Status of the Thermal Neutron Constant Data Base

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Technical Meeting on Neutron Data Standards, January 2025

Estimated « target » TNC values

"Target" TNC values established from Axton data, reference integrals, SAMMY and CONRAD evaluations

	^{233}U	^{235}U	^{239}Pu	^{241}Pu
σ_{tot}	≈590(2)	≈699.8(20)	≈1029(5)	≈1399(2)
σ_f	≈533(2)	≈586.2(30)	≈751(2)	≈1024(2)
σ_γ	≈45(1)	≈99.5(15)	≈270(3)	≈363(7)
σ_n	≈12.3(7)	≈14.1(2)	≈8(1)	≈11.9(25)
υ_{tot}	2.484-2.490	2.414-2.436	2.868-2.878	2.940(13)
I_3		≈245.7(40)		

Not uncertainty, but range of variation

Final TNC values will be given by **GMAPY** ⇒ **consistent description between TNC and high energy cross sections !**

Actions listed during the last STD meeting in 2023

TNC evaluation strategy

- TNC evaluation should be considered as an independent work and not included in a fitting procedure that combines the full GMA database ?
- If yes, remove TNC data from the GMA database
- Identify data sets in the GMA database that cover the thermal range

Recommendation and actions for Code and Database

- Provide input data for TNC including covariance matrices to IAEA for an evaluation with GMAPY
- Include reference integral ratios I1/I3, σ_{th}/I1 and σ_{th}/I3 to get correlation information
- Re-evaluation of $\nu(^{252}Cf)$ with updated uncertainties, especially for the Spencer and Smith data

Suggestions for possible future work

- Follow up what half live values was used in the past
- Use R-matrix to calculate integrals I1 and I3 to get correlation information
- Determine I1 and I3 directly in the evaluation procedure with GMAPY ?

New data sets for TNC evaluation

U233

M. Bacak, Développement d'un détecteur pour la mesure simultanée et l'étude des rendements de capture et de fission de l'uranium-233 auprès de la source de neutrons n_TOF au CERN, PhD thesis Université Paris Saclay, 2019
https://theses.hal.science/tel-02358659v1/document

⇒ Not yet available (needed for reference integral evaluation ?)

U235

N. Patronis et al., Measurement of the fission cross-section of 243Am at EAR-1 and EAR-2 of the CERN n_TOF

⇒ For the measurement, additional samples of 235U, 238U and 10B were used as reference for the neutron flux determination

⇒ Is this data available and already taken into account ?

Pu239

Adrian Sanchez-Caballero et al., Experimental setup of the 239Pu neutron capture and fission cross-section measurements at n_TOF, WONDER2023
https://doi.org/10.1051/epjconf/202429401003

⇒ Not yet available (needed for STD evaluation !)

Pu241

⇒ n_TOF measurements of the capture and fission cross sections in preparation

New/Final TNC will be delivered as soon as n_TOF data for Pu239 will be available …

New data sets for TNC evaluation

Include tof data used to established reference integral in the TNC evaluation procedure

I. Duran et al., Normalization of ToF (n,f) Measurements in Fissile Targets: Microscopic cross-section integrals, NDS 193 (2024) 95–104

Exemple : U235(n,f)

Experimental dataset	EXFOR entry	Integrals I_1 (b·eV)	Integrals I_3 (b·eV)	Integrals I_3/I_1	Renormalized integrals renormal. factor	Renormalized integrals I_1 (b·eV)	Renormalized integrals I_3 (b·eV)	Analytical fit σ_0^f (b)	Analytical fit fitted b (see Eq.(2))	Analytical fit I_1^{anal} (b·eV)
^{235}U(n,f) selected data and results of the fit to Eq.(1)										
Adamchuk 1955	40063	17.27			1.088	18.79		581.3	-0.554	18.77
Amaducci 2019	23453	18.82	247.5	13.15	1.0	18.82	247.50	582.2	-0.567	18.72
Bowman 1966	12433	18.36	246.1	13.40	1.018	18.69	250.53	587.8	-0.600	18.68
Deruytter 1971	20131	18.60	239.5	12.88	1.004	18.67	240.46	586.9	-0.594	18.69
Gwin 1984	12905	18.82	249.5	13.26	1.0	18.82	249.50	589.7	-0.585	18.84
Melkonian 1958	12403	18.49			1.01	18.71		587.5	-0.589	18.74
Mihailescu 1972	30269	18.70			1.009	18.87		585.2	-0.569	18.80
Schrack 1988	13198	18.83	240.7	12.78	1.004	18.91	241.70	585.9	-0.567	18.84
Wagemans 1988	22080	18.83	246.3	13.08	1.0	18.83	246.30	586.9	-0.572	18.83
Wagemans 1979	21522	18.71	244.2	13.05	1.005	18.71	244.24	587.2	-0.577	18.81
Mean values				13.08		18.78	245.7	586.1	-0.577	18.77
Absolute std.dev.				0.20		0.08	4.1	2.6	0.014	0.06
Relative std.dev.(%)				1.5		0.4	1.7	0.4	2.5	0.3

Adamchuk data not considered by Axton, not used in the CONRAD evaluation of RRR

⇒ **Need for a consistent database between TNC, reference integrals and RRR analysis**

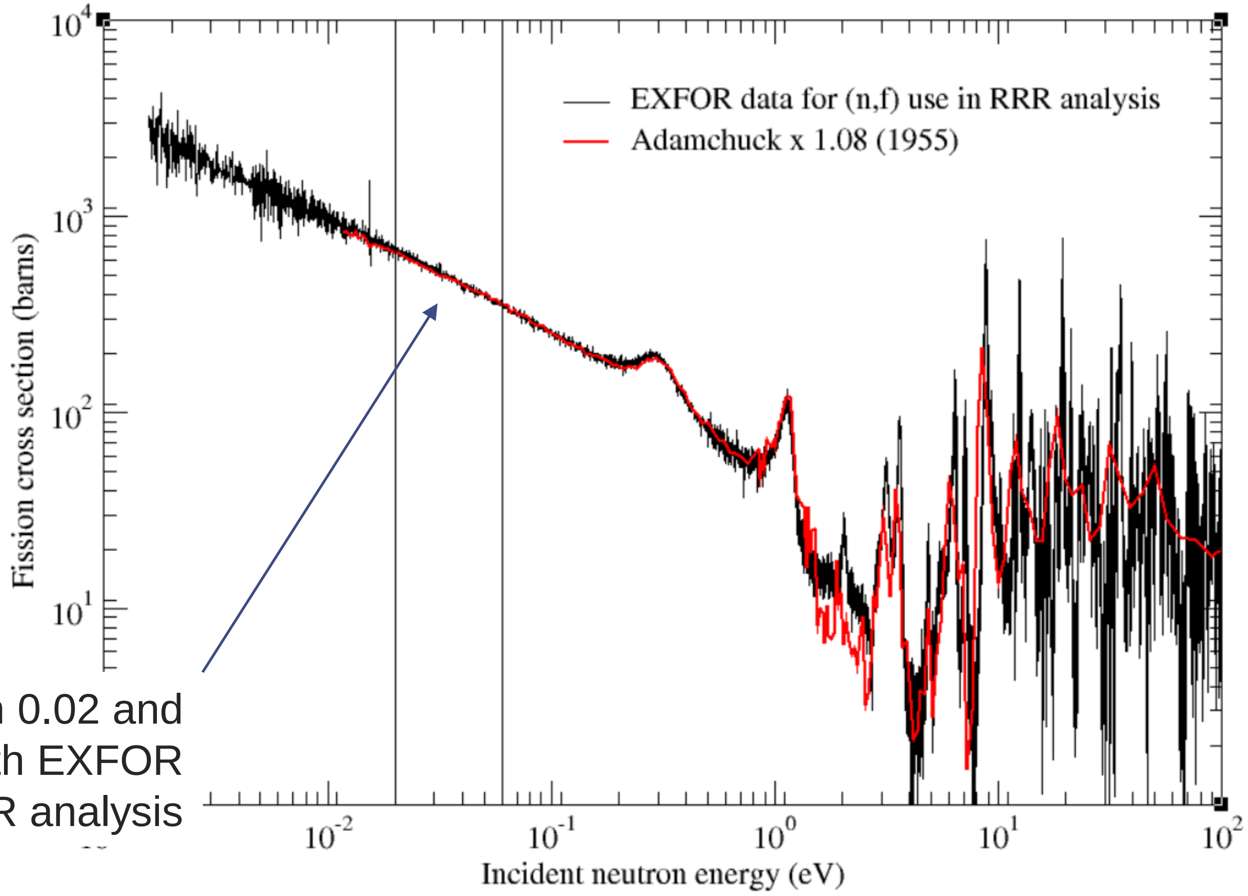
⇒ See Talk of Ignacio

New data sets for TNC evaluation

Include tof data used to established reference integral in the TNC evaluation procedure

I. Duran et al., Normalization of ToF (n,f) Measurements in Fissile Targets: Microscopic cross-section integrals, NDS 193 (2024) 95–104

Exemple : U235(n,f)



Slope of Adamchuck between 0.02 and 0.06 eV not consistent with EXFOR data used in the RRR analysis

New data sets for TNC evaluation

Include tof data used to established reference integral in the TNC evaluation procedure

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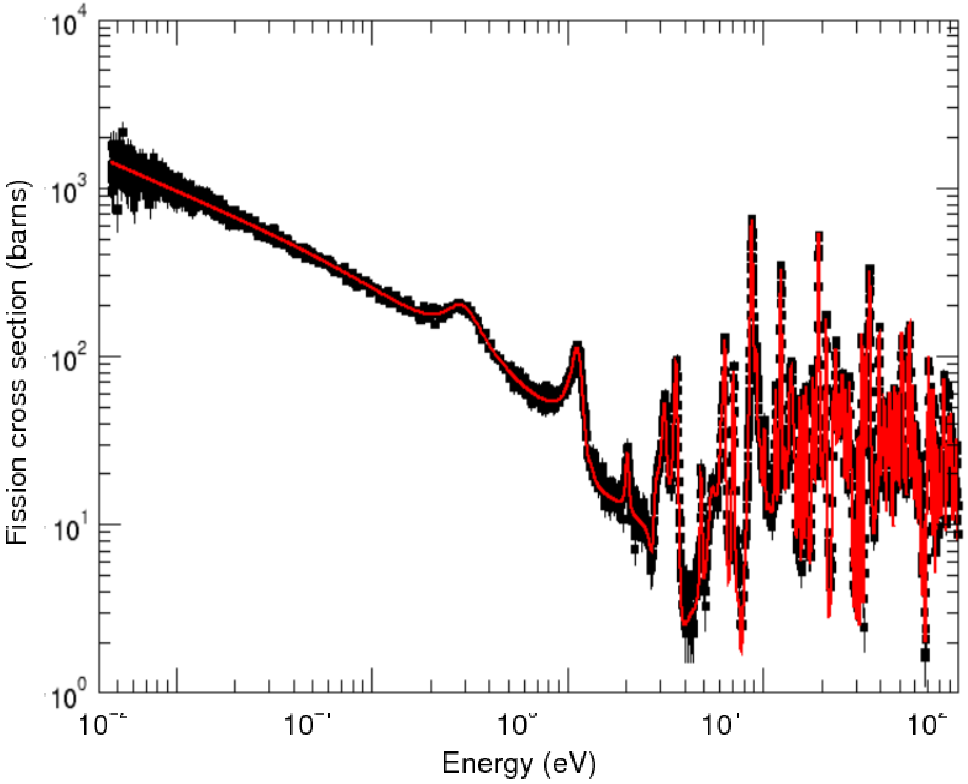
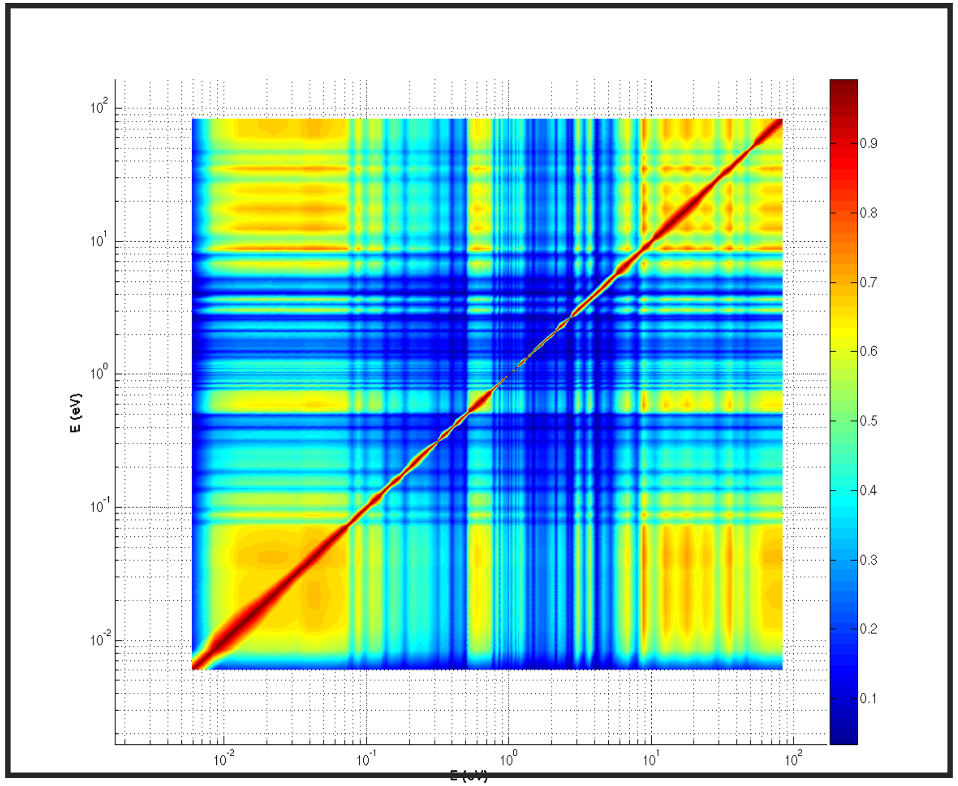
Exemple : U235(n,f) ⇒ use unpublished fission cross section measured at JRC-Geel ?





Axton data vs. EXFOR data

Naohiko Otuka, "Experiments in the EXFOR library for evaluation of thermal neutron constants », ND2016

ID	Quantity	X4/Axton	EXFOR #	Reference reporting the original value
3	$\bar{\sigma}_{\gamma,3}$	1.044	12335.002	J.Halperin+,J,NSE,16,245,1963
13	$\bar{\sigma}_{f,9}/\bar{\sigma}_{f,5}$	1.020	21494.008	P.H.White+,C,66PARIS,2,29,1966
14	$\bar{\sigma}_{f,1}/\bar{\sigma}_{f,5}$	1.021	21494.009	P.H.White+,C,66PARIS,2,29,1966
23	$\sigma_{\gamma,9}/\sigma_{f,9}$	1.012	10013.004	M.Lounsbury+,C,70HELSINKI,1,287,1970
79	$\sigma_{a,3}+\sigma_{sm,3}$	0.989	21065.003	N.J.Pattenden,J,JNE,3,28,1956
107	$\sigma_{f,5}$	1.020	12392.002	A.Saplakoglu,C,58GENEVA,16,103,1958
108	$\sigma_{f,1}$	0.976	12529.005	T.Watanabe+,R,IDO-16995,1964

Non negligible differences ranging from 1 to 4% on some **«old» TNC data** reported in the Axton report

⇒ **Should we replace Axton data by EXFOR data ?**

« Old » TNC data 1944-1960

Cross sections and neutron yields for

U^{233}, U^{235} and Pu^{239} at 2200 m/sec.

N.G. Sjöstrand and J.S. Story

AKTIEBOLAGET ATOMENERGI

STOCKHOLM · SWEDEN · 1960

History of data selection/correction made by Axton for data measured before 1960 difficult to trace

Report from Sjostrand contains usefull information (total cross sections, elastic cross section, uncertainties, origin of the data …)

⇒ But, quality of the data is questionable …

Unfortunately, many of the earlier measurements have not yet been described in the open literature, and we must still use some of them. In such cases we have often had to rely on secondhand information and may have misinterpreted it.

Some data reported by Sjostrand (close to the TNC-17 value) are not included in the Axton report

⇒ **Should we take them into account ?**

« Old » TNC data 1944-1960

Some data reported by Sjostrand (close to the TNC-17 value) are not included in the Axton report
⇒ Should we take them into account ?

Scattering cross section not used by Axton

total cross-sections. The most reliable values of the scattering cross-sections for subtraction seem to be the following:

U^{233}	12.5 ± 1.0 b	OLEKSA (1958)
U^{235}	15 ± 2.5 b	FOOTE (1958)
Pu^{239}	10 b	Calculated potential scattering.

However, as HAVENS and MELKONIAN (1958) have observed, these values may be somewhat high at 2200 m/sec, as a result of molecular and crystallic binding effects in the coherent scattering.

Taken into account by Axton, should be corrected (relative to Gold)

Absorption cross section not used by Axton

Reference	U^{233}	U^{235}	Pu^{239}
MAY (1944)		687 ± 15 695 ± 20	
ANDERSON et al. (1944)			1057
PALEVSKY & MUETHER (1954)	585 ± 10		
PALEVSKY et al. (1954)		685 ± 5	
EGELSTAFF (1954) (Revised)		709 ± 15	
ZIMMERMAN & PALEVSI Y (1955)			1020 ± 10
PATTENDEN (1956)	595 ± 15		1005 ± 30
NIKITIN et al. (1956)	570 ± 20	695 ± 20	1030 ± 30
KUKAVADSE et al. (1956)	618 ± 30		
GREEN et al. (1957)	578 ± 17		
SCHWARTZ (1958)		683 ± 6 681 ± 6	
BOLLINGER et al. (1958)			988 ± 10

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Neutron scattering cross section at thermal energy depends on the structure and dynamics of the molecule

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ANDERSON et al. (1944)			1057
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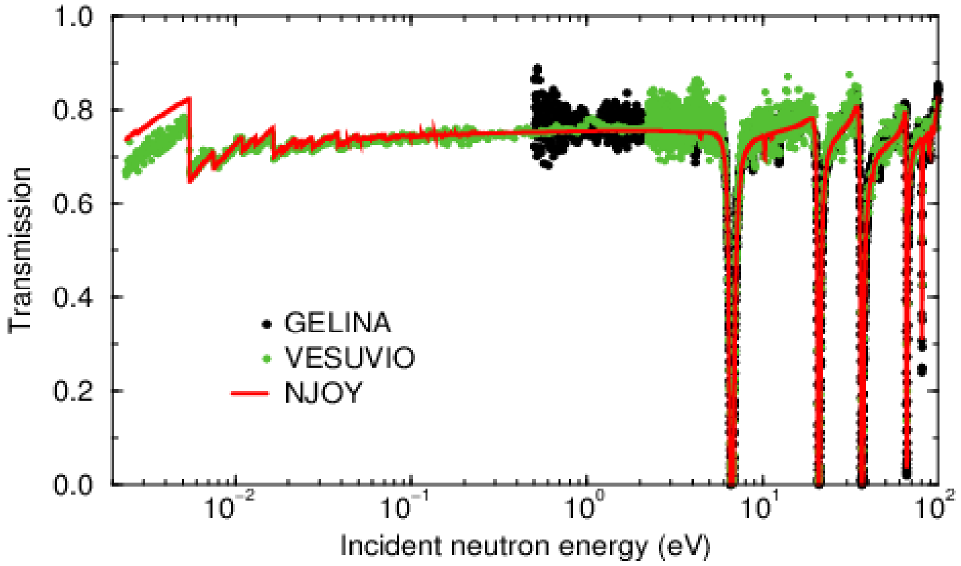
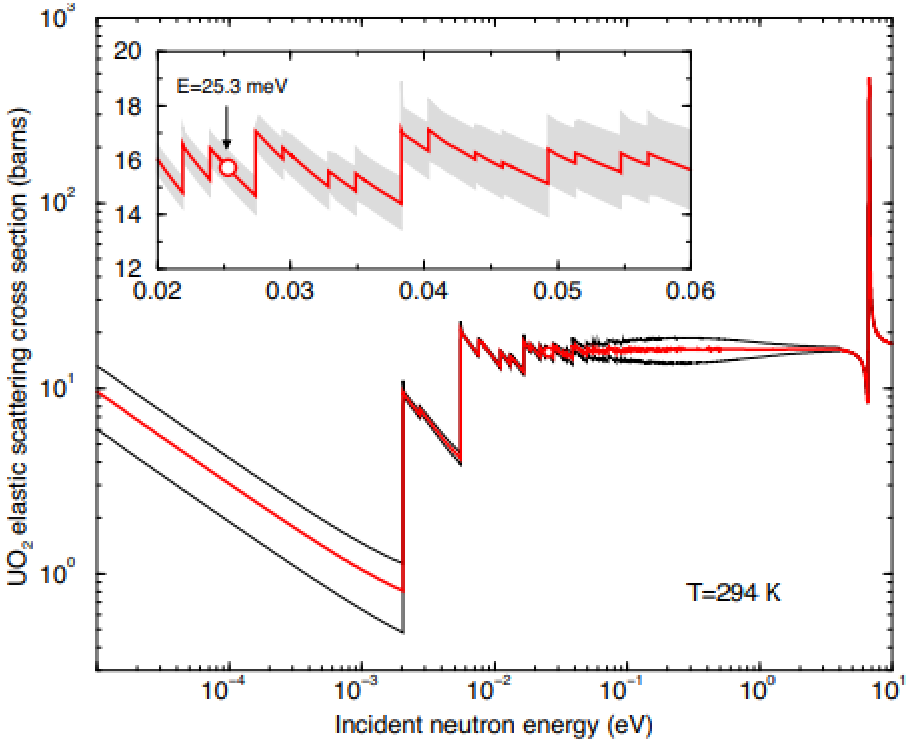
Issues with neutron scattering cross section

Neutron scattering cross section and Bragg Edges observed in a UO2 powder sample

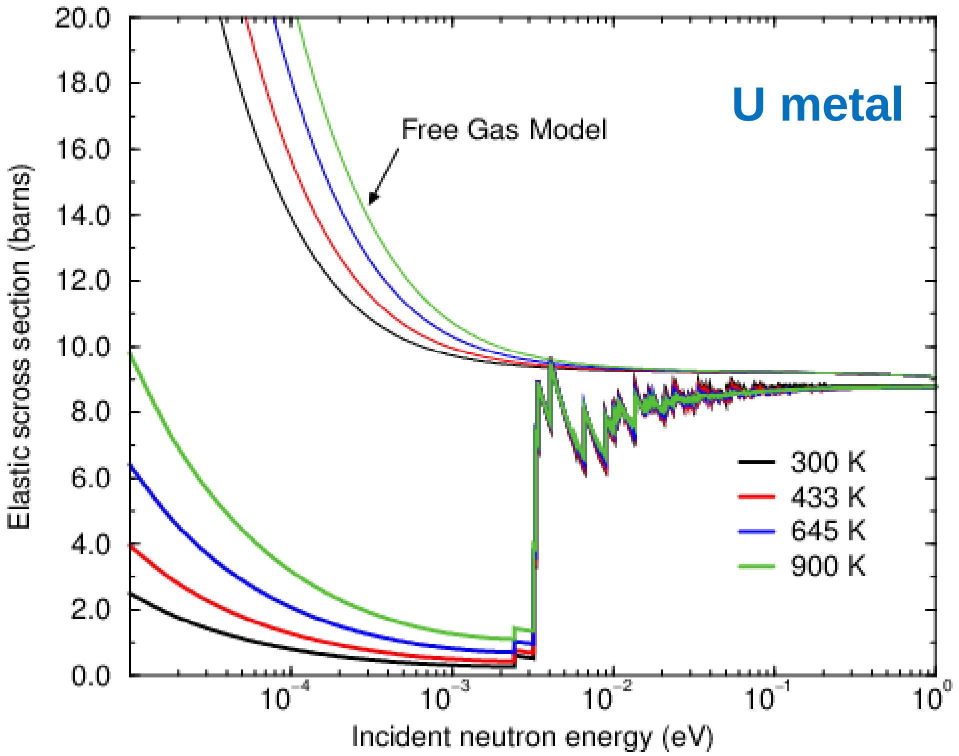
Total cross section of UO2 measured at the VESUVIO facility (ISIS, UK)

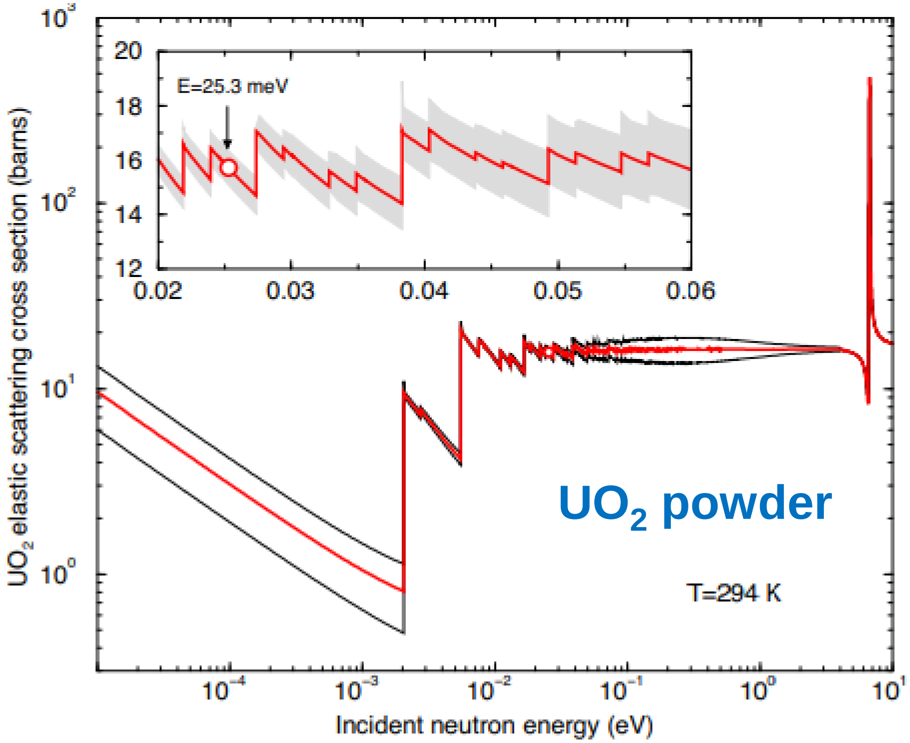




Issues with neutron scattering cross section

Neutron scattering cross section depends of the material





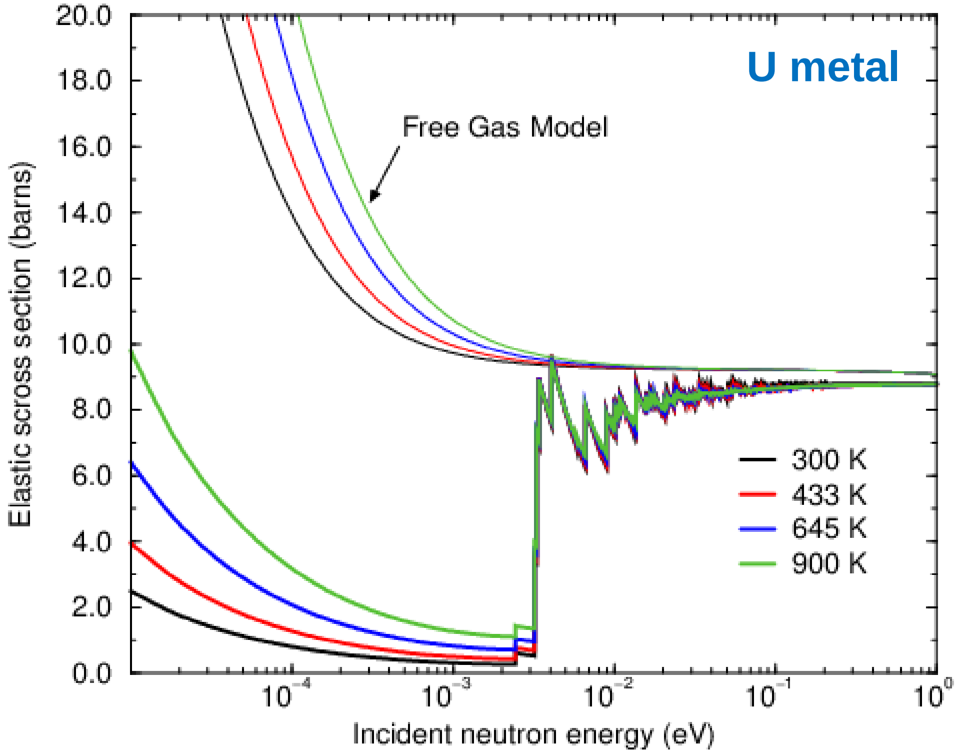
Free Gas Model used in the evaluations available in the ENDF libraries ⇒ consistency with TNC work ?

Issues with neutron scattering cross section

"Crystal extinction effects" due to the structure and dynamics of the molecule in the crystal

Block, NSE 8, 112 (1960) ⇒ In order to arrive at the "effective" scattering cross section, σ_{sc} in Eq. (2), it is necessary to take into account both the true scattering cross section and the crystal extinction effects. These crystal extinction effects are the result of Bragg scattering in samples where there is a preferred orientation of crystals; this preferred orientation can be brought about in the rolling process. The net result of this effect is generally to lower the measured cross section. In thermal measurements with gold samples it has been noted (*1*) that rolled samples give thermal total cross section values which are ~2 barns lower than those obtained with powdered samples. Since gold has a thermal scattering cross section of ~9 barns, this represents an extinction effect of ~20 % of the scattering cross section.

« Crystal extinction effects taken into account in the TNC evaluation



⇒ Consistency with the work performed on the reference integrals $\sigma_\gamma = \sigma_{tot} - \sigma_f - \sigma_n$?

⇒ The neutron scattering cross section at **zero Kelvin** is the common value that should be taken into account (more complex evaluation procedure, with additional sources of uncertainties ☹)

Input for TNC evaluation : Half-live values

TNC calculations have to performed with updated half-lives, which are needed to compute some quantities reported in the Axton's report:

Values taken in CONRAD evaluation:

- $T_{1/2}$(U233) = (1.592 $\pm$ 0.002).10^5 y (ENSDF
- $T_{1/2}$(U234) = (2.455 $\pm$ 0.006).10^5 y (LNHB = ENSDF)
- $T_{1/2}$(Pu239) = (2.4100 $\pm$ 0.0011).10^4 y (LNHB)
- $T_{1/2}$(Pu241) = 14.33 $\pm$ 0.04 y (LNHB)

$\Rightarrow$ Other suggestions ? **Which Half-live values should we adopt?**

Input for TNC evaluation : USU on ν_{tot}(Cf252)

	STD meeting 2017 CONRAD (1)	NDS 2018 A.D. Carlson et al. (2)	Difference (1)-(2)
υ_{tot}	3.7660(70)	3.7637(158)	+0.0023

$\overline{\nu}_{tot}$ for ^{252}Cf from the GMAP analysis is 3.7637 (or 3.764) $\pm$ 0.42 %. This includes a 0.4 % unrecognized sys-

Reduce USU from **0.4%** to **0.25%** ?

$\Rightarrow$ In CONRAD, USU is taken into account via the marginalization procedure of nuisance parameters

$\Rightarrow$ **Which USU value should we adopt (see talk of Denise) ?**

Input for TNC evaluation : "Evaluator dependent biases"

Trivial sources of bias that can be taken into account ⇒ fitting strategy and data selection

For the second category of biases, we can distinguished the contribution of the sample characteristics (oxide powder vs. rolled metal samples), "mic-mac" data, contribution of the differences between the Axton and EXFOR data …

Thermal constants		Sources of uncertainties (in %)				Total (in %)
		fitting model	rolled metal	mac. data	EXFOR data	
U233	σ_s	-	0.05	0.98	-	**0.98**
	σ_f	0.04	0.21	0.09	0.01	0.23
	σ_γ	0.50	0.36	0.89	0.17	**1.20**
	υ_t	0.05	-	0.07	-	0.09
U235	σ_s	1.36	3.04	2.93	0.03	**4.44**
	σ_f	0.16	0.51	0.11	0.01	**0.55**
	σ_γ	0.47	0.04	0.51	0.01	**0.69**
	υ_t	0.10	0.02	0.07	-	0.12
Pu239	σ_s	0.04	0.22	0.06	-	0.23
	σ_f	0.05	0.19	0.18	0.01	0.27
	σ_γ	0.11	0.17	0.23	-	0.31
	υ_t	0.02	-	0.02	-	0.03
Pu241	σ_s	0.19	0.10	0.96	-	**0.98**
	σ_f	0.34	-	0.45	-	**0.56**
	σ_γ	0.02	0.10	0.25	0.01	0.27
	υ_t	0.04	-	0.06	-	0.07
Cf252	υ_t	0.02	-	0.02	-	0.03

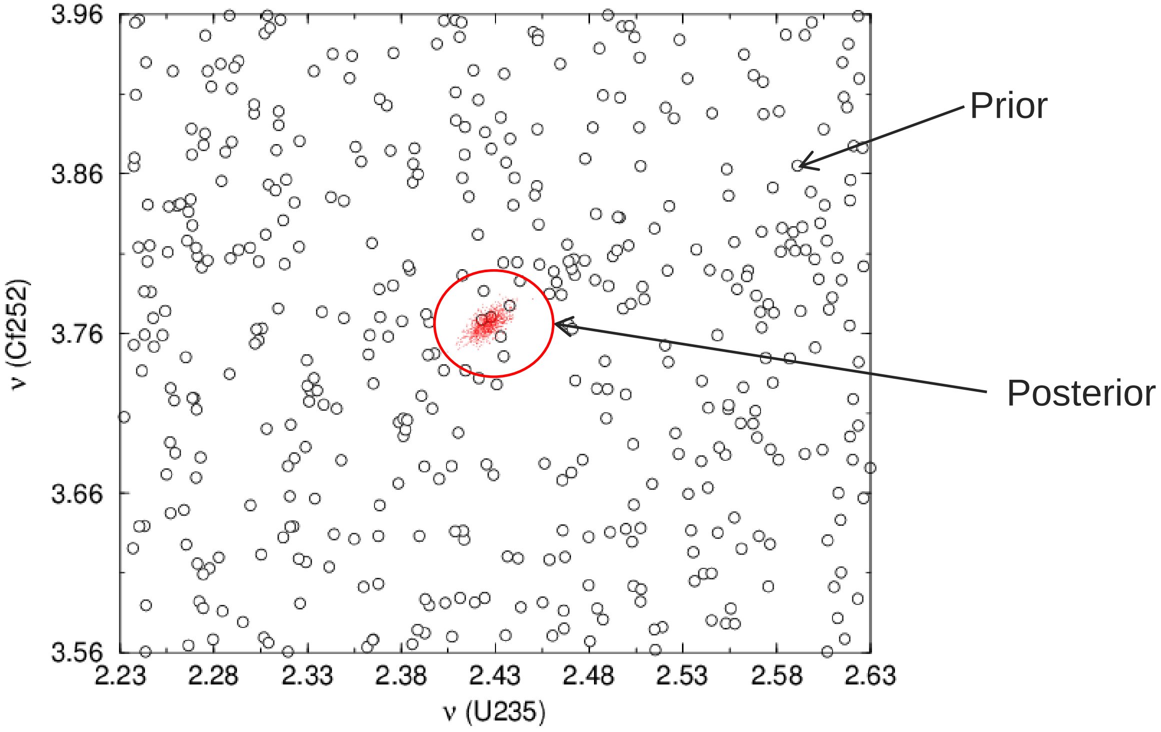
Impact of these types of biases ranges from 0.5% to 4% depending of the TNC

⇒ Provide a lower uncertainty limit (included in the CONRAD analysis)

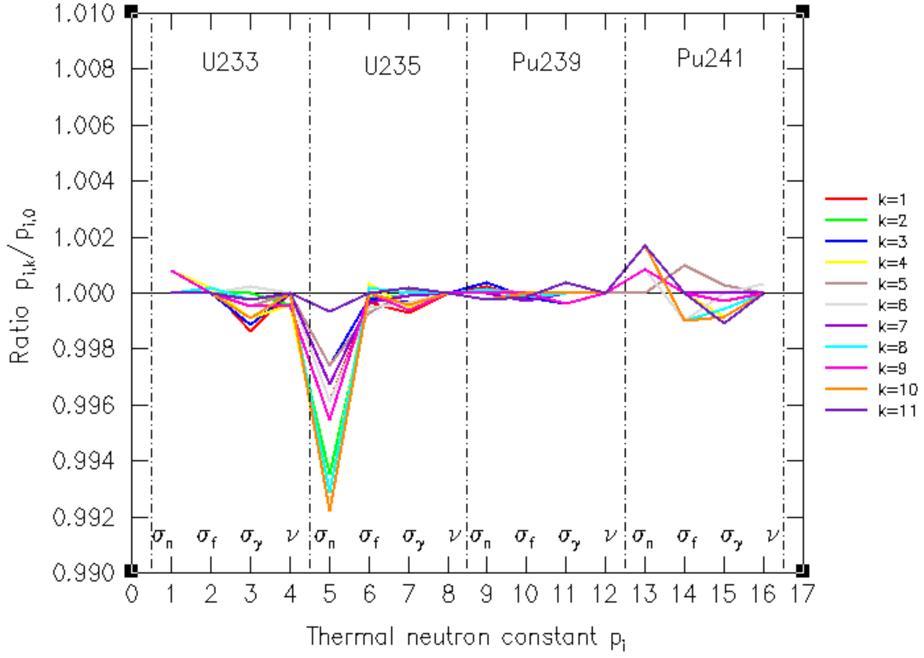
⇒ **Should we consider these sources of biases in GMAPY ?**

Input for TNC evaluation : prior uncertainties

Non-informative prior values were introduced in the fitting procedure (prior relative uncertainties of 100%, uniform sampling of the priors)



Example of dispersion of the Monte-Carlo results for N=1000 iterations



Reliable posterior correlation between the U235 and Cf252 neutron multiplicities (red dot) obtained after a Monte-Carlo data assimilation procedure by randomly choosing the prior values (open circle).

Input for TNC evaluation : AGS/IDC data format

Number of correlated uncertainties

Uncorrelated uncertainties

```
[/Spectrum]
 Energy          =   0
 Uncertainty     =   1
 Sensitivity     =  64
 NumberOfIter    =   3
 Values          =
```

" ^ 0.100000E+01	0.222757E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.169106E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.137858E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.120000E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.920000E-03	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
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0.100000E+01	0.142800E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.295700E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.139100E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.359000E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
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0.100000E+01	0.359000E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.208900E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.127100E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.297800E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.136900E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.300200E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.726600E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.234400E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
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0.100000E+01	0.348300E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.799900E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.989900E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.409900E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.511000E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.360500E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.289600E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.143300E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.568600E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.499600E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.787400E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.440900E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.124900E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.216500E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.306703E-02	0.207000E-02	0.232000E-02	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.228567E-02	0.207000E-02	0.232000E-02	0.185000E-02	0.000000E+00	0.000000E+00
0.100000E+01	0.130453E-01	0.000000E+00	0.232000E-02	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.925081E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.122500E-01	0.000000E+00
0.100000E+01	0.121974E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.122500E-01	0.000000E+00
0.100000E+01	0.721334E-02	0.000000E+00	0.000000E+00	0.300000E-02	0.000000E+00	0.000000E+00
0.100000E+01	0.329960E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.309100E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.284030E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.599900E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
0.100000E+01	0.104862E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.100000E-01
0.100000E+01	0.990871E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	-0.200000E-01

« sparse » matrix

Example GMA format

```
BLCK     0    0
DATA  8050    1    0    1   10    0    0    0
 2016    1    0 P.Salvador-Casti~neira,F.-J       .Hambsch ND2016
  0.7  0.5  2.6  0.5  1.0  0.0  0.0  0.0  0.0  0.0  1  1  1  1  2  2  2  0  0  0
 0.00 0.00 0.00  0
 0.00 0.00 0.00  0
 0.00 0.00 0.00  9
 0.50 0.50 0.50  9
 0.50 0.50 0.50  1
 0.50 0.50 0.50  2
 0.50 0.50 0.50  2
 0.50 0.50 0.50  2
 0.50 0.50 0.50  0
 0.50 0.50 0.50  0
 0.00 0.00 0.00  1
0.1800E+010.4952E+00  0.0  0.0  2.5  0.8  0.4  0.3  0.0  0.0  0.0  0.0  0.0  0.0
0.2000E+010.5451E+00  0.0  0.0  2.5  0.8  0.4  0.3  0.0  0.0  0.0  0.0  0.0  0.0
0.2400E+010.5600E+00  0.0  0.0  2.5  0.8  0.4  0.3  0.0  0.0  0.0  0.0  0.0  0.0
0.0000E+000.0000E+00  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
EDBL     0    0
```

Same uncertainty format in GMA data base

$$C = SS^T + D$$

Questions

- TNC evaluation should be considered as an independent work and not included in a fitting procedure that combines the full GMA database ?
- Should we replace Axton data by EXFOR data ?
- Should we take data reported by Sjostrand which are not included in the Axton report ?
- Which Half-live values should we adopt?
- Which USU value for ν_{tot}(Cf252) should we adopt?
- Should we consider "evaluator dependent biases" in GMAPY ?
- Use non-informative prior values and uncertainties in GMAPY ?
- Determine I1 and I3 directly in the evaluation procedure with GMAPY ?
- …