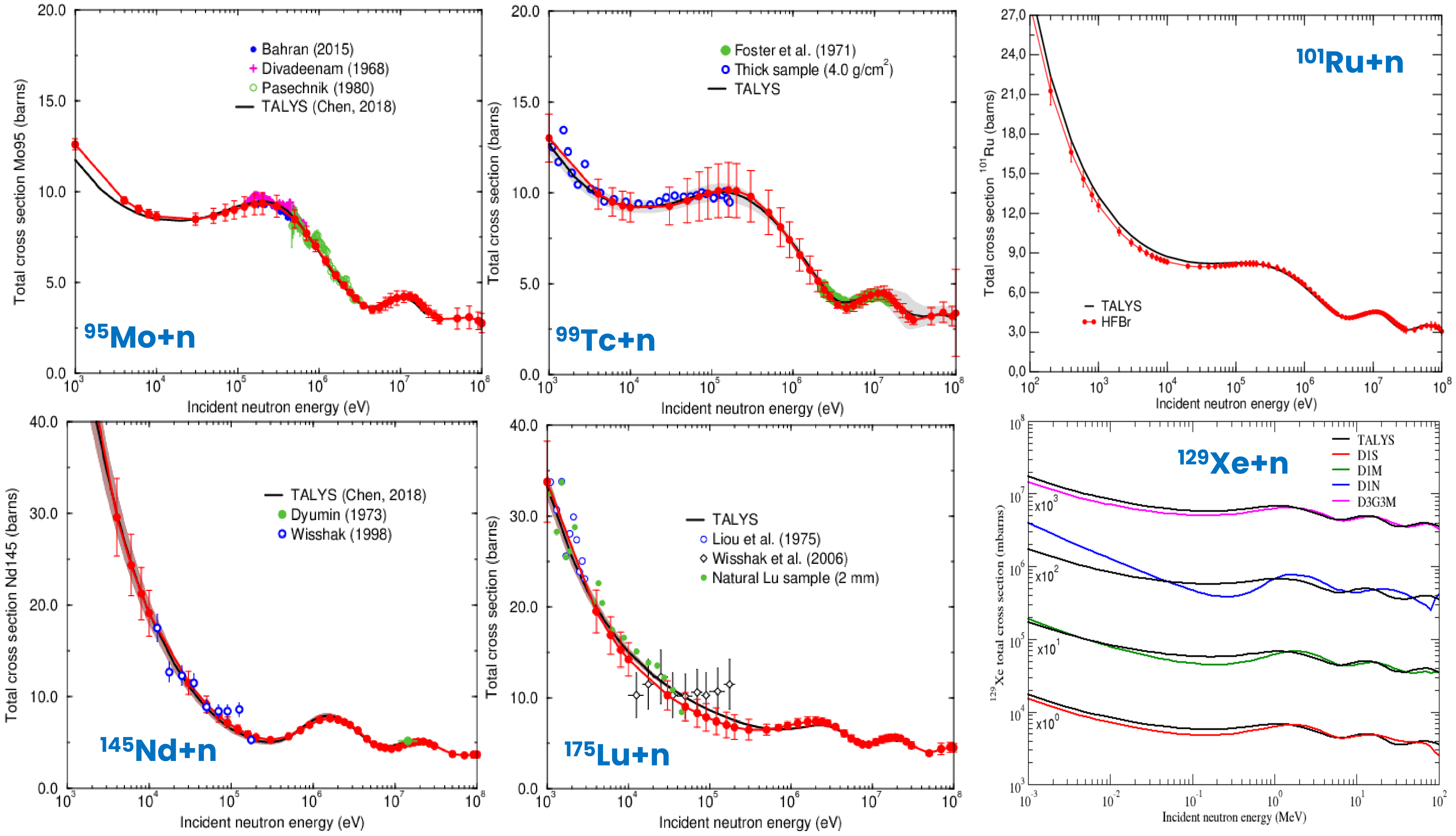
$$\Delta k(E) = k(E_{\text{eff}}) - k(E)$$

For the volume contribution, introducing a positive time shift increases the effective dwell time of the neutron inside the nucleus

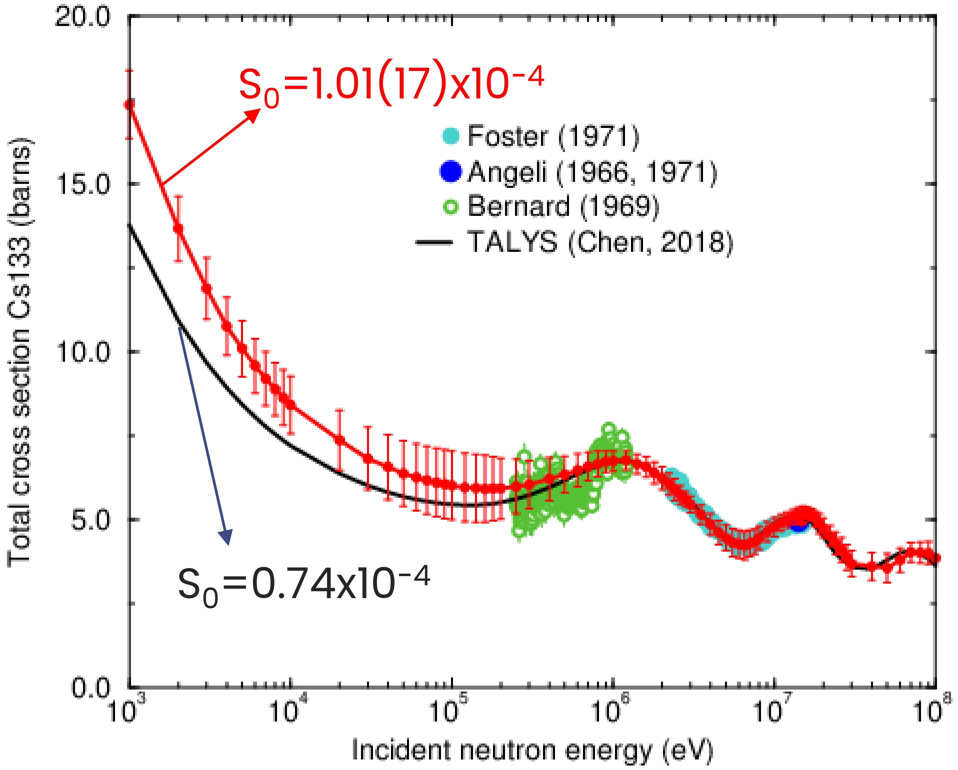
For the surface contribution, introducing a negative time shift shortens the effective propagation contribution



Total cross section using Skyrme and Gogny interactions

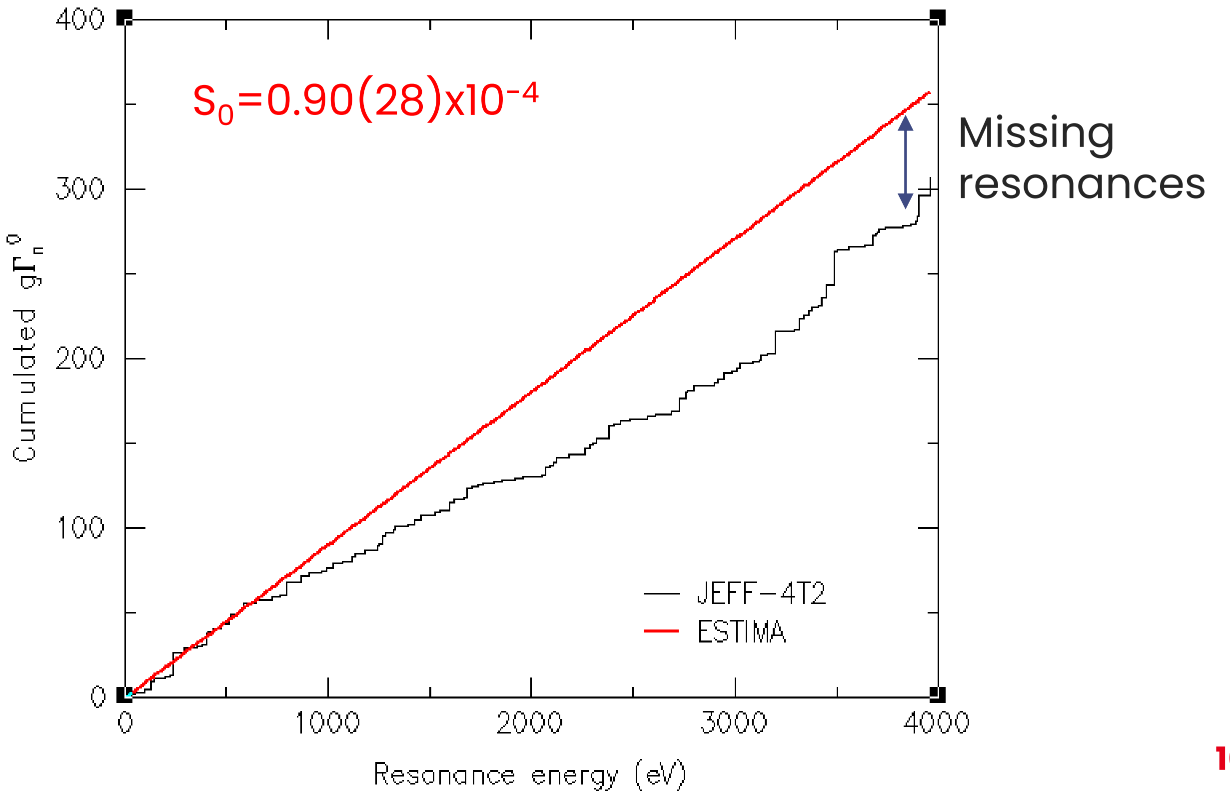


Focus on $^{133}Cs+n$



Not possible to reproduce the TALYS calculations (Chen, 2018) based on a neutron strenght function of S_0=0.74x10^{-4} (Atlas of Neutron Resonances)

Statistical analysis of the RRR with the **ESTIMA method** seems to confirm the underestimation of S_0 in the Atlas of Neutron Resonances



⇒ HFBr results can help identify issues in the resonance range

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Capture cross section formalism

Below the inelastic threshold:

$$\sigma_{\gamma_{lJ}}(E) = \frac{\pi}{k^2}\frac{T_{lJ}(E)T_{\gamma_{lJ}}(E)}{T_{lJ}(E)+T_{\gamma_{lJ}}(E)}W_{n\gamma}(E)$$

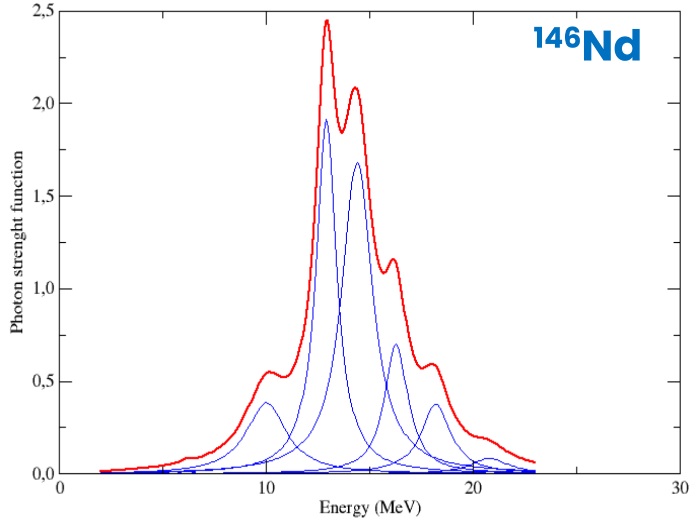
Neutron transmission coefficients $T_{lJ}(E)$ provided by HFBr+ECIS calculations

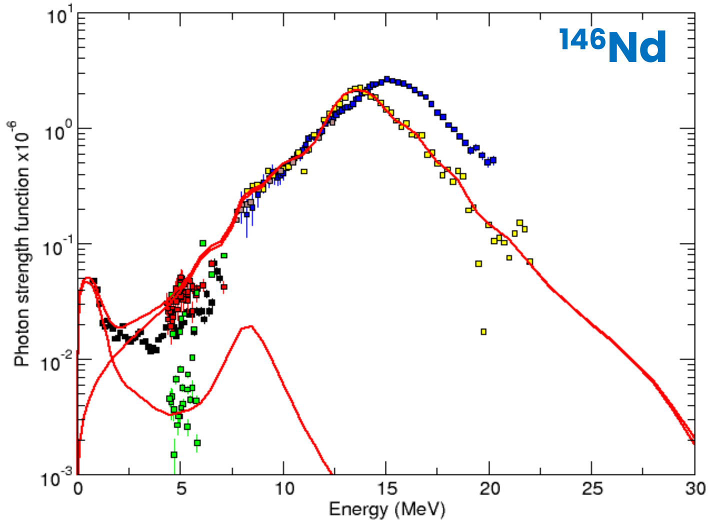
γ-ray transmission coefficients $T_{\gamma lJ}(E)$ depend on photon strenght function (PSF). For electric dipole transistion E1, the relationship between γ-ray transmission coefficient and PSF is given by:

$$T_{E1}(E\gamma)=2\pi\, f_{E1}(E\gamma)E_{\gamma}^{3}$$

QRPA photon strenght function $f_{E1}(E\gamma)$ and $f_{M1}(E\gamma)$ are calculated with the panacea code using effective Gogny-type interaction D1M and D1S and the computationnaly efficient Finite Amplitude Method (FAM)

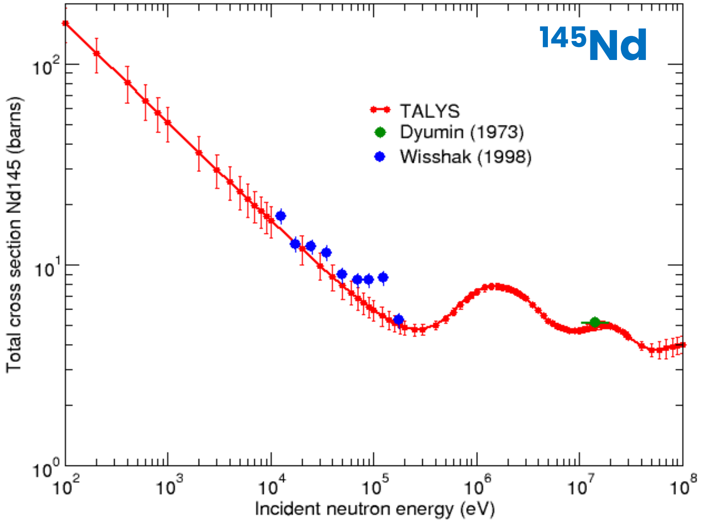
QRPA-FAM photon strenght function

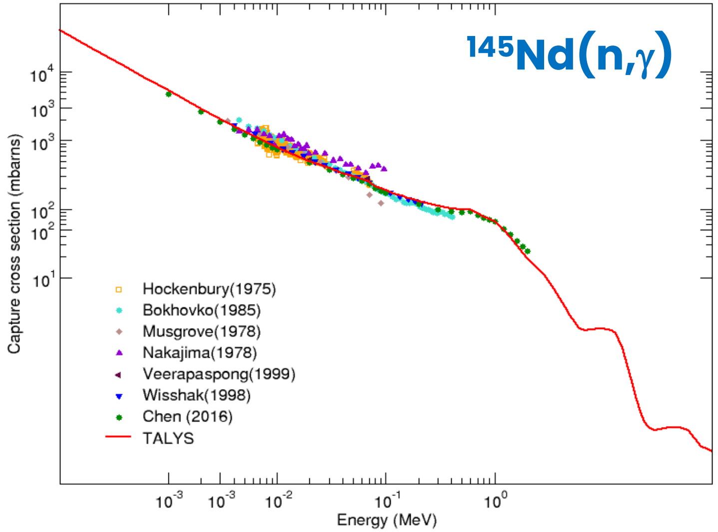




Local Lorentzian decomposition of the PSF

Local deviation from the experimental capture cross section can be solved by a Lorentzian décomposition of the QFAM photon strenght functions





QRPA-FAM photon strenght function

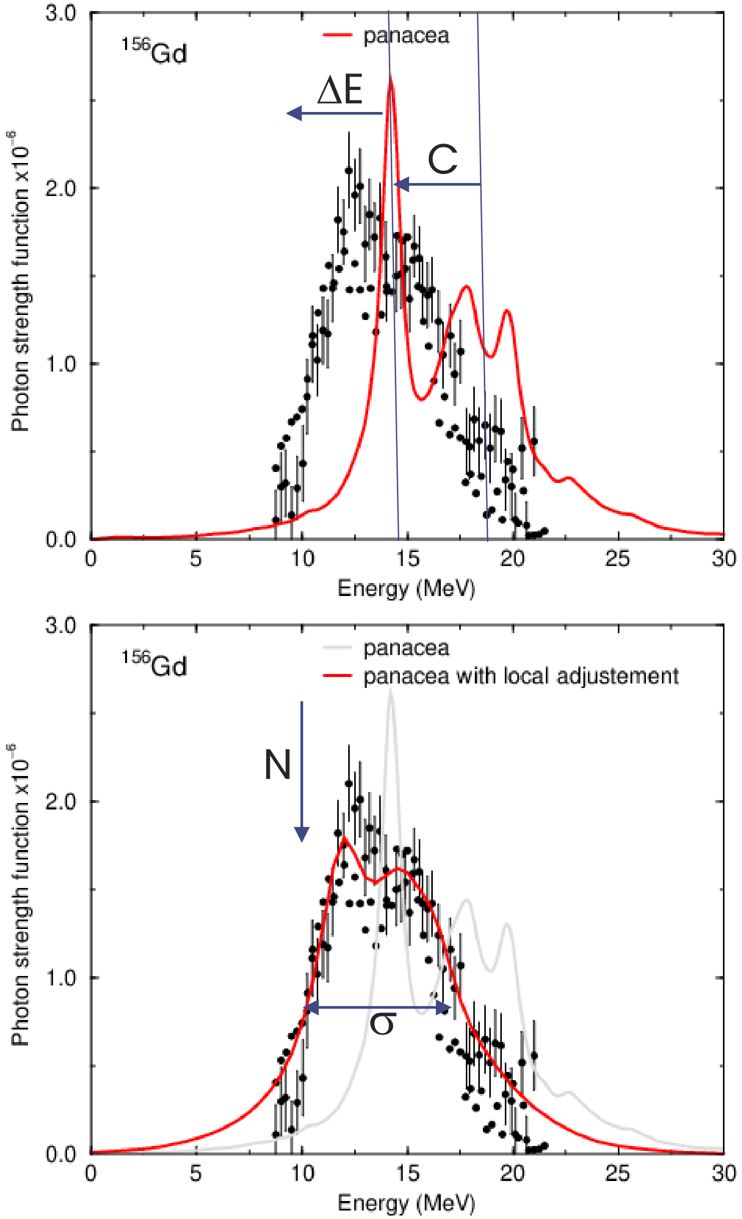
Global model calibration to correct for systematic biases inherent to QRPA results

Experimental data base

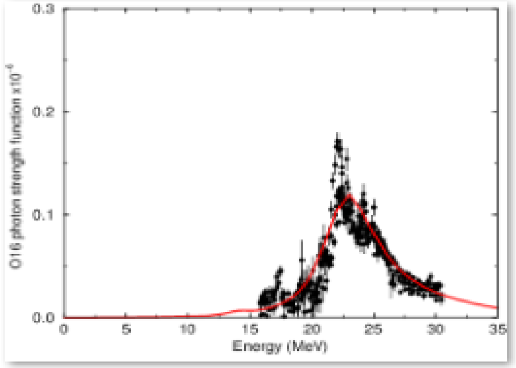
- https://nds.iaea.org/CRP-photonuclear/
- Ajustment performed on 142 photon strenght functions
- Use photon strenght function at S_n as constraint

4 free mass dependent parameters

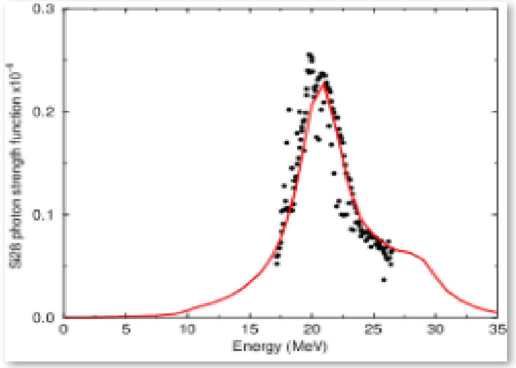
- ΔE: energy shift
- N: normalisation
- C: compression factor
- σ: lorentzian broadening width



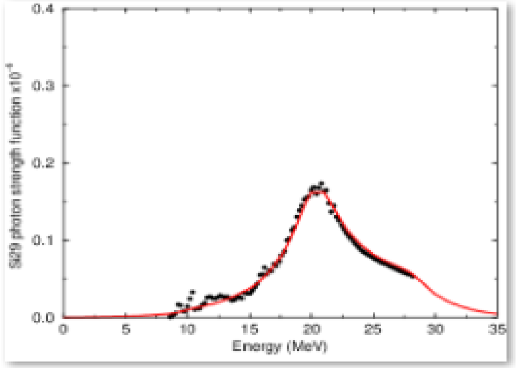
PSF with a global model calibration



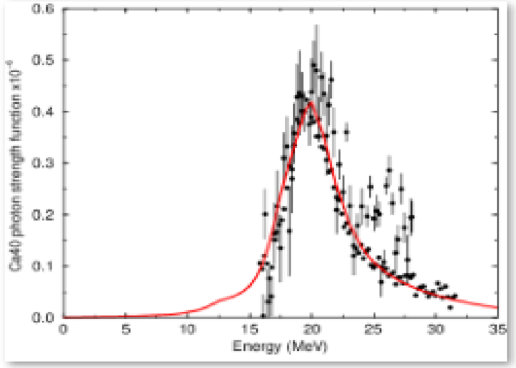
o16



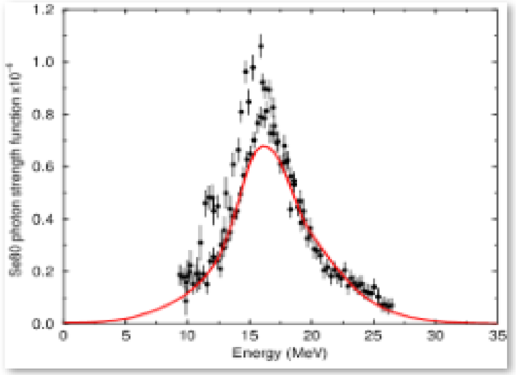
si28



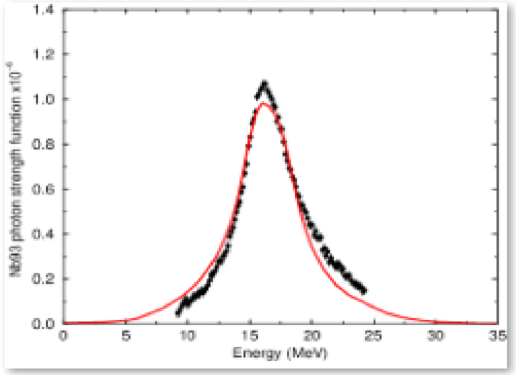
si29



ca40



se82



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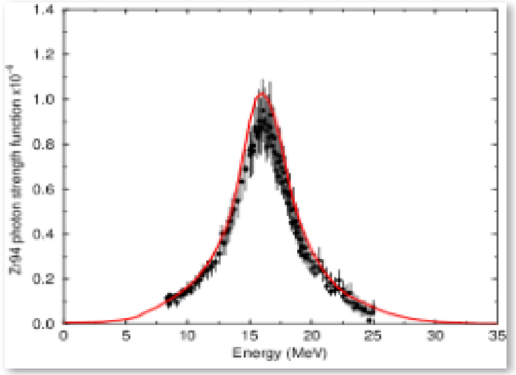
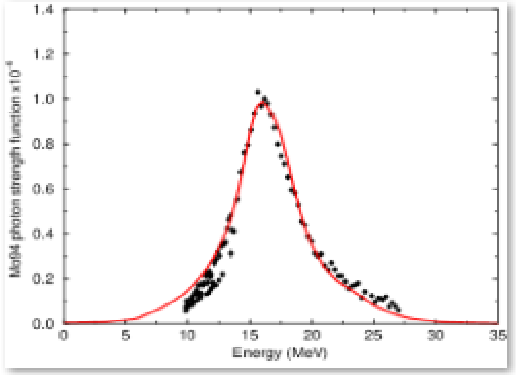


zr94



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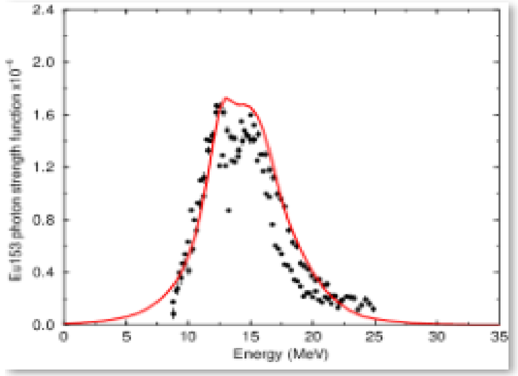
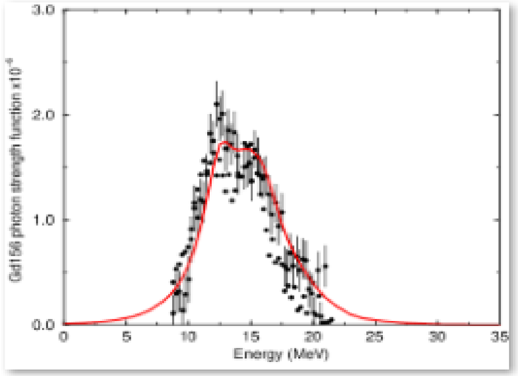
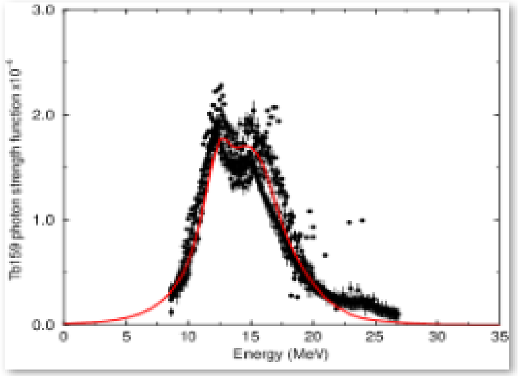


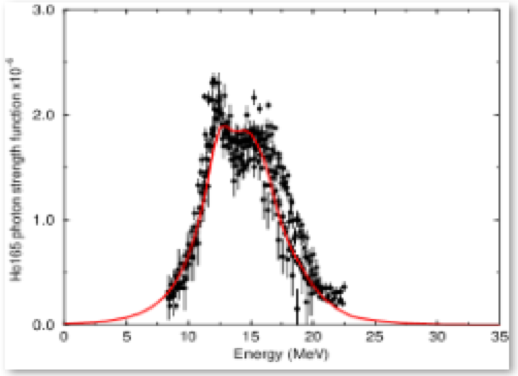
eu153



gd156

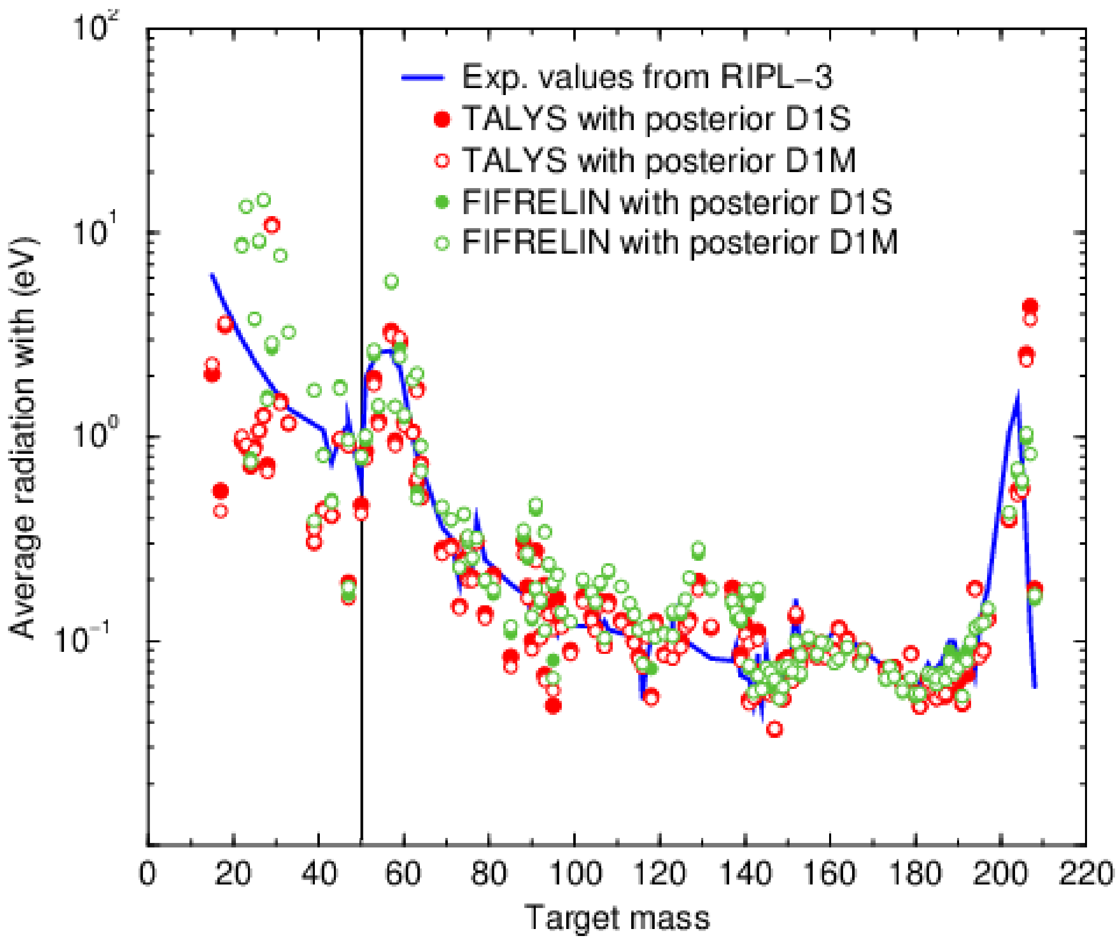


tb159



ho165

Average radiation width



TALYS and FIFRELIN results obtained with a global parametrisation of ΔE, N, C and σ as a function of the compound nucleus mass

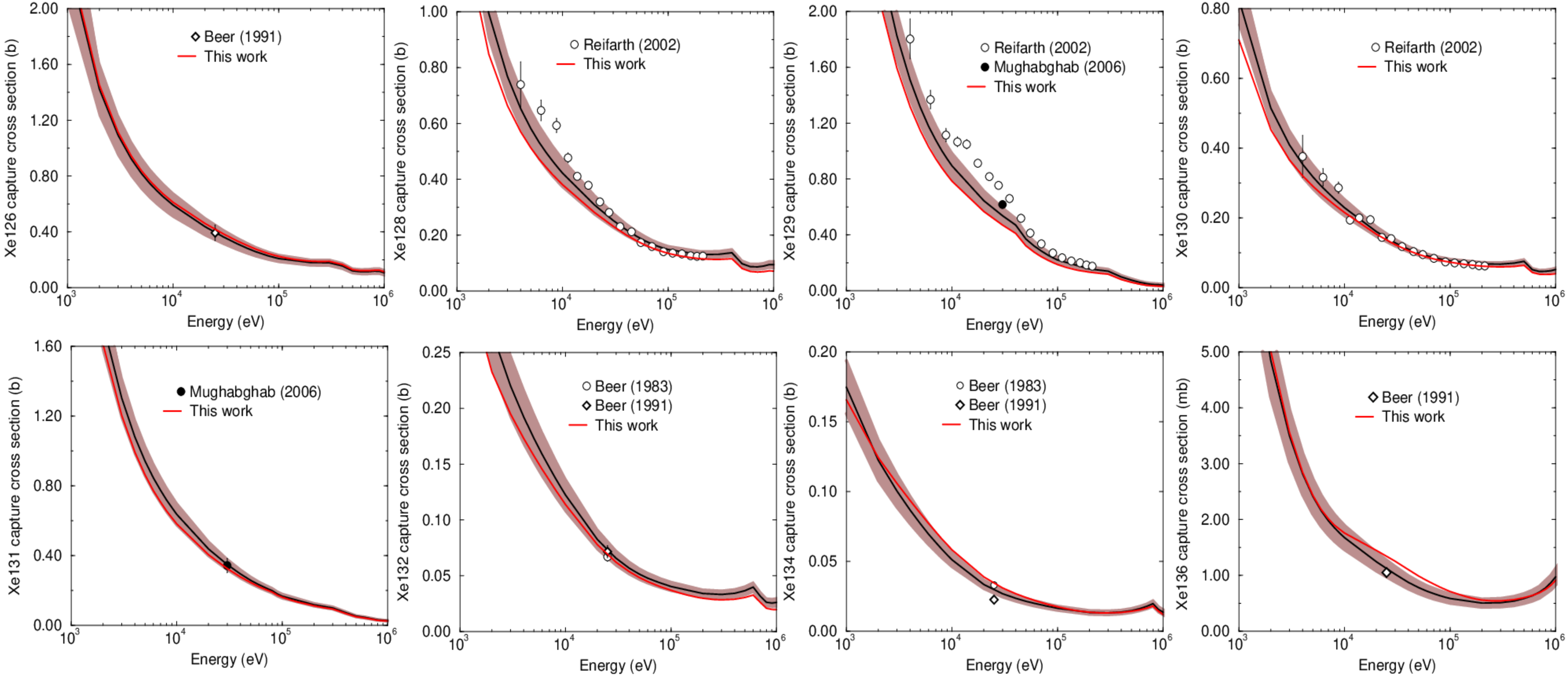
☐ **Systematic A<50**

- Average radiation width not a relevant osbervable for light elements

☑ **Systematic A> 50**

- Encouraging results but local deviation between the experimental and theoretical average radiation widths will induce sizeable effects on the capture cross section
- Differences between TALYS and FIFRELIN due to the level density

Xenon capture cross section



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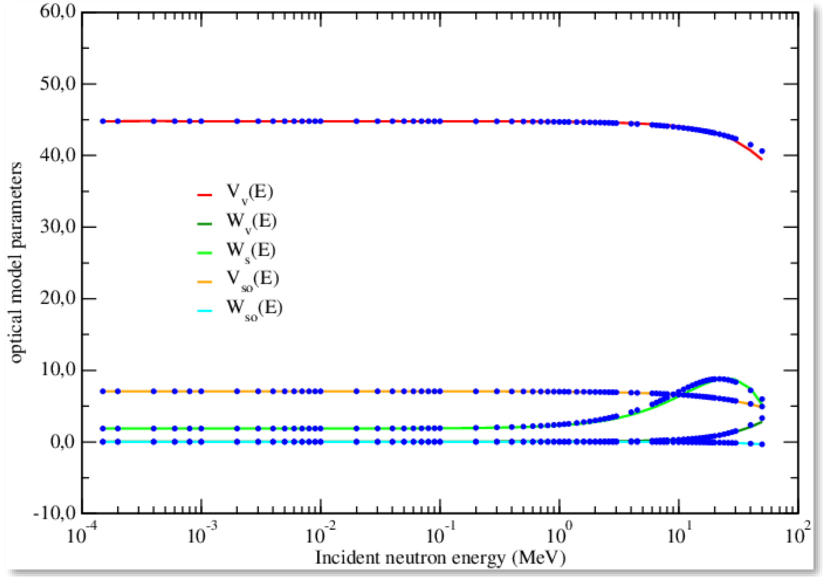
HFBr optical model parameters in RIPL format

OMP from HFBr



RIPL format

```
   1
 200.000
   1.24550   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
   0.63522   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
   1.00000   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0  4.88500+1   .00600+0   .00000+0   .00000+0
           -1.59000+1   .00000+0   .00000+0   .00000+0  1.00000+0   .00000+0
   1
 200.000
   1.24550   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
   0.63522   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
  20.00000   .00000+0  1.25000+2   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0  2.00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0  3.85000+2   .00000+0   .00000+0  1.00000+0   .00000+0
   0
   1
 200.000
   1.23590   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
   0.56869   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
  30.00000  2.35000-2   .00000+0   .00000+0   .00000+0  1.90000+1   .00000+0
           -2.35000+1   .00000+0   .00000+0   .00000+0   .00000+0  2.00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0  1.00000+0   .00000+0
   1
 200.000
   1.15798   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
   0.50558   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
    .00000   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0  7.35000+0   .00000+0  4.00000-3   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0  1.00000+0   .00000+0
   1
 200.000
   1.15798   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
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   0.50558   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
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  -3.00000   .00000+0  1.60000+2   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0  2.00000+0
             .00000+0   .00000+0   .00000+0   .00000+0   .00000+0   .00000+0
             .00000+0   .00000+0   .00000+0   .00000+0  1.00000+0   .00000+0
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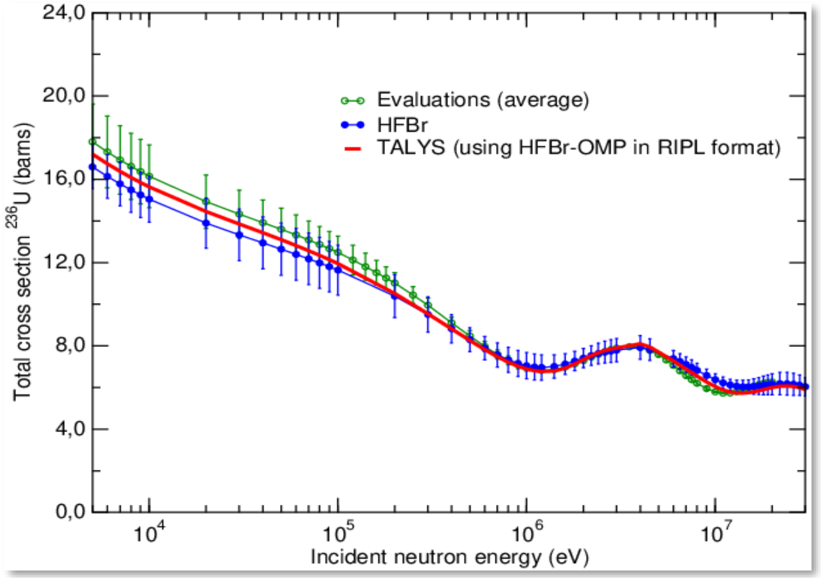
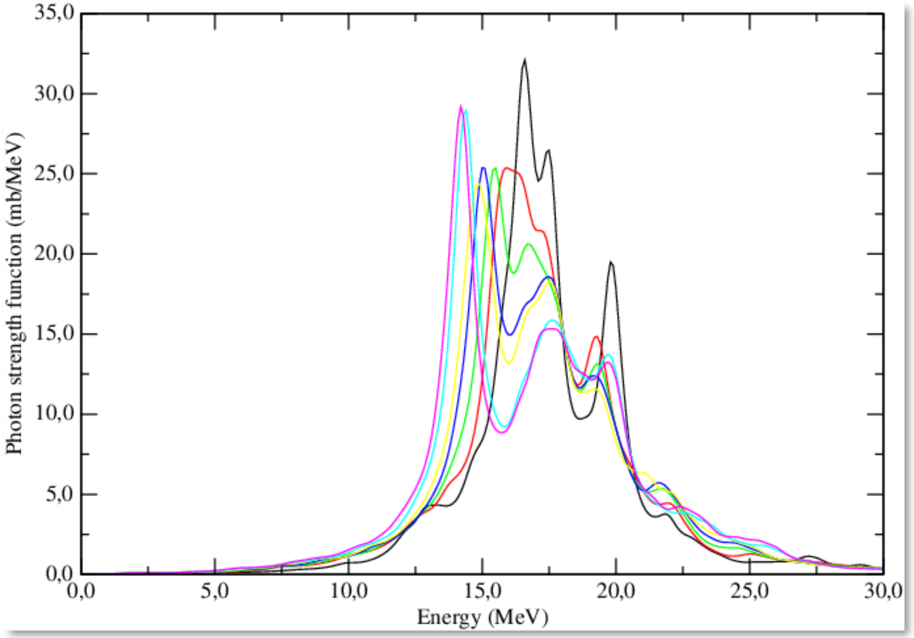
The parameters of the HFBr optical model can be stored in RIPL format for later use via OMGET in standard TALYS calculations (see red solid line)



QFAM photon strenght function in FIFRELIN or TALYS-like format

Raw QRPA-FAM PSF



FIFRELIN of TALYS-like format

Z= 62 A= 144

U[MeV]	fE1[mb/MeV]	fM1[mb/MeV]
0.100	2.867E-03	1.519E-04
0.200	5.303E-03	3.047E-04
0.300	7.217E-03	4.593E-04
0.400	8.801E-03	6.165E-04
0.500	1.027E-02	7.774E-04
0.600	1.221E-02	9.429E-04
0.700	1.375E-02	1.114E-03
0.800	1.529E-02	1.293E-03
0.900	1.687E-02	1.479E-03
1.000	1.904E-02	1.676E-03
1.100	2.064E-02	1.884E-03
1.200	2.227E-02	2.106E-03
1.300	2.395E-02	2.344E-03
1.400	2.567E-02	2.600E-03
1.500	2.743E-02	2.879E-03
1.600	2.921E-02	3.183E-03
1.700	3.156E-02	3.517E-03
1.800	3.334E-02	3.888E-03
1.900	3.515E-02	4.301E-03
2.000	3.700E-02	4.764E-03
2.100	3.887E-02	5.289E-03
2.200	4.126E-02	5.888E-03
2.300	4.314E-02	6.577E-03
2.400	4.505E-02	7.377E-03
2.500	4.699E-02	8.314E-03
2.600	4.896E-02	9.425E-03
2.700	5.119E-02	1.075E-02

- Raw QRPA-FAM photon strength function are stored in a FIFRELIN or TALYS-like format
- Default empirical corrections are implemented in the TALYS source code, allowing user fitting of the parameters for a better uncertainty propagation

Average radiation widths in ENDF format

In MF=2 MT=151, for poorly known isotope, the radiative width of each resonance is fixed to the average radiative width

Example: ^{130}**Xe** (JEFF4)

```
 0.000000+0 0.000000+0          0          0          0          05443 1  099999
 0.000000+0 0.000000+0          0          0          0          05443 0  0     0
 5.413000+4 1.287880+2          0          0          1          05443 2151     1
 5.413000+4 1.000000+0          0          0          1          05443 2151     2
 1.000000-5 4.000000+3          1          2          0          15443 2151     3
 0.000000+0 7.028000-1          0          0          2
 1.287880+2 7.028000-1          0          0         96
-1.380000+1 5.000000-1 1.047110-1 4.711000-3 1.000000-1 0.00000
 4.304100+2 5.000000-1 2.067400-1 1.538000-1 5.294000-2 0.00000
 7.038100+2 5.000000-1 1.843000-1 1.268000-1 5.750000-2 0.00000
 9.415800+2 5.000000-1 2.530000-1 1.955000-1 5.750000-2 0.00000
 1.114900+3 5.000000-1 1.425000-1 8.500000-2 5.750000-2 0.00000
 1.372700+3 5.000000-1 2.463000-1 1.888000-1 5.750000-2 0.00000
 1.400100+3 5.000000-1 2.355000-1 1.780000-1 5.750000-2 0.00000
 1.485200+3 5.000000-1 2.255500+0 2.198000+0 5.750000-2 0.00000
 2.432800+3 5.000000-1 2.167500+0 2.110000+0 5.750000-2 0.00000
 2.579600+3 5.000000-1 5.845000-1 5.270000-1 5.750000-2 0.00000
 2.614900+3 5.000000-1 4.875000-1 4.300000-1 5.750000-2 0.00000
 2.648100+3 5.000000-1 1.727500+0 1.670000+0 5.750000-2 0.00000
 2.980400+3 5.000000-1 2.407500+0 2.350000+0 5.750000-2 0.00000
 3.003200+3 5.000000-1 2.197500+0 2.140000+0 5.750000-2 0.00000
 3.259200+3 5.000000-1 1.671500+0 1.614000+0 5.750000-2 0.00000
 3.566900+3 5.000000-1 4.687500+0 4.630000+0 5.750000-2 0.00000
```

Resonance energies

Γγ=57.5 meV

^{130}Xe with average radiation width from panacea/FIFRELIN results

```
 0.000000+0 0.000000+0          0          0          0          05443 1  099999
 0.000000+0 0.000000+0          0          0          0          05443 0  0     0
 5.413000+4 1.287880+2          0          0          1          05443 2151     1
 5.413000+4 1.000000+0          0          0          1          05443 2151     2
 1.000000-5 4.000000+3          1          3          0          15443 2151     3
 0.000000+0 7.028000-1          0          0          2          25443 2151     4
 1.287880+2 7.028000-1          0          0         96         165443 2151     5
-1.380000+1 5.000000-1 4.711000-3 1.000000-1 0.000000+0 0.000000+05443 2151     6
 4.304100+2 5.000000-1 1.538000-1 0.05068000 0.000000+0 0.000000+05443 2151     7
 7.038100+2 5.000000-1 1.268000-1 0.05068000 0.000000+0 0.000000+05443 2151     8
 9.415800+2 5.000000-1 1.955000-1 0.05068000 0.000000+0 0.000000+05443 2151     9
 1.114900+3 5.000000-1 8.500000-2 0.05068000 0.000000+0 0.000000+0
 1.372700+3 5.000000-1 1.888000-1 0.05068000 0.000000+0 0.000000+0
 1.400100+3 5.000000-1 1.780000-1 0.05068000 0.000000+0 0.000000+0
 1.485200+3 5.000000-1 2.198000+0 0.05068000 0.000000+0 0.000000+0
 2.432800+3 5.000000-1 2.110000+0 0.05068000 0.000000+0 0.000000+0
 2.579600+3 5.000000-1 5.270000-1 0.05068000 0.000000+0 0.000000+0
 2.614900+3 5.000000-1 4.300000-1 0.05068000 0.000000+0 0.000000+0
 2.648100+3 5.000000-1 1.670000+0 0.05068000 0.000000+0 0.000000+0
 2.980400+3 5.000000-1 2.350000+0 0.05068000 0.000000+0 0.000000+0
 3.003200+3 5.000000-1 2.140000+0 0.05068000 0.000000+0 0.000000+0
 3.259200+3 5.000000-1 1.614000+0 0.05068000 0.000000+0 0.000000+0
 3.566900+3 5.000000-1 4.630000+0 0.05068000 0.000000+0 0.000000+0
```

Γγ=50.68 meV

Capture resonance integral I_0

Isotopes	I_0 (JEFF4) (a)	I_0 with panacea results (b)	Ratio (b)/(a)
Xe124	3512 b	3245 b	**0.92**
Xe126	37.3 b	32.4 b	**0.87**
Xe128	8.4 b	8.6 b	**1.02**
Xe129	253.8 b	251.6 b	**0.99**
Xe130	5.4 b	5.2 b	**0.96**
Xe131	878.7 b	878.5 b	**1.00**
Xe132	1.21 b	1.13 b	**0.93**
Xe134	0.47 b	0.46 b	**0.98**
Xe136	0.15 b	0.17 b	**1.13**

Max differences lower than ±15% ←

Nuclear model codes for fission product evaluation

From optical model parameters to total neutron cross section

From photon strength function to neutron capture cross section

Dissemination of the results

Conclusions

Conclusions

☑ « on the fly » HFBr and panacea calculations in association with TALYS

☑ Encouraging results obtained on the total cross section thanks to 2 free parameters (applied on the imaginary part of the nuclear potential) for spherical nuclei + 2 deformation parameters (β_2, β_4) for deformed nuclei + 1 free parameter for time-delay correction (finite interaction time Δt or distant level parameter shift R_{shift})

☑ Encouraging results obtained for the capture cross section thanks to 4 free parameters applied on the QFAM photon strenght function. Local deviation from the experimental capture cross section can be alternatively solved by a Lorentzian décomposition of the QFAM photon strenght functions

Perspectives

Codes	Optical Model Parameters	Deformation parameters	Level density	Photon strength function	Average radiation width	Fission barrier parameters	Resonance parameters
TALYS A. Koning et al.	From OMP RIPL-3 library	From FRDM	From Gilbert-Cameron composite formula	From GDR models	From HF γ-decay formula	From Empirical Hill–Wheeler–type fission barriers	From URR option
HFBr code suite A. Pastore	From 160 Skyrme forces + 4 Gogny forces	From FRDM	✓	✓		✓	
Panacea M. Frosini, P. Tamagno et al.	From 160 Skyrme forces + 4 Gogny forces	Natural outcome of the code	✓	From QFAM with D1S and D1M forces			
HFBaxial L. Robledo (in-house version of R. Bernard)		Natural outcome of the code				From TDGCM (not presented in this talk)	
FIFRELIN O. Litaize					From Monte-Carlo de-excitation		
CONRAD C. de Saint Jean P. Tamagno		From FRDM					From R-Matrix formalism

For JEFF-4.x ....