BRC neutron evaluations of actinides with TALYS code

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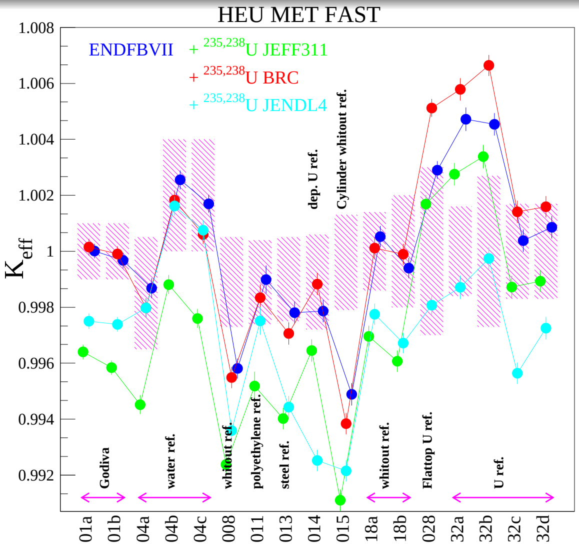
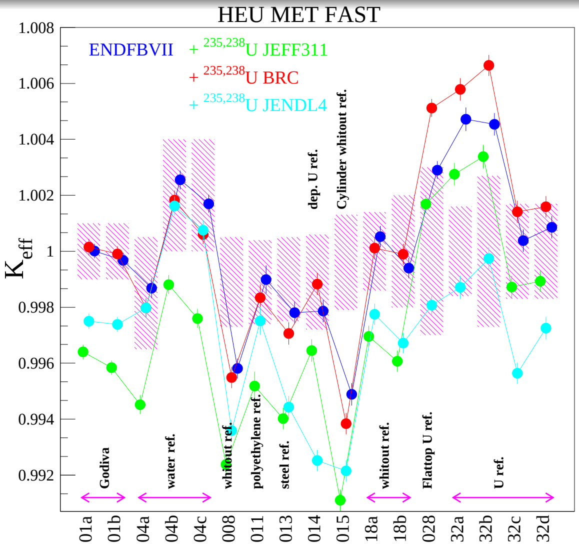
Criticality benchmarks



B. Morillon

MCNP5

Criticality benchmarks



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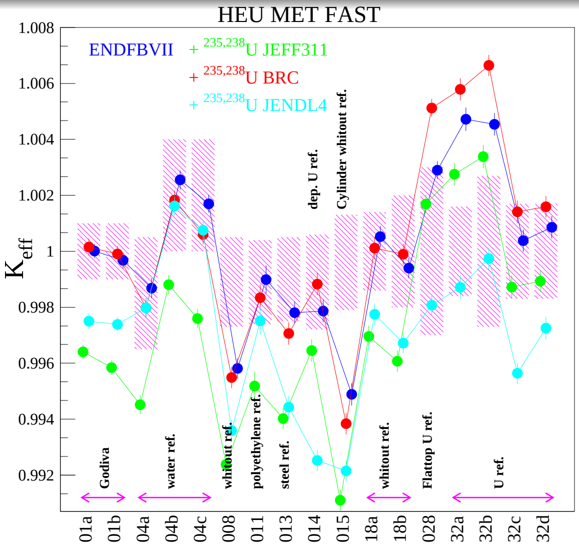
The major evaluated libraries predict measured criticality benchmarks extremely well !

Compensating errors



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BUT

These good agreements are certainly due to compensating errors

Optical Model $\leftrightarrow \sigma_{tot}, \sigma_{SE}, \sigma_{DI}, \sigma_R$ et $T_{l,j}^{J\pi}$

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Statistical Model $\leftrightarrow \sigma_{n,\gamma}, \sigma_{n,f}, \sigma_{n,xn}, \cdots$

+ P.E. $(\sigma_R = \sigma_{CN} + \sigma_{PE} + \sigma_{DI})$

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$+$ P.E. $(\sigma_R = \sigma_{CN} + \sigma_{PE} + \sigma_{DI})$

good Opt. Pot. $\equiv$ good tank σ_R and also $T_{l,j}^{J\pi}$

Optical Model $\leftrightarrow \sigma_{tot}, \sigma_{SE}, \sigma_{DI}, \sigma_R$ et $T_{l,j}^{J\pi}$

But !

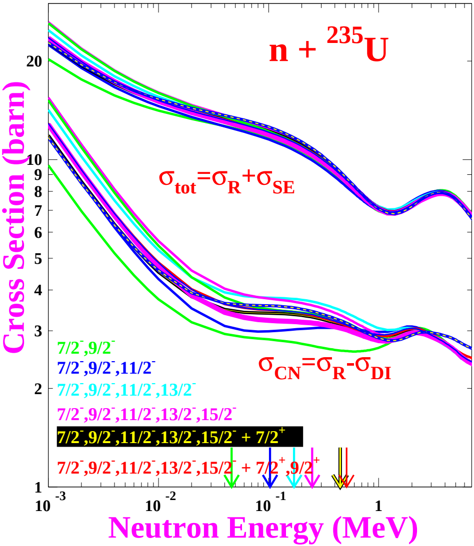
Are we sure to use the "best" coupling scheme ?

Statistical Model $\leftrightarrow \sigma_{n,\gamma}, \sigma_{n,f}, \sigma_{n,xn}, \cdots$

$+$ P.E. $(\sigma_R = \sigma_{CN} + \sigma_{PE} + \sigma_{DI})$

good Opt. Pot. $\equiv$ good tank σ_R and also $T_{l,j}^{J\pi}$

OMP - CCC ↔ which coupling scheme ?



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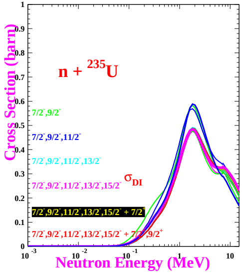

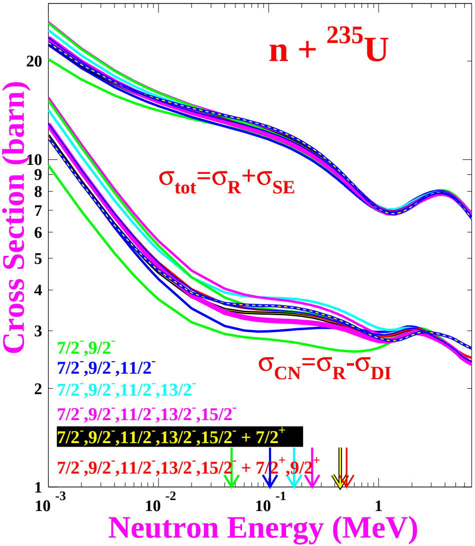

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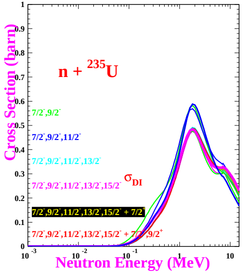

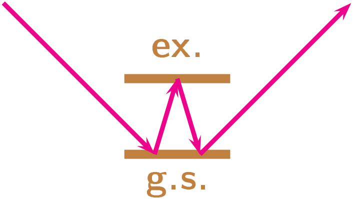

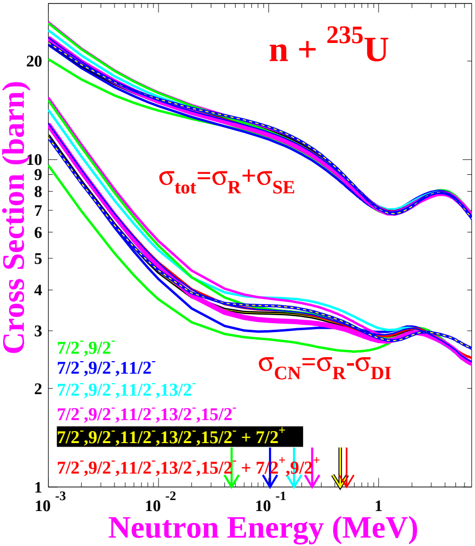

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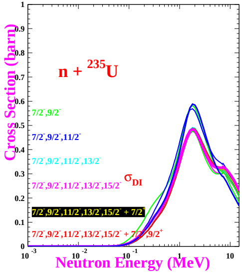

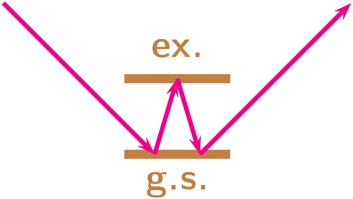

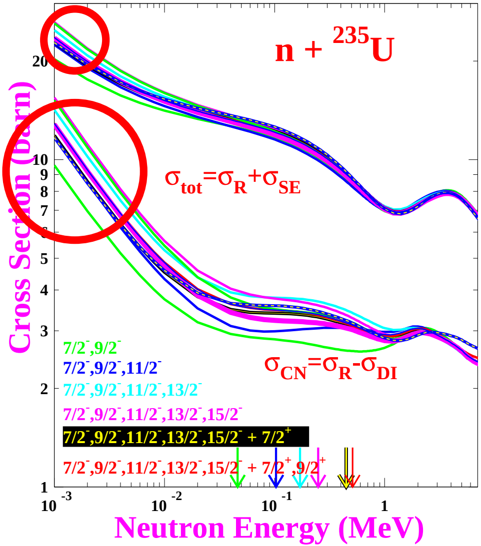

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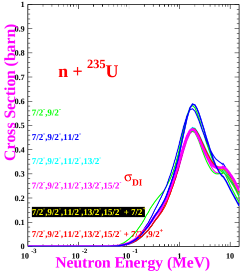
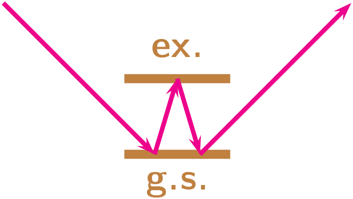
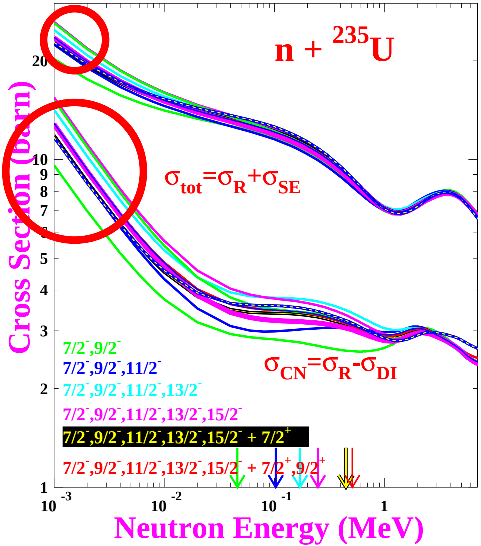
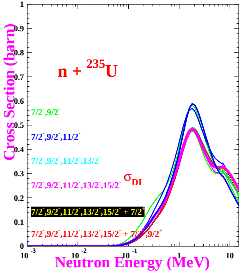


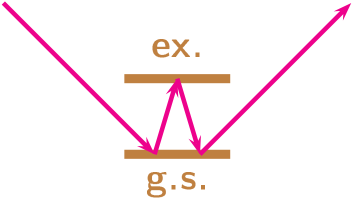


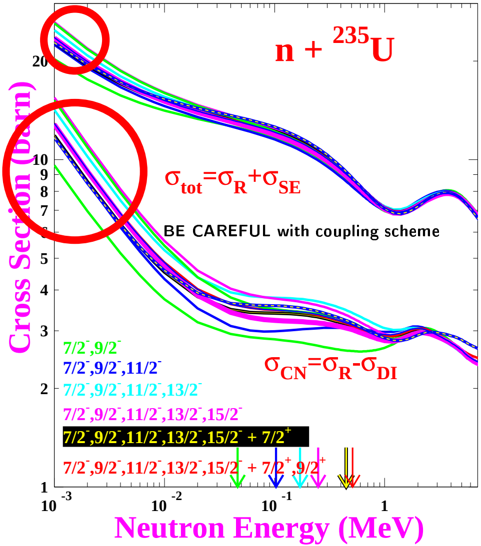


SPRT (= Ch. LAGRANGE BRC 1973) 1 -10 keV ? ? ? ?

OMP - CCC ↔ which coupling scheme ?



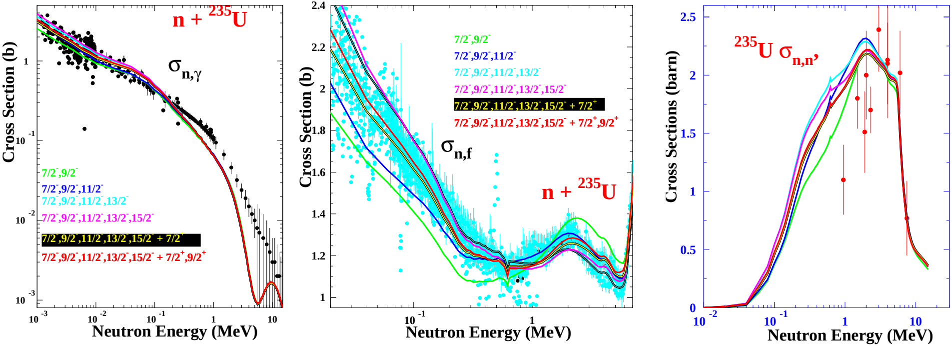




SPRT (= Ch. LAGRANGE BRC 1973) 1 -10 keV ? ? ? ?

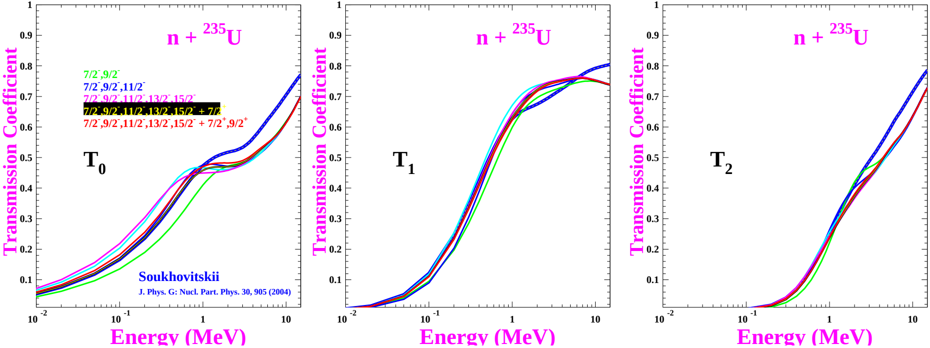
CCC : coupling scheme effects on statistical model caculations

Cross Sections behaviour



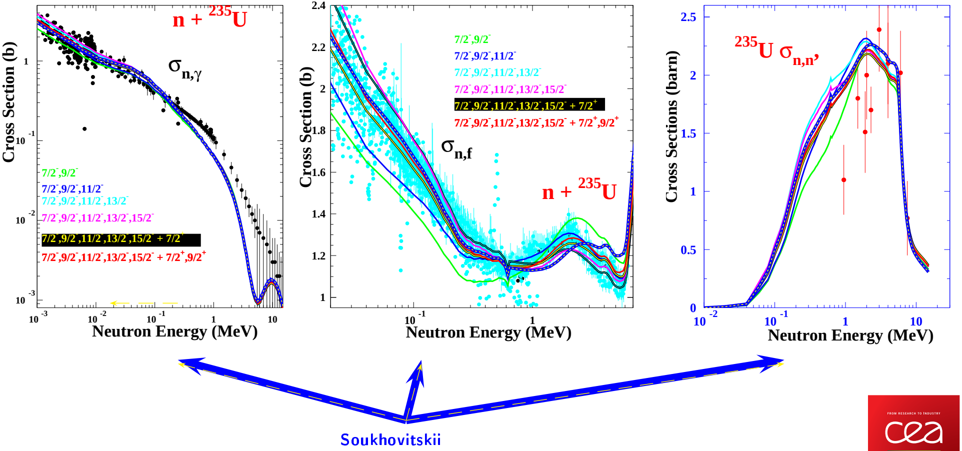
CCC : coupling scheme effects on statistical model caculations

Transmission Coefficients used



CCC : optical potentiel effects on statistical model caculations

Cross Sections behaviour



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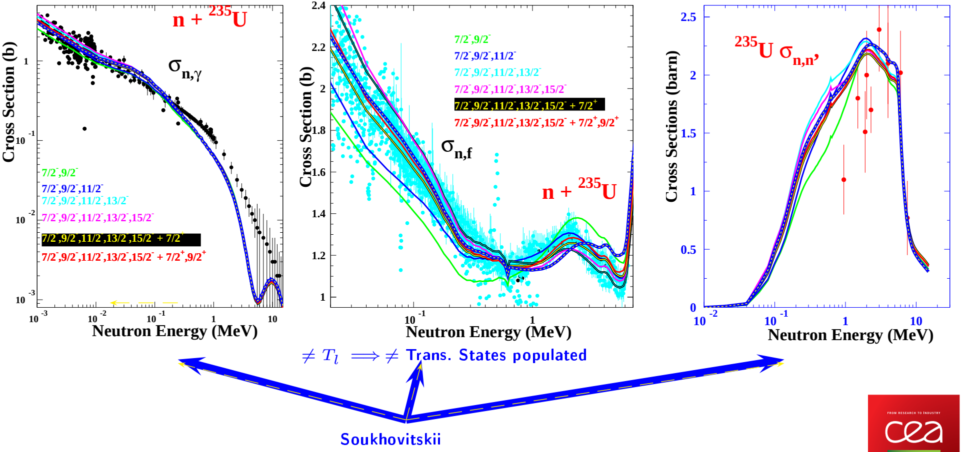
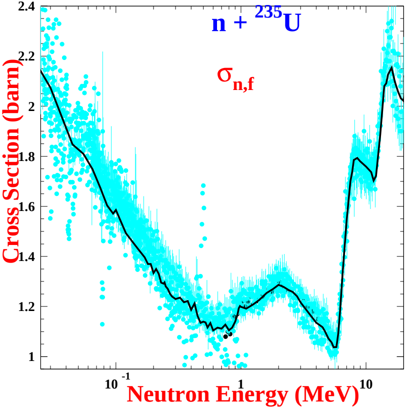


Once Optical Potentiel and coupling scheme adopted ...

^{235}U $\sigma_{n,f}$: standard cross section



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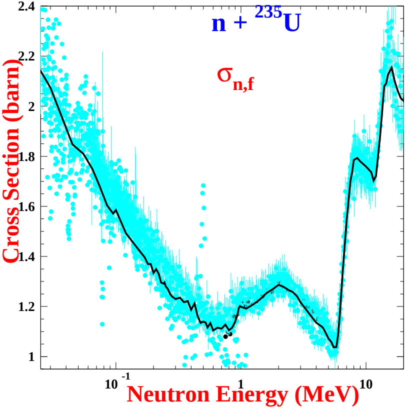

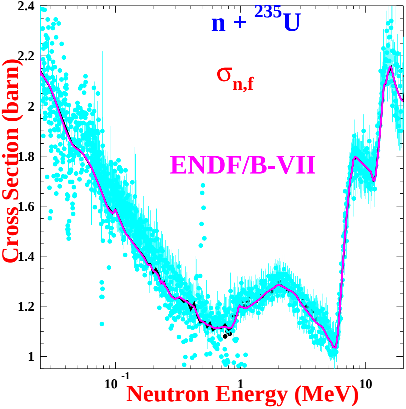

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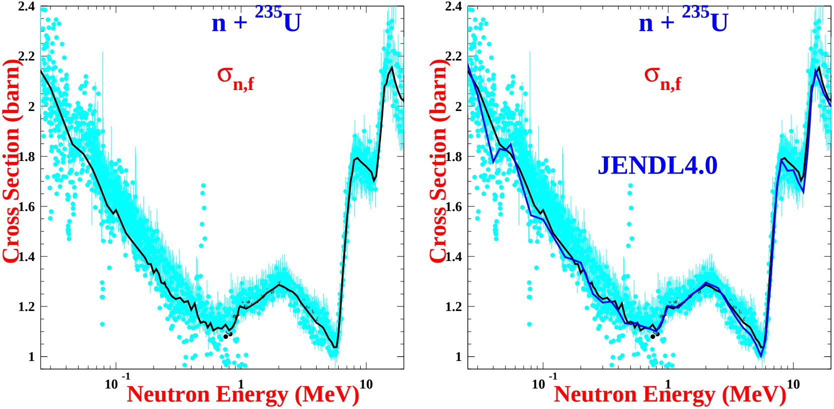

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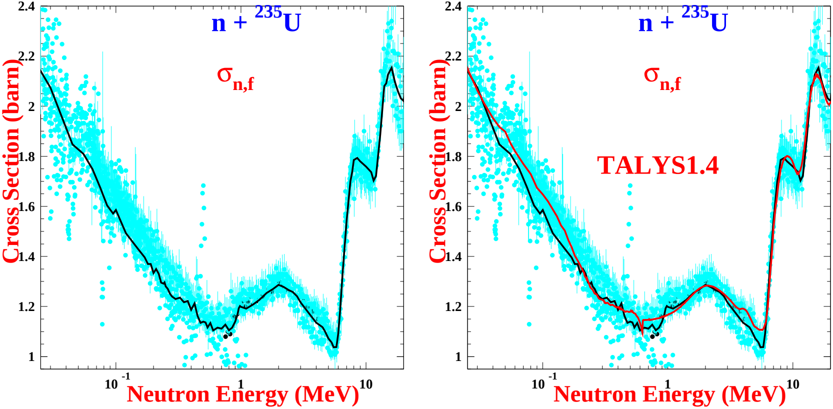


For energies $E < E_{(n,2n)}^{threshold}$, we can write :

$$\sigma_R = \sigma_{CE} + \sigma_{n,n'} + \sigma_{n,\gamma} + \sigma_{n,f}$$

and finally :

$$\sigma_R - \sigma_{CE} = \sigma_{n,n'} + \sigma_{n,\gamma} + \sigma_{n,f} = \sigma_{non-elas}$$

$$\Longleftrightarrow \quad 1 = \frac{\sigma_{n,n'}}{\sigma_R - \sigma_{CE}} + \frac{\sigma_{n,\gamma}}{\sigma_R - \sigma_{CE}} + \frac{\sigma_{n,f}}{\sigma_R - \sigma_{CE}}$$

$$1 = \frac{\sigma_{n,n'}}{\sigma_{non-elas}} + \frac{\sigma_{n,\gamma}}{\sigma_{non-elas}} + \frac{\sigma_{n,f}}{\sigma_{non-elas}}$$

By defining a probability for each non-elastic process occuring in this energy range :

$$1 = P_{n,n'}^{non-elas} + P_{n,\gamma}^{non-elas} + P_{n,f}^{non-elas}$$

And these probabilities can be directly deduced from evaluated files :

$$\sigma_{non-elas} = MF_3MT_4 + MF_3MT_{102} + MF_3MT_{18}$$

$$1 = \frac{MF_3MT_4}{\sigma_{non-elas}} + \frac{MF_3MT_{102}}{\sigma_{non-elas}} + \frac{MF_3MT_{18}}{\sigma_{non-elas}}$$

Dalitz plot

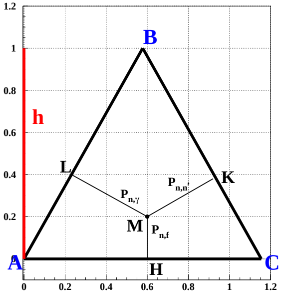


Fig.: *Dalitz plot of non-elastic processes in the energy range* 1 *keV* $< E < E^{threshold}_{(n,2n)}$

For these three open channels a Dalitz plot can be used. Indeed for an equilateral triangle ABC $(AB = AC = BC)$ with height h, each point M inside this triangle satisfies the following property :

$$MH + MK + ML = h$$

where H, K, L are the M orthogonal projections on each side $[AC]$, $[BC]$ et $[AB]$ respectivly. When assuming :

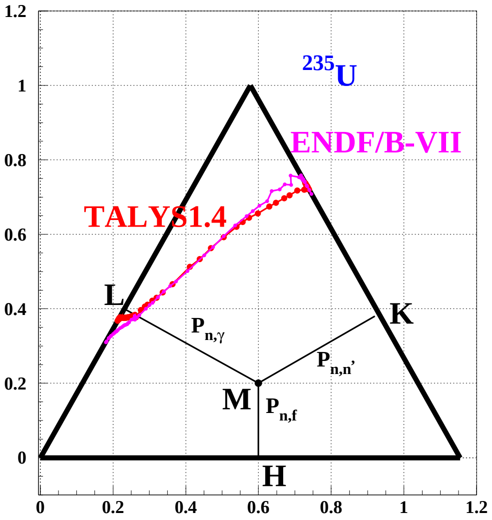
$$MH = P^{non-elas}_{n,f}, ML = P^{non-elas}_{n,\gamma}, MK = P^{non-el}_{n,n'}$$
$$MH + MK + ML = P^{non-elas}_{n,n'} + P^{non-elas}_{n,\gamma} + P^{non-}_{n,f}$$

Then each set

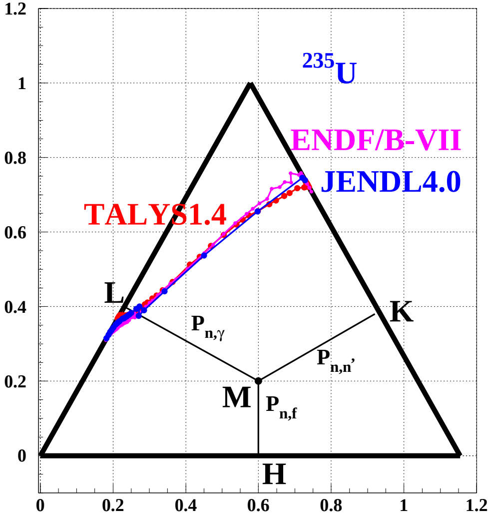
$$(E, \sigma_{n,n'}, \sigma_{n,\gamma}, \sigma_{n,f}) = (E, MF_3MT_4, MF_3MT_{102}, MF_3$$

of an evaluated file can be represented by a corresponding point M inside an equilateral triangle ABC $(AB = AC = BC)$ with unitary height $(h = 1)$. And finally an evaluated file will display a path inside this equilateral triangle.

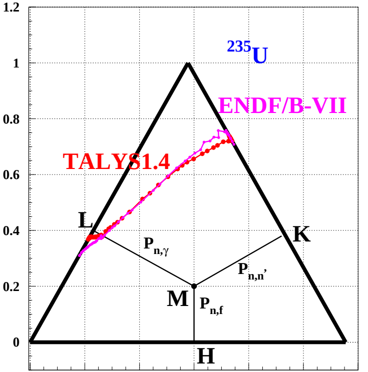
Dalitz plot of non-elastic processes probabilities on the 1 keV $< E < E^{seuil}_{(n,2n)}$ energy range



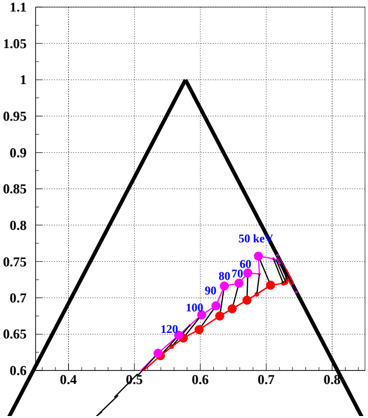
Dalitz plot of non-elastic processes probabilities on the $1 \text{ keV} < E < E^{seuil}_{(n,2n)}$ energy range



Dalitz plot

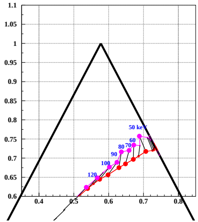


235U
ENDF/B-VII
TALYS1.4
L
K
M
H
$P_{n,\gamma}$
$P_{n,n'}$
$P_{n,f}$



50 keV
60
80 70
90
100
120

Dalitz plot



$$P_f(TALYS1.4) < P_f(BVII)$$

whereas

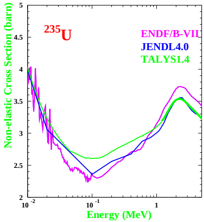
$$\sigma_f(TALYS1.4) > \sigma_f(BVII)$$

in the $50 < E < 100$ keV energy range ! But as shown

$$P_\gamma(TALYS1.4) > P_\gamma(BVII)$$

and

$$\sigma_{non-el}(TALYS1.4) > \sigma_{non-el}(BVII)$$

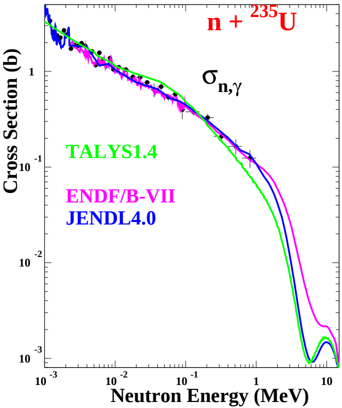


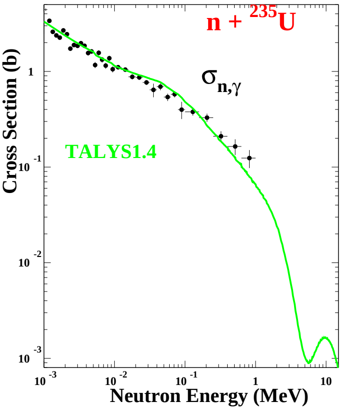
seek :

$$\sigma_\gamma(TALYS1.4)$$

Neutron Capture Cross Section

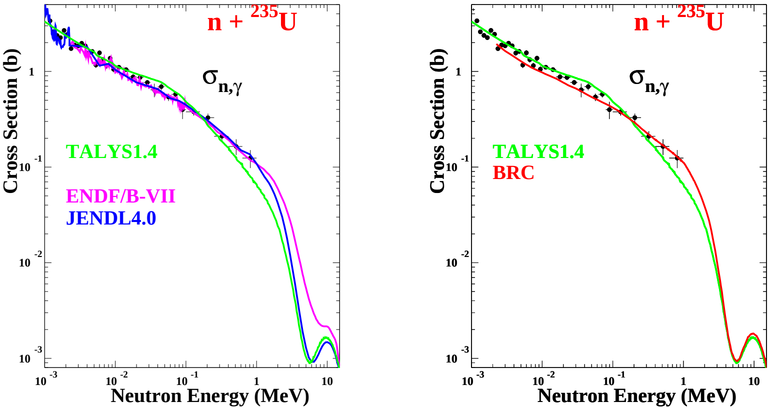
Jandel *et al.* 2012





Jandel *et al.* 2012

In fact $\sigma_{n,\gamma}^{BRC}$ adjusted on particular benchmarks



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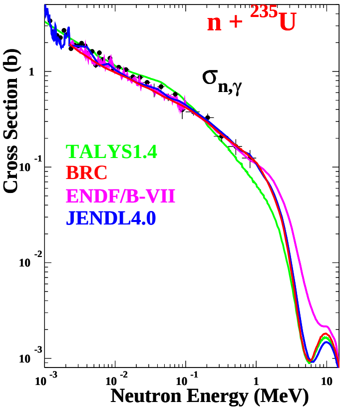

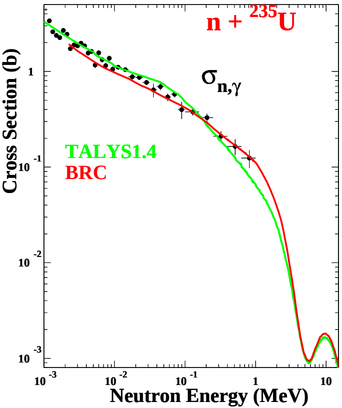

Neutron Capture Cross Section

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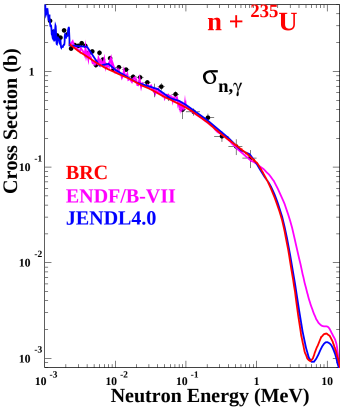
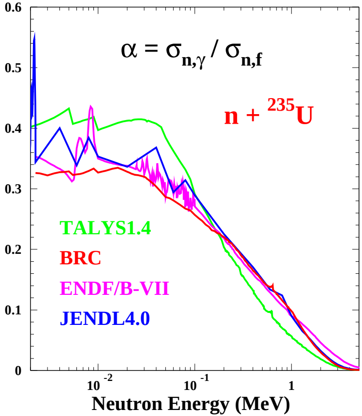
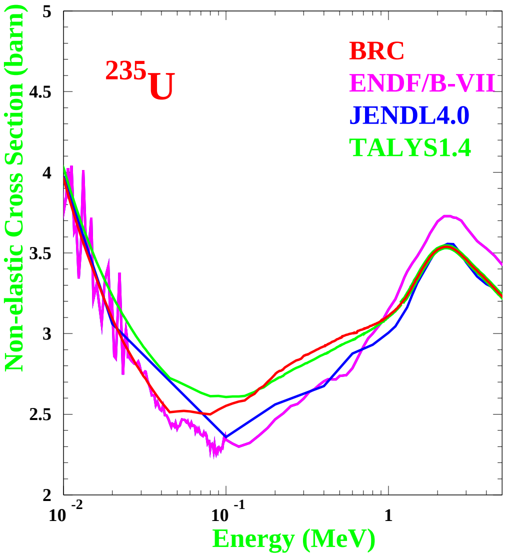
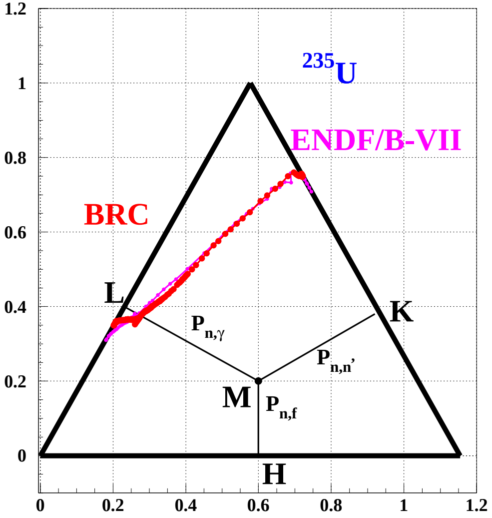




non-elastic cross sections on the $1\ \text{keV} < E < E^{seuil}_{(n,2n)}$ energy range



Dalitz plot of non-elastic processes probabilities on the 1 keV $< E < E^{seuil}_{(n,2n)}$ energy range



Use of Shannon theorem

From another point of view, we can also define the lack of information on the non-elastic emission processes for an emitting system A. When using the same notations as previous Dalitz plots, according to the Shannon theorem [1], the lack of information (also called entropy) or the uncertainties on the non-elastic emission processes for an emitting nucleus A can be defined as :

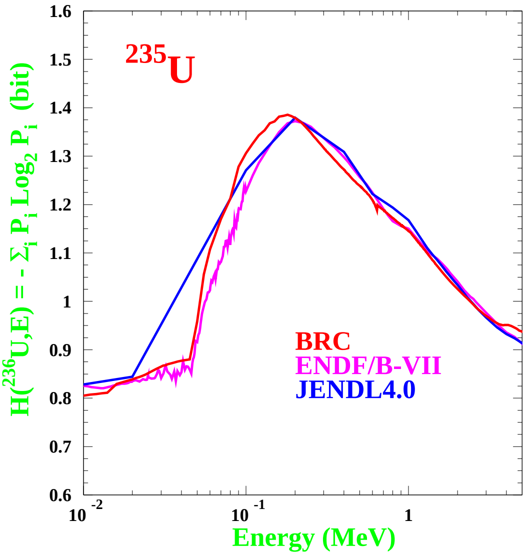
$$\begin{aligned} H_n(A,E) = \quad & -P_{n,\gamma}(E)\log_2 P_{n,\gamma}(E) \\ & -P_{n,n}(E)\log_2 P_{n,n}(E) \\ & -P_{n,f}(E)\log_2 P_{n,f}(E). \end{aligned}$$

Instead of plotting each probabibality of all exit channels for each studied evaluations versus energy, this representation is more compact, and so, more clearly to read.
If two evaluations are close together, the uncertainties on their non-elastic emission processes should be identical :

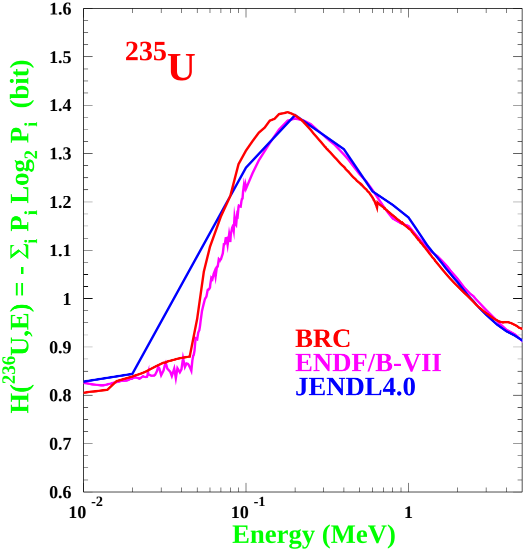
$$H_{Eval_1}(A,E) = H_{Eval_2}(A,E).$$

[1] C.E Shannon, Bell System Technical Journal, 27 , 379 and 623, (1948).

Use of Shannon theorem for non-elastic processes probabilities on the 1 keV $< E < E^{seuil}_{(n,2n)}$ energy range



Use of Shannon theorem for non-elastic processes probabilities on the 1 keV $< E < E^{seuil}_{(n,2n)}$ energy range



More

uncertainties for BRC

partly due to the

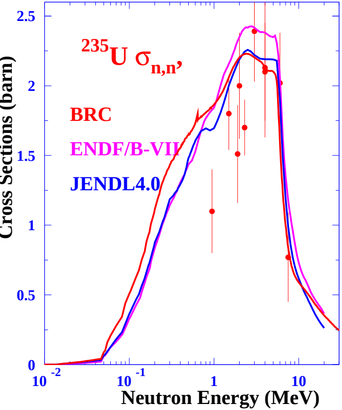
Inelastic Scattering

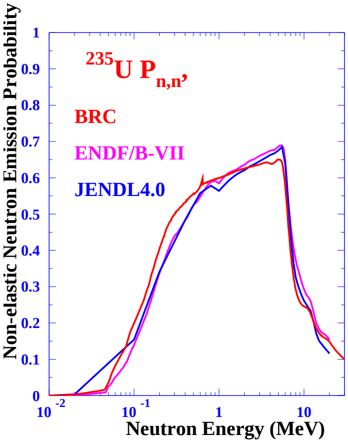
in $60 < E < 300keV$ **range**

ENDF/B-VII and JENDL4.0

same Coupling Scheme

Inelastic Scattering





Non-elastic neutron emission probability

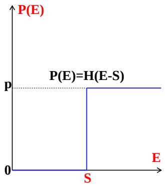


Fig.: *Non-elastic neutron emission probability for populating an $E = S$ energy state (Heaviside function)= threshold reaction.*

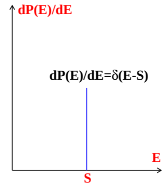


Fig.: *Energy derivative of the non-elastic neutron emission probability for populating an $E = S$ energy state (Dirac distribution $=$* energy distribution of populated states*).*

Energy distribution of populated states

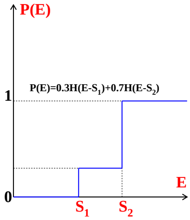


Fig.: *Non-elastic neutron emission probability for populating two energy states $E = S_1$ and $E = S_2$ (Heaviside functions)= threshold reactions.*

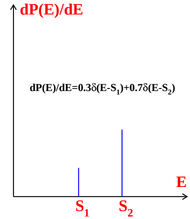
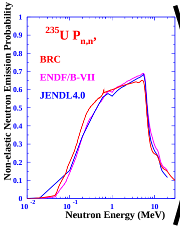


Fig.: *Energy derivative of the non-elastic neutron emission probability for populating two energy states $E = S_1$ and $E = S_2$ (Dirac distributions* $=$ energy distribution of populated states).

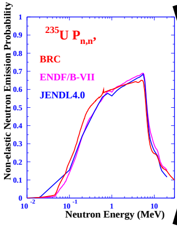
Energy distribution of populated states

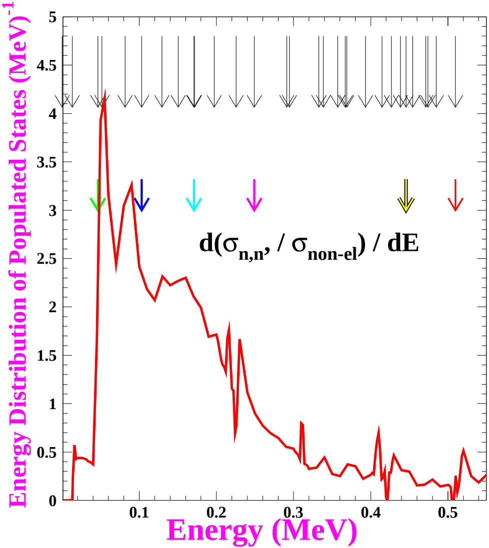
$$\frac{d}{dE}\left(\quad \right)$$



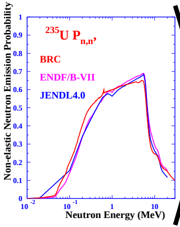
Energy distribution of populated states

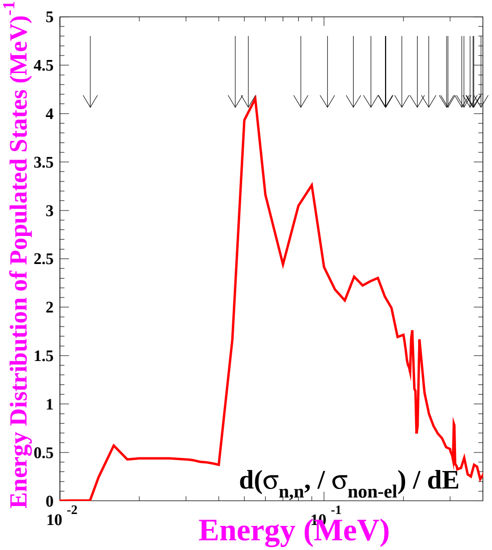
$$\frac{d}{dE}$$



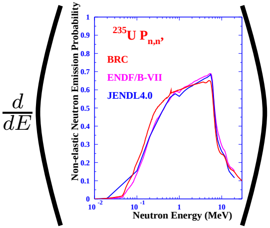


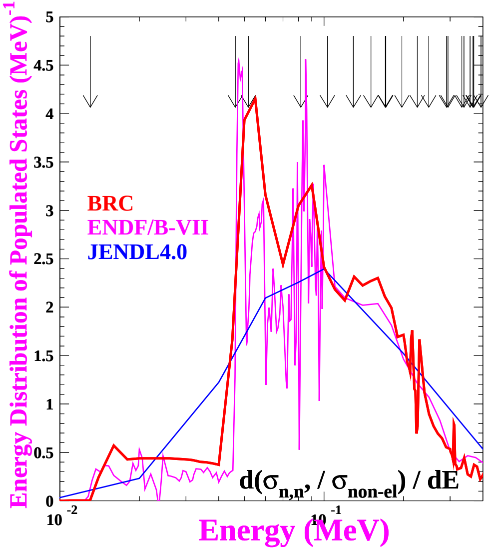
Energy distribution of populated states

$\frac{d}{dE}\left(\right.$  $\left. \right)$

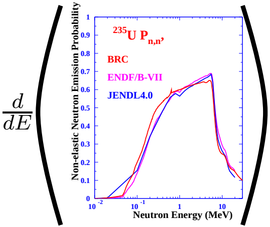


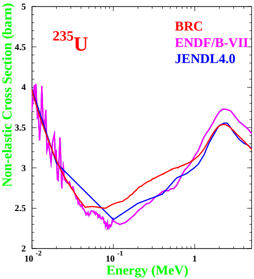
Energy distribution of populated states

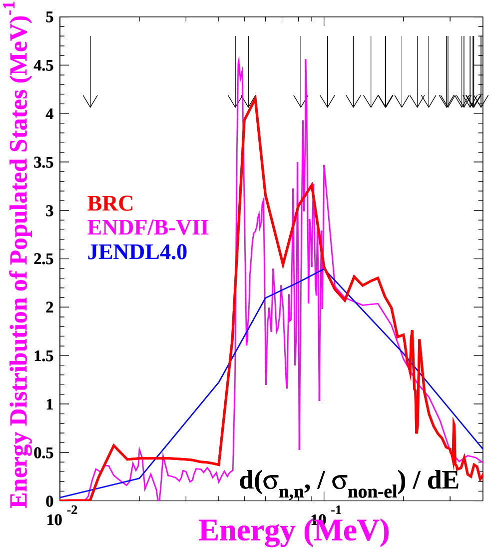




Energy distribution of populated states







DI in the URR

- Problem with DI in the URR for certain actinides (not so large for 235U)

- How can one take it into account in the URR (when not negligible) ?

Pseudo-states

- Problem with ENDF format with pseudo-states (MT51 -> MT90) for nucleus like ^{235}U (worse with ^{241}Am) with compressed spectrum.

- Which kind of approach to treat them ?

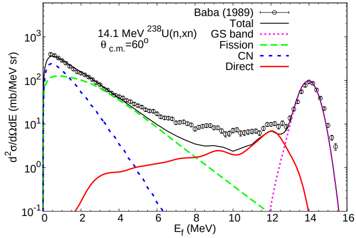
Pseudo-states

Collective states in the continuum that increase the inelastic scattering to the continuum.

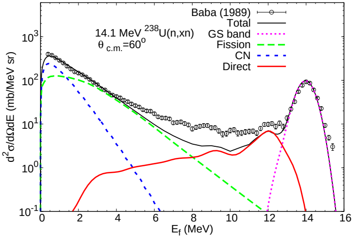
- These states were introduced in order to better reproduce the neutron leakage spectra from pulsed spheres measured using TOF techniques. L. F. Hansen *et al.* 1978 LLNL

- They were also adopted in JENDL3.2 by T. Kawano (1994) in order to better fit Baba's data.

Pseudo-states



Recent calculation by M. Dupuis (BRC) based on one step direct + QRPA (red curve) all the other contributions were calculated using T. Kawano (LANL) codes.



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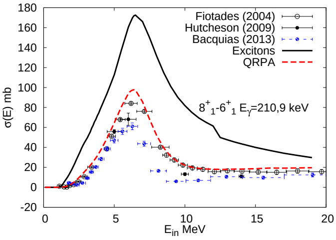
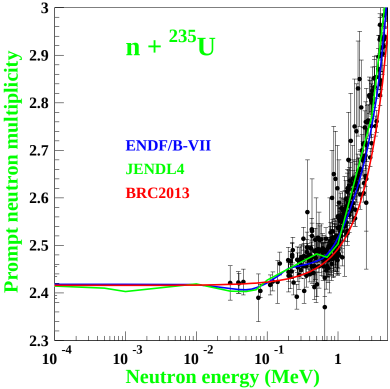


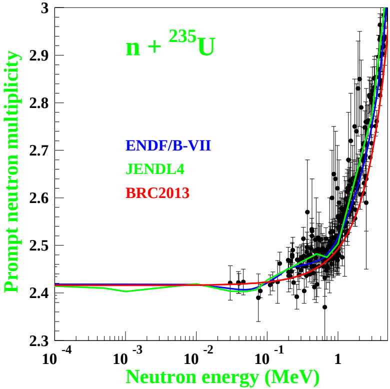
In this M. Dupuis (BRC) approach (one step direct + QRPA) the spin distribution of the composite nucleus differs strongly from the exciton model spin distribution. In fact, in (one step direct + QRPA) lower spins are preferentially populated. As shown there (red dashed curve), this improves considerably the $(n, xn\gamma)$ cross sections.

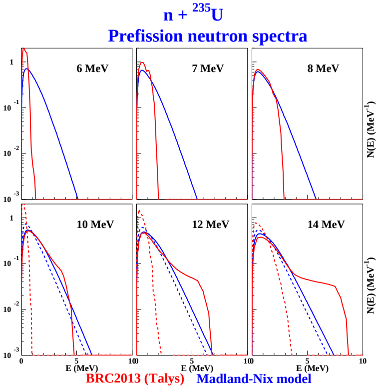
B. Morillon


n + ^{235}U
ENDF/B-VII
JENDL4
BRC2013
Prompt neutron multiplicity
Neutron energy (MeV)
3
2.9
2.8
2.7
2.6
2.5
2.4
2.3
10^{-4}
10^{-3}
10^{-2}
10^{-1}
1

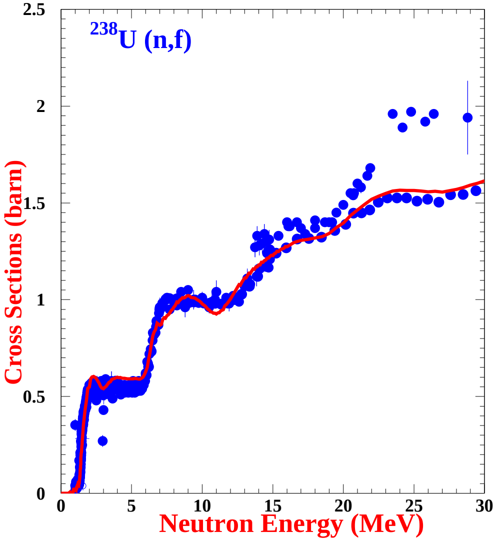
B. Morillon

includes pre-fission neutron spectra issued from TALYS





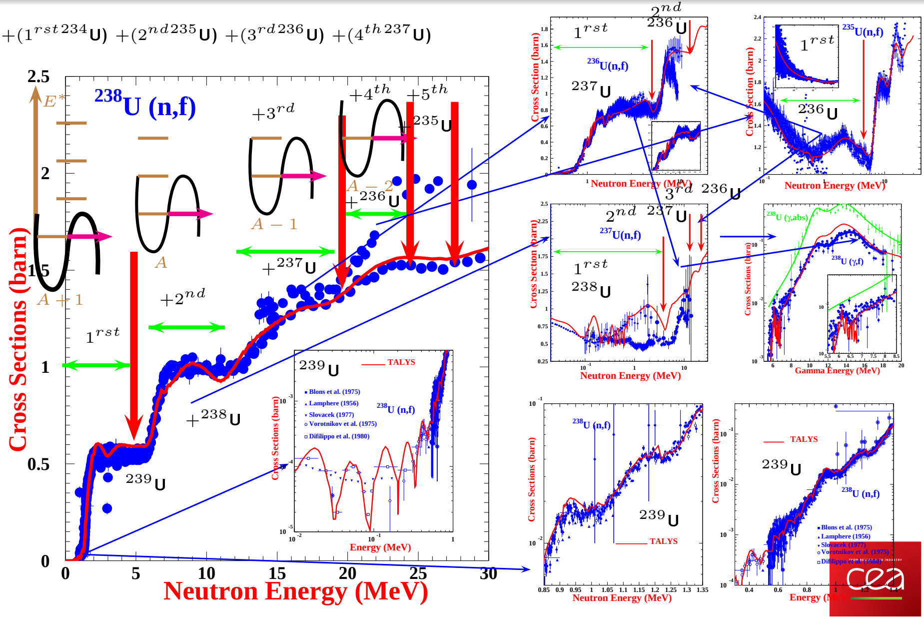
fission modeling $\leftrightarrow$ consistent parameters



^{238}U (n,f)
Cross Sections (barn)
Neutron Energy (MeV)
0
0.5
1
1.5
2
2.5
0
5
10
15
20
25
30

fission modeling ↔ consistent parameters

$+(1^{rst}\,{}^{234}U)\ +(2^{nd}\,{}^{235}U)\ +(3^{rd}\,{}^{236}U)\ +(4^{th}\,{}^{237}U)$



Conclusion or what should be done...

OMP :	*Dispersive OP* *Choice of Coupling Scheme*
URR :	*when extended to "high energies" problem with DI component*
Pseudo − states :	*which approach?* *how many states can be supported* (*MT*51 − 90)
InelasticXS	(*waste XS?*) *Measurements of this XS would be of great interest* *But effectivly experimental limits* (*to separate Inel. scat.* *to the low − lying states from the elast. scat.*)
PFNS	*Pre − fission neutron spectra have to be included.*
Evaluations just from models???	*sometimes adjustment of certain XS*
Consistent parameters!	*Is this the ultimate goal?*
Standard fission XS imposed?	*Is this also not a way for compensating errors?*

Would it be possible to eliminate all compensating errors?