European Commission

Description and usage of experimental data for evaluation in the resolved resonance region

SG - 36

Objective

Produce accurate cross section data together with reliable covariance information in the resonance region

$\Rightarrow$ **Reduce bias effects**

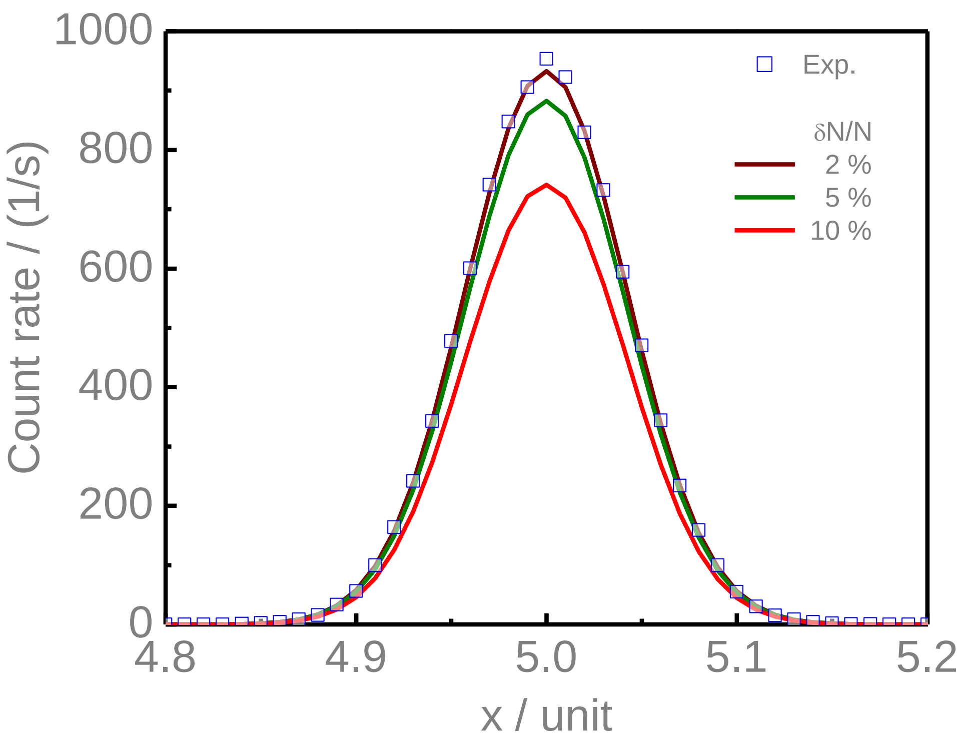
$\Rightarrow$ **Produce reliable and realistic covariance data**

IRMM contribution

- **Problems with PPP**
- **Uncertainty components of experimental data (IRMM, INFN Bari)**
  - **Transmission**
  - **Capture**
- **Evaluation models (IRMM, CEA Cadarache)**
- **Case studies**
- **Reporting data**
  - **Reporting response functions of TOF-spectrometers (IRMM, IAEA)**
  - **Reporting experimental data (IRMM, IAEA)**

Model parameters from experimental data
a) reaction experiment

$$Z_{exp} = N\,C_{exp} \qquad V_{Z_{exp}}(\delta C_{exp}, \delta N)$$



shape is not affected

$$\chi^2(\vartheta) = (Z_{exp} - F_m(x,\theta))^T\, V_{Z,exp}^{-1}\, (Z_{exp} - F_m(x,\theta))$$

$$\frac{\delta N}{N} = 2\%$$

A	=	98.9	(1.98)
x_o	=	5	(0.00013)
σ^2	=	0.00180	(0.0000080)

$$\frac{\delta N}{N} = 5\%$$

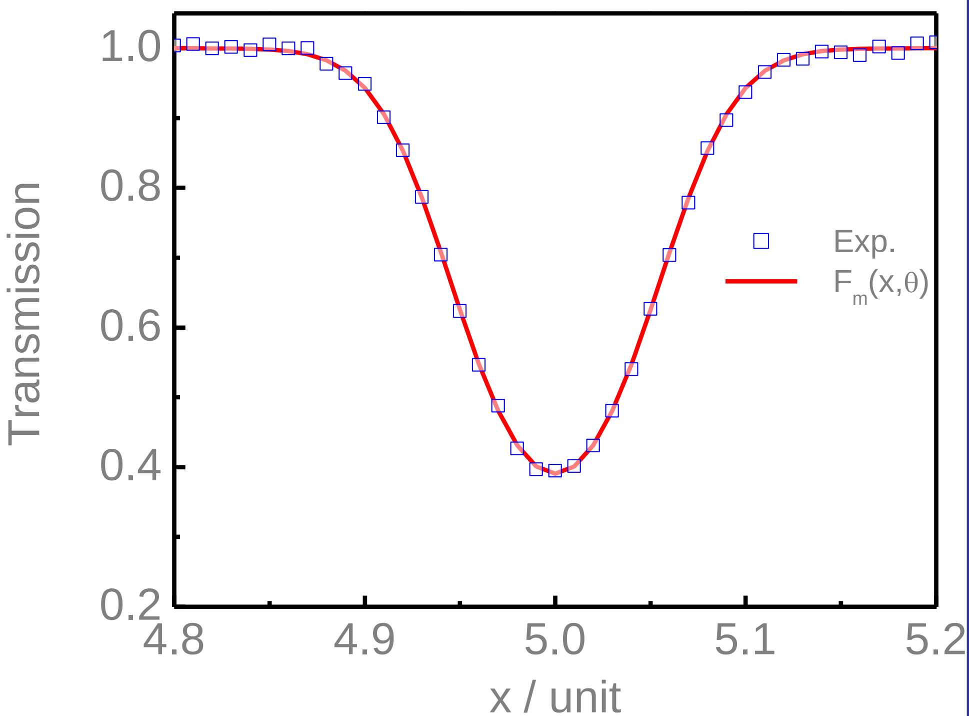
A	=	93.62	(4.85)
x_o	=	5	(0.00014)
σ^2	=	0.00179	(0.0000084)

$$\frac{\delta N}{N} = 10\%$$

A	=	78.60	(8.87)
x_o	=	5	(0.00017)
σ^2	=	0.00179	(0.000010)

Model parameters from experimental data
b) transmission experiment

$T_{exp} = N\,C_{exp}$ $V_{Z_{exp}}(\delta C_{exp}, \delta N)$



$$\chi^2(\vartheta) = (T_{exp} - F_m(x,\theta))^T\, V_{Z,exp}^{-1}\, (T_{exp} - F_m(x,\theta))$$

$$\frac{\delta N}{N} = 10\%$$

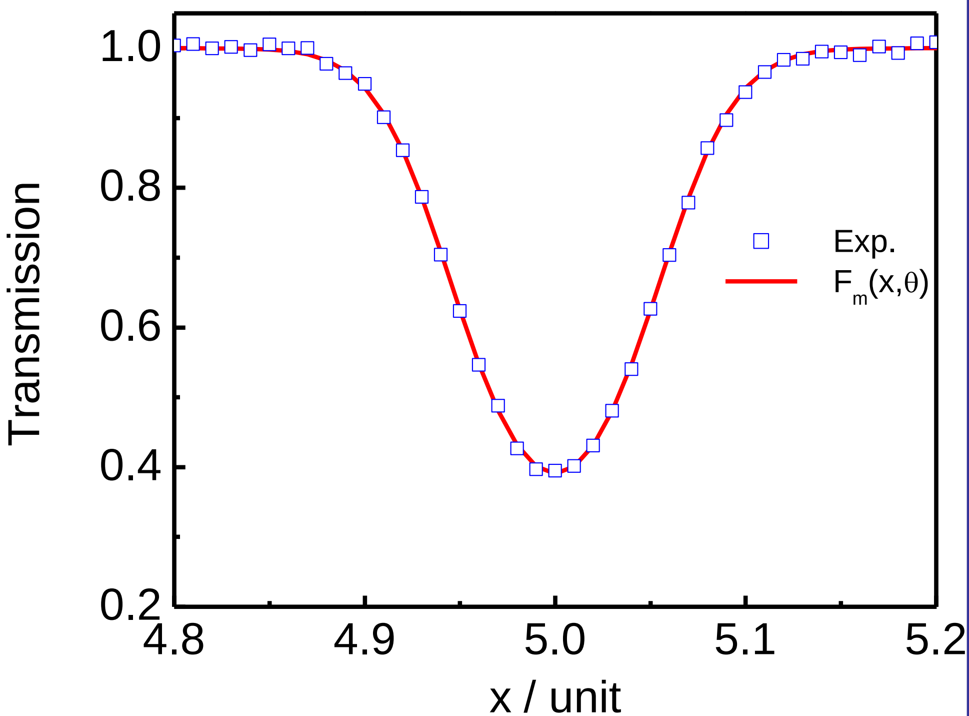
A	=	100	(0.63)	1	0	0.41
x_o	=	5	(0.00030)	0	1	0
σ^2	=	0.0018	(0.000024)	0.41	0	1

only counting statistics

A	=	100	(0.61)	1	0	0.38
x_o	=	5	(0.00030)	0	1	0
σ^2	=	0.0018	(0.000024)	0.38	0	1

Model parameters from experimental data
b) transmission experiment

$$T_{exp} = B + C_{exp} \qquad V_{Z_{exp}}(\delta C_{exp}, \delta B)$$



$$\chi^2(\vartheta) = (T_{exp} - F_m(x,\theta))^T \, V_{Z,exp}^{-1} \, (T_{exp} - F_m(x,\theta))$$

$$\frac{\delta B}{B} = 10\% \qquad \frac{B}{P} = \frac{1}{2}$$

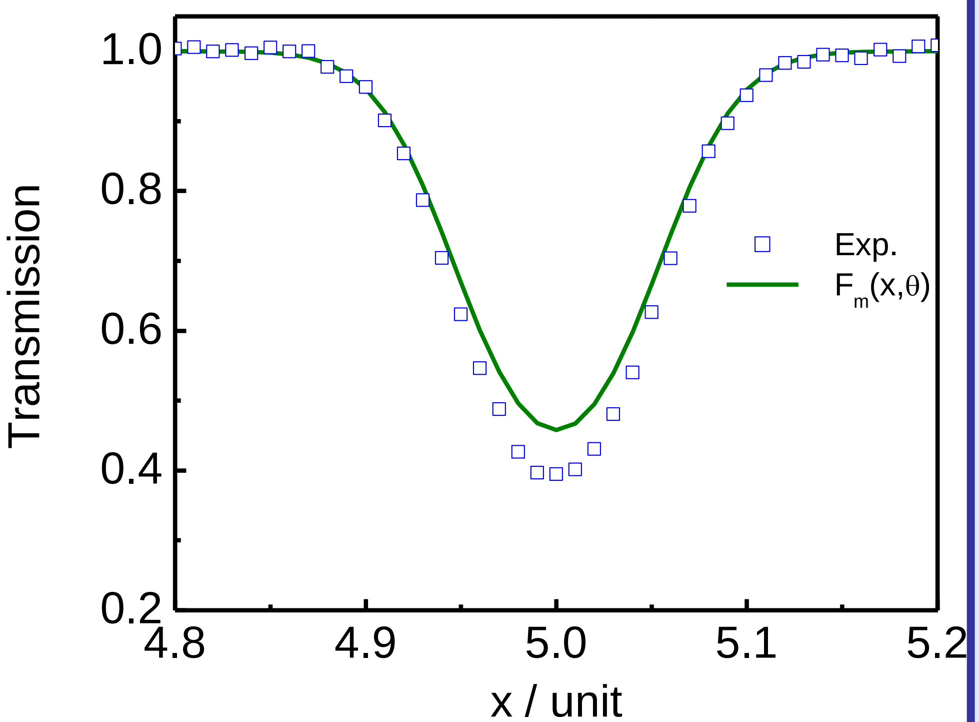
A	=	100	(0.66)	1	0	0.41
x_o	=	5	(0.00030)	0	1	0
σ^2	=	0.0018	(0.000024)	0.41	0	1

only counting statistics

A	=	100	(0.61)	1	0	0.38
x_o	=	5	(0.00030)	0	1	0
σ^2	=	0.0018	(0.000024)	0.38	0	1

Model parameters from experimental data
b) transmission experiment

$T_{exp} = B + N\,C_{exp}$ $\qquad V_{Z_{exp}}(\delta C_{exp}, \delta B, \delta N)$



$$\chi^2(\vartheta) = (T_{exp} - F_m(x,\theta))^T\, V_{Z,exp}^{-1}\, (T_{exp} - F_m(x,\theta))$$

$$\frac{\delta N}{N} = 10\% \qquad \frac{\delta B}{B} = 10\% \qquad \frac{B}{P} = \frac{1}{2}$$

A	=	85.0	(5.2)	1	0	−0.61
x_o	=	5	(0.00034)	0	1	0
σ^2	=	0.0018	(0.00038)	−0.61	0	1

only counting statistics

A	=	100	(0.61)	1	0	0.38
x_o	=	5	(0.00030)	0	1	0
σ^2	=	0.0018	(0.000024)	0.38	0	1

Solution : include N in adjustment procedure

Zhao & Perey ORNL/TM-12106

D'Agostini, NIM A346 (1994) 306

Fröhner, NSE 126 (1997) 1 - 18

Conclusion

$$(Z_{exp}, V_Z) \text{ and } (\kappa, V_\kappa) \Rightarrow (\eta, V_\eta) \Rightarrow (\sigma, V_\sigma)$$

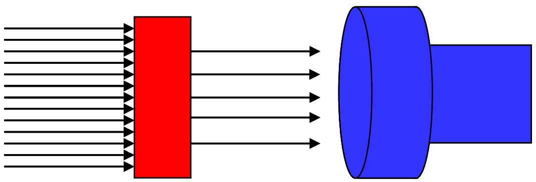
To deduce unbiased resonance parameters and cross section data with reliable covariances, (η, V_η) , we need:

- **a detailed understanding of the experiment (unbiased Z_{exp})**
- **covariance of the experimental observables (V_Z)**
- **to report all parameters involved in the measurement, data reduction and analysis process: (κ, V_κ)**
- **resonance shape analysis codes accounting for experimental conditions**

Uncertainty components of experimental observables

Transmission

$$T_m \propto e^{-n_X \sigma_{tot}}$$

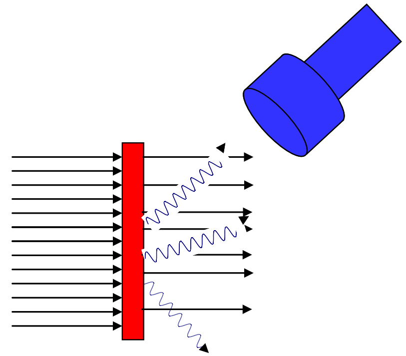


$$T_{exp} = N \frac{C'_{in} - B'_{in}}{C'_{out} - B'_{out}}$$

$$\frac{\delta N}{N} \approx 0.5\% \qquad \frac{\delta B_{out}}{B_{out}} \approx 5\% \qquad \frac{\delta B_{in}}{B_{in}} \approx 5-10\%$$

Reaction cross section

$$Y_m \propto \frac{\sigma_r}{\sigma_{tot}}(1-e^{-n_x \sigma_{tot}}) + \dots$$



$$C = \varepsilon_r \, \Omega_r \, F_r \, Y_r \, A_r \, \varphi$$

$$Y_{exp} = N \frac{\sigma_\varphi}{\varepsilon_r} \frac{C'_r - B'_r}{C'_\varphi - B'_\varphi}$$

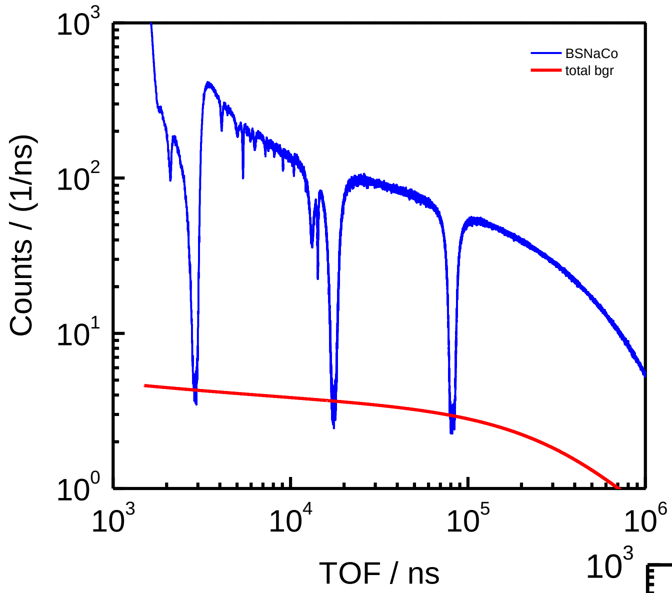
$$\frac{\delta N}{N} \approx 2\% \qquad \frac{\delta B_\varphi}{B_\varphi} \approx 5\% \qquad \frac{\delta B_r}{B_r} \approx 5-10\%$$

Ideal conditions + experimental verification of uncertainties (IRMM, INFN)

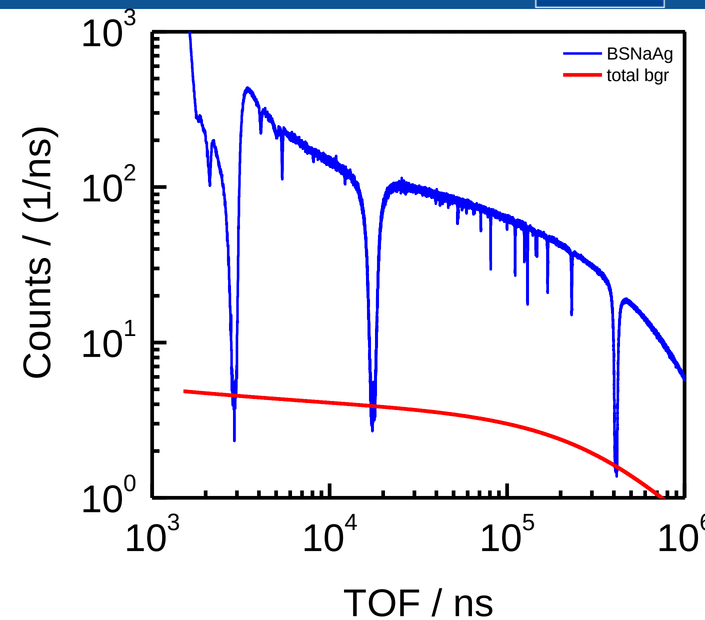
Capture: Borella et al., NIMA 577 (2007) 626

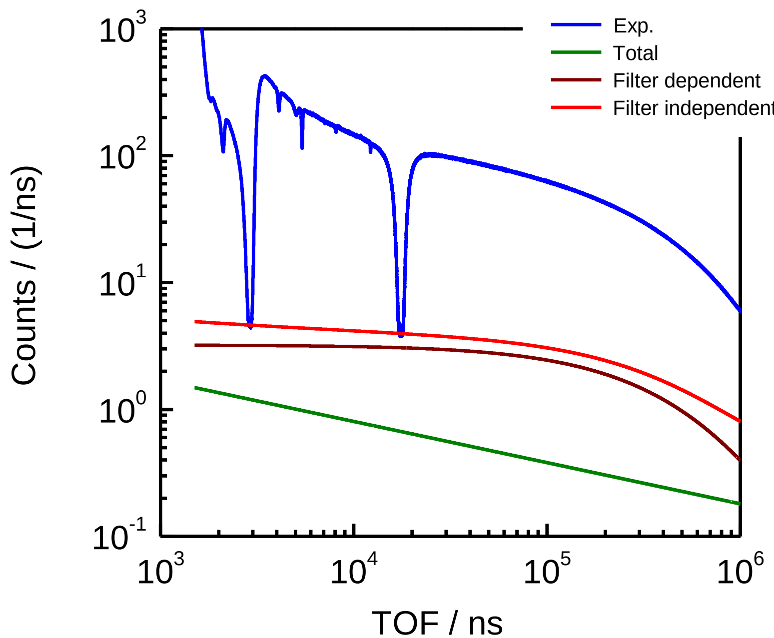
Massimi et al., in preparation

Flux : background



$$C'_{\varphi} - B'_{\varphi}$$





Use of fixed background filters

$\Rightarrow \delta B'_{\varphi} / B'_{\varphi} \leq 3\%$

with

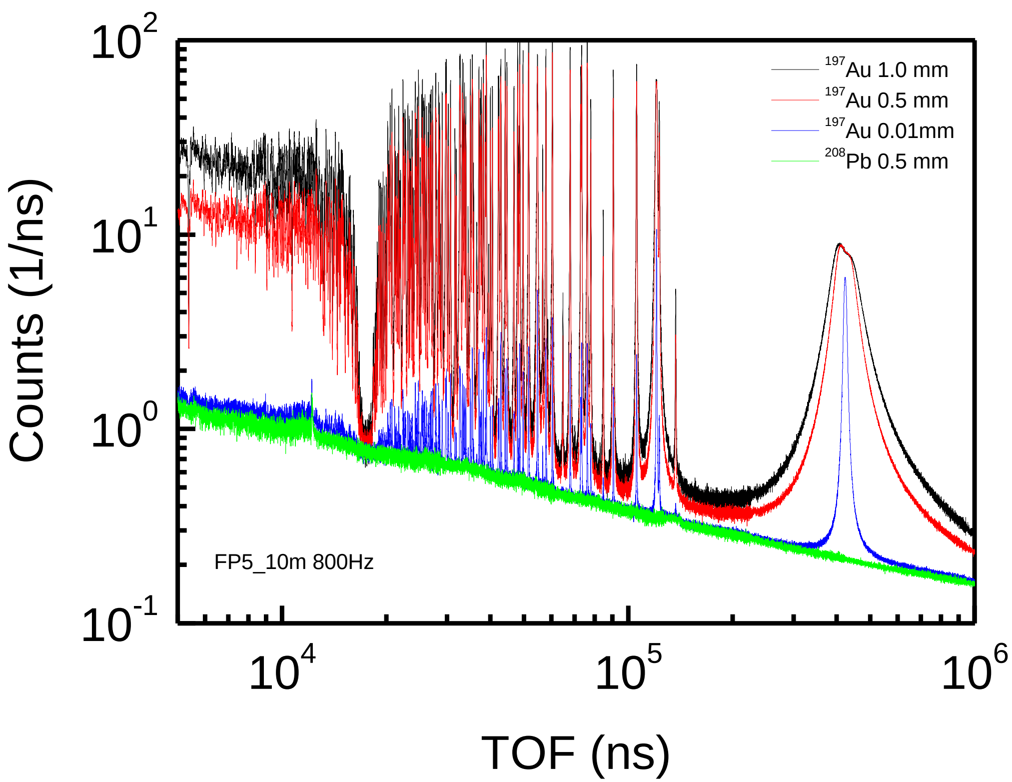
$B'_{\varphi} / C'_{\varphi} \leq 7\%$ at 5 eV

$\leq 4\%$ in URR

Capture : background e.g. $^{197}Au(n,\gamma)$

$$B_c(t) = b_0 + B_1(t) + B_2(t)$$

b_0 : ambient (or activity)
B_1 : sample independent   without sample
B_2 : sample dependent   n and γ-scattering

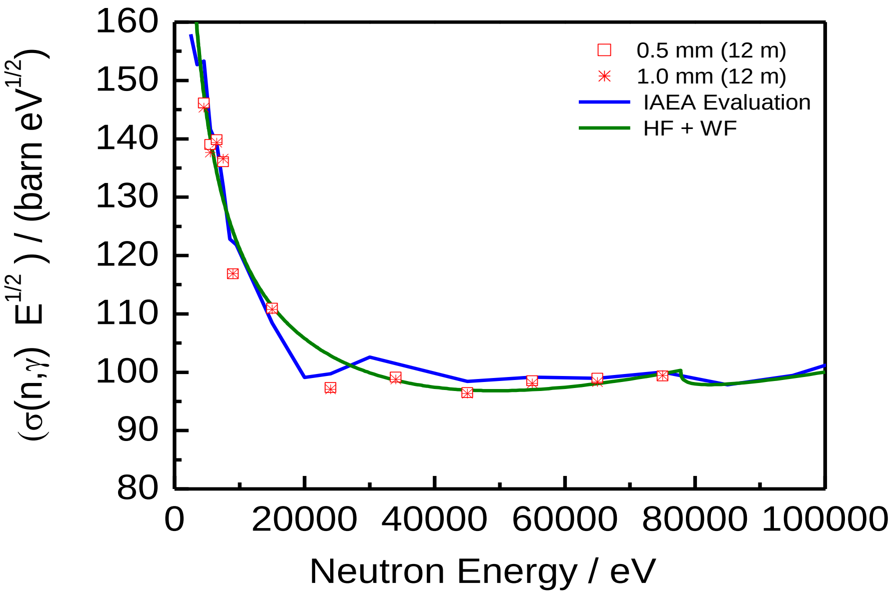


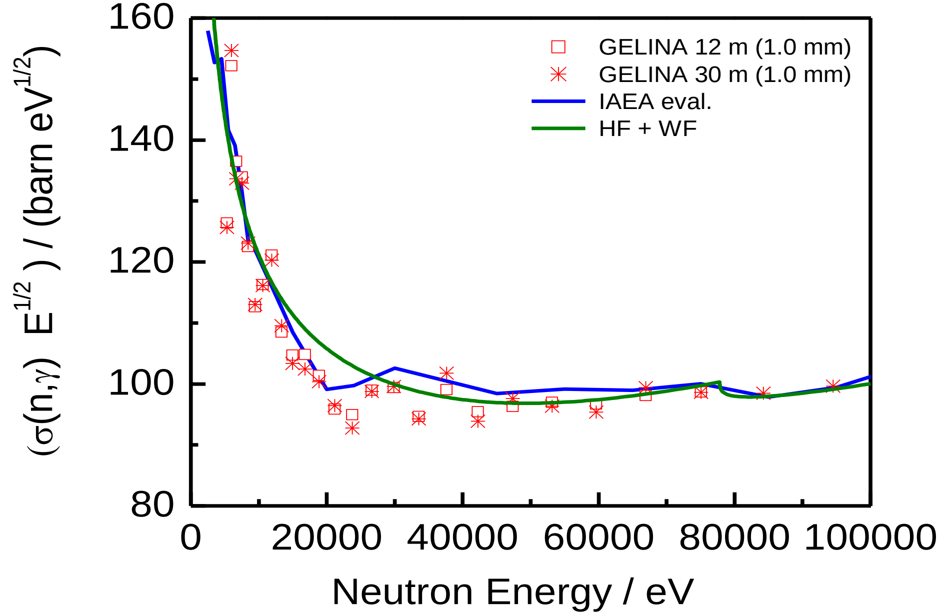
Use of fixed background filters
$\Rightarrow \delta B_c / B_c \leq 5$ %
with
B_c / C_c ≤ 2.5 % at 5 eV
≤ 10% in URR (0.5 mm)

GELINA : (n,γ) methodology ⇒ 1.5%

Borella et al., NIMA 577 (2007) 626

- Total energy principle: C_6D_6 with weighting functions
- Weighting functions which account for the threshold
- Verify experimentally the effect of WF and threshold
- Correction for γ-ray attenuation in the sample
- Use fixed background filters
- Perform background measurements with additional filters
- Perform additional background measurements with Pb
- Determine neutron flux with a double ionization chamber 2 thin layers of ^{10}B
- Normalization at a saturated resonance (account for gamma-ray attenuation)





Model parameters from fitting exp. data

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LSQ adjustment or Maximum Likelihood (Max. Entropy)

$$\text{minimize} \quad \chi^2(\vec{\theta}) = (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))^T \, V^{-1}_{\vec{z}_{exp}} \, (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))$$

$$\vec{z}_m = f(\vec{\theta}) \qquad \vec{\theta} = (\vec{\eta}, \vec{\kappa}) \begin{cases} \vec{\eta} : \text{theoretical model parameters} \\ \vec{\kappa} : \text{experimental parameters} \end{cases}$$

$$\vec{\theta} = (\underline{G}^T_{\vec{\theta}} \underline{V}^{-1}_{\vec{z}_{exp}} \underline{G}_{\vec{\theta}})^{-1} (\underline{G}^T_{\vec{\theta}} \, \underline{V}^{-1}_{\vec{z}_{exp}} \, \vec{z}_{exp})$$

$$\underline{V}_{\vec{\theta}} = (\underline{G}^T_{\vec{\theta}} \underline{V}^{-1}_{\vec{z}_{exp}} \, \underline{G}_{\vec{\theta}})^{-1}$$

(linear model)

Note on LSQ adjustment

Include all model parameters in adjustment procedure Fröhner, NSE 126 (1997) 1 – 18

is a full Bayesian approach $\vec{z}_{exp} = (Z_{exp}(t), \vec{\theta})$

$$\chi^2(\vec{\theta}) = (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))^T \, V_{\vec{z}_{exp}}^{-1} \, (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))$$

$$\vec{\theta} = (\underline{G}_{\vec{\theta}}^T \underline{V}_{\vec{z}_{exp}}^{-1} \underline{G}_{\vec{\theta}})^{-1} (\underline{G}_{\vec{\theta}}^T \underline{V}_{\vec{z}_{exp}}^{-1} \vec{z}_{exp})$$

$$\underline{V}_{\vec{\theta}} = (\underline{G}_{\vec{\theta}}^T \underline{V}_{\vec{z}_{exp}}^{-1} \underline{G}_{\vec{\theta}})^{-1}$$

The equations

$$\vec{\theta} = \vec{\theta}_o + V_{\vec{o}} \, \underline{G}_{\vec{\theta}}^T \, (\underline{G}_{\vec{\theta}} \, V_{\vec{o}} \, \underline{G}_{\vec{\theta}}^T + \underline{V})^{-1} (\vec{z} - \vec{z}_m(\vec{\theta}_o))$$

Linear model

$$\underline{V}_{\vec{\theta}} = V_{\vec{o}} - V_{\vec{o}} \, \underline{G}_{\vec{\theta}}^T (\underline{G}_{\vec{\theta}} \, V_{\vec{o}} \, \underline{G}_{\vec{\theta}}^T + \underline{V})^{-1} \underline{G}_{\vec{\theta}} \, V_{\vec{o}}$$

with $(\vec{\theta}_o, V_o)$ **the prior information (parameters + covariance)**

are only valid when the prior and the new data are not correlated

Accounting for experimental parameters

European Commission

LSQ adjustment or Maximum Likelihood (Max. Entropy)

$$\chi^2(\vec{\theta}) = (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))^T \, V_{\vec{z}_{exp}}^{-1} \, (\vec{z}_{exp} - \vec{z}_m(\vec{\theta}))$$

$$\vec{z}_m = f(\vec{\theta})$$

$$\vec{\theta} = (\vec{\eta}, \vec{\kappa}) \begin{cases} \vec{\eta} : \text{theoretical model parameters} \\ \vec{\kappa} : \text{experimental parameters} \end{cases}$$

$$\vec{\theta} = (\underline{G}_{\vec{\theta}}^T \underline{V}_{\vec{z}_{exp}}^{-1} \underline{G}_{\vec{\theta}})^{-1} (\underline{G}_{\vec{\theta}}^T \, \underline{V}_{\vec{z}_{exp}}^{-1} \, \vec{z}_{exp})$$

$$\underline{V}_{\vec{\theta}} = (\underline{G}_{\vec{\theta}}^T \underline{V}_{\vec{z}_{exp}}^{-1} \, \underline{G}_{\vec{\theta}})^{-1}$$

(linear model)

Methods to account for all uncertainty components and avoid PPP

- **Include all model parameters in adjustment procedure** Fröhner, NSE 126 (1997) 1 – 18
- **Monte Carlo** De Saint Jean et al., NSE 161 (2009) 363 - 370
- **Marginalization** Habert et al., NSE 166 (2010) 276 - 287

Differ in the way the uncertainty of experimental parameters are taken into account

⇒ At IRMM all tools available

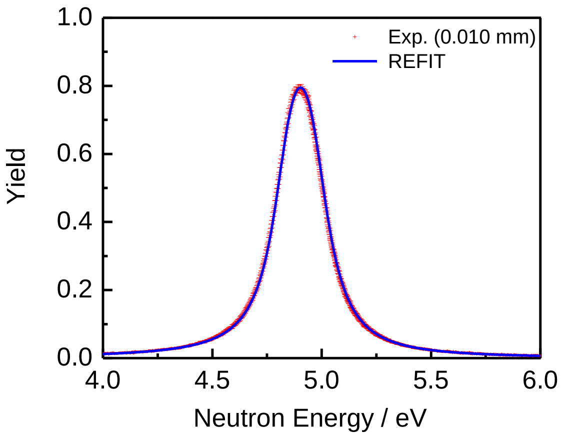
Experimental parameters κ

- **Non-model parameters (data reduction)**
  - **Dead time**
  - **Background**
  - **Normalization *(can also be considered as model parameter)***
- **Model parameters (RSA)**
  - **Target characteristics**
    - **Thin targets (fission studies, flux measurements)**
    - **Thick targets (transmission and capture)**

      Study particle size ongoing at IRMM (report 2013, IRMM, JAEA)
  - **Multiple collision models**
    - **Models (see meeting 2011)**

      Report in preparation (Becker et al., CEA, IRMM, KIT, RPI)
  - **Doppler**
    - **Temperature ($\Delta T \sim 5\ ^{o}C$)**
    - **Model**
  - **TOF - response function**

Comparison 3 methods : 4.9 eV $^{197}Au(n,\gamma)$

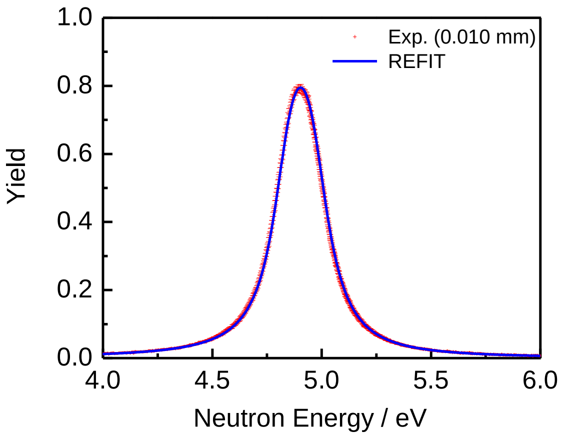


E = 4.9 eV
Γ_γ = 122 meV
Γ_n = 15 meV

	Sample thickness : 0.01 mm		
Peak uncertainty (counting statistics)	0.1 %	1 %	10 %
	Fit -all	Fit -all	Fit -all
E	0.0	0.0	0.0
Γ_γ	0.1	1.0	2.5
Γ_n	0.2	1.5	3.1
N (2%)	0.1	1.0	1.9

Relative uncertainty in %

Comparison 3 methods : 4.9 eV $^{197}Au(n,\gamma)$



	Peak uncertainty (counting statistics) : 1%					
Sample thickness	0.001 mm			0.01 mm		
	Fit -all	MC	Marg.	Fit -all	MC	Marg.
E	0.0	0.0	0.0	0.0	0.0	0.0
Γ_γ	0.4	0.4	0.5	1.0	2.3	2.7
Γ_n	2.3	2.3	2.3	1.5	3.9	4.0
N (2%)	2.0			1.0		

$E = 4.9$ eV
$\Gamma_\gamma = 122$ meV
$\Gamma_n = 15$ meV

Relative uncertainty in %

^{113}Cd+n : 0.179 eV (IRMM – CEA Cadarache)

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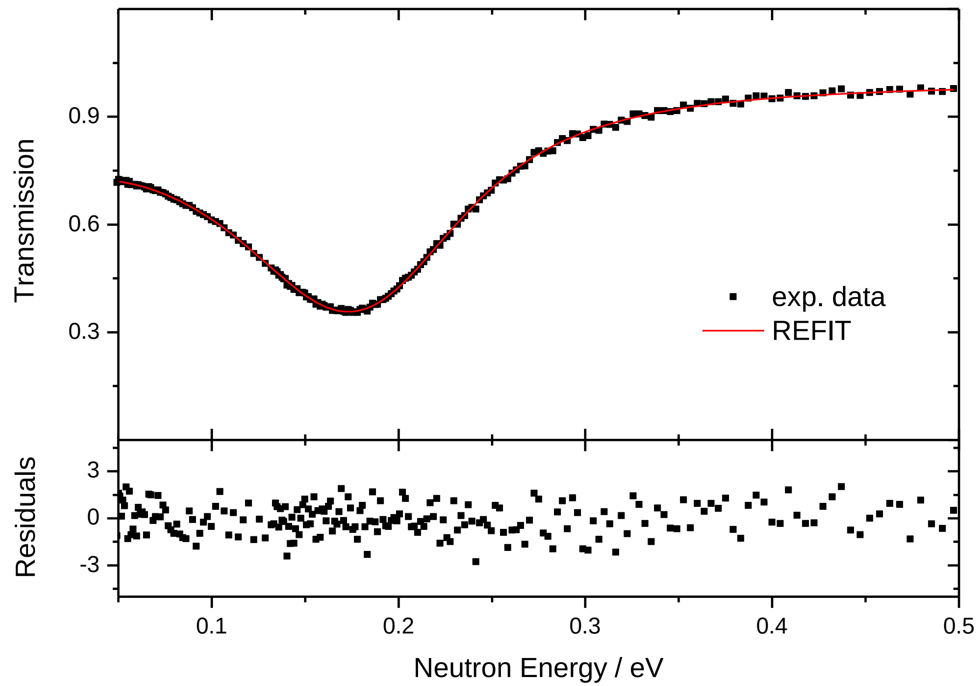
Experiment ⇒ Data reduction with AGS ⇒ REFIT + GLUP

Thin – Thick transmission
($1.36 10^{-4}$ – $2.24 10^{-4}$ at/b)
Metal discs

$\ell = 0$ J =1 $\chi^2 = 0.98$

$\ell = 0$ J =0 $\chi^2 = 1.30$

Parameter	p / meV			ρ(p_i,p_j)	
E_R	178.7	± 0.1	1.00	0.53	0.28
Γ_γ	113.5	± 0.2		1.00	0.26
Γ_n	0.640	± 0.004			1.00



$\Delta_D \sim 20$ meV
$\Delta_R \sim 0.2$ meV (L = 50 m)

Kopecky et al., NIMB 267 (2009) 2345 - 2350

^{113}Cd : uncorrelated uncertainty components

(REFIT – SAMMY – Monte Carlo)

REFIT + GLUP (numerical derivatives)

Parameter	p / meV		ρ(p_i,p_j)		
E_R	178.7	± 0.068	1.00	0.43	0.79
Γ_γ	113.5	± 0.15		1.00	0.43
Γ_n	0.640	± 0.0007			1.00

SAMMY + GLUP (analytical derivatives)

Parameter	p / meV		ρ(p_i,p_j)		
E_R	178.7	± 0.098	1.00	0.45	0.80
Γ_γ	113.5	± 0.19		1.00	0.43
Γ_n	0.640	± 0.0010			1.00

Monte Carlo (CEA Cadarache)

Parameter	p / meV		ρ(p_i,p_j)		
E_R	178.7	± 0.099	1.00	0.38	0.63
Γ_γ	113.5	± 0.27		1.00	0.65
Γ_n	0.640	± 0.0010			1.00

^{113}Cd : + correlated uncertainty components
(REFIT – SAMMY – Monte Carlo)

REFIT

$$T_m(t) \approx \frac{e^{-n\,\sigma_{tot}}}{N}$$

Parameter	δp_{ini}	p	δp	$\rho(p_i,p_j)$: E_R	Γ_γ	Γ_n	L	n	T_D	N
E_R / meV	-	178.7	± 0.074	1.00	0.53	0.28	0.13	0.00	0.00	-0.34
Γ_γ / meV	-	113.5	± 0.22		1.00	0.26	0.20	0.02	-0.04	-0.70
Γ_n / meV	-	0.640	± 0.0036			1.00	0.11	-0.91	-0.00	-0.28
L / m	0.006	26.4439	± 0.006				1.00	-0.00	0.01	-0.09
n / (at/b)	0.5 %		± 0.5 %					1.00	0.00	-0.00
T_D / meV	0.5 %	25.46	± 0.5 %						1.00	0.00
N (norm)	0.5 %	1.000	± 0.0013							1.00

SAMMY

$$T_m(t) \approx N e^{-n\,\sigma_{tot}}$$

Parameter	δp_{ini}	p	δp	$\rho(p_i,p_j)$: E_R	Γ_γ	Γ_n	L	n	T_D	N
E_R / meV	-	178.7	± 0.098	1.00	0.60	0.43	0.35	0.00	0.02	0.09
Γ_γ / meV	-	113.5	± 0.26		1.00	0.38	0.17	0.01	-0.04	0.51
Γ_n / meV	-	0.640	± 0.0039			1.00	0.13	-0.85	0.00	0.29
L / m	0.006	26.4439	± 0.006				1.00	0.00	0.00	0.00
n / (at/b)	0.5 %	$1.360\ 10^{-4}$	± 0.5 %					1.00	0.00	0.00
T_D / meV	0.5 %	25.46	± 0.5 %						1.00	0.00
N (norm)	0.5 %	1.000	± 0.0007							1.00

^{113}Cd : + correlated uncertainty components

(REFIT – SAMMY – Monte Carlo)

REFIT

$$T_m(t) \approx \frac{e^{-n\,\sigma_{tot}}}{N}$$

Parameter	δp_{ini}	p	δp	$\rho(p_i,p_j)$: E_R	Γ_γ	Γ_n	L	n	T_D	N
E_R / meV	-	178.7	± 0.074	1.00	0.53	0.28	0.13	0.00	0.00	-0.34
Γ_γ / meV	-	113.5	± 0.22		1.00	0.26	0.20	0.02	-0.04	-0.70
Γ_n / meV	-	0.640	± 0.0036			1.00	0.11	-0.91	-0.00	-0.28
L / m	0.006	26.4439	± 0.006				1.00	-0.00	0.01	-0.09
n / (at/b)	0.5 %		± 0.5 %					1.00	0.00	-0.00
T_D / meV	0.5 %	25.46	± 0.5 %						1.00	0.00
N (norm)	0.5 %	1.000	± 0.0013							1.00

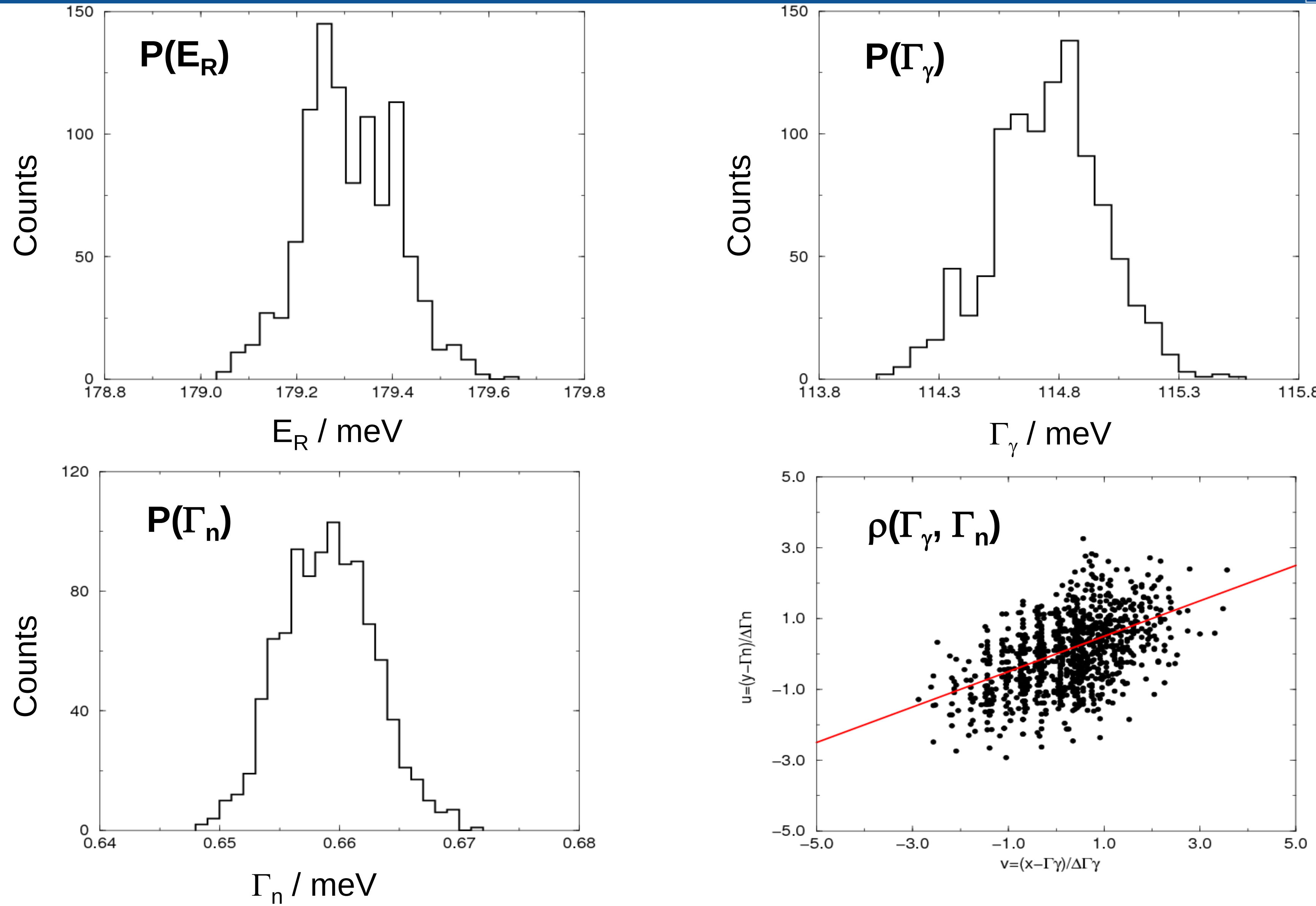
Monte Carlo (+ REFIT)

$$T_m(t) \approx \frac{e^{-n\,\sigma_{tot}}}{N}$$

Parameter	δp_{ini}	p	δp	$\rho(p_i,p_j)$: E_R	Γ_γ	Γ_n	L	n	T_D	N
E_R / meV	-	178.7	± 0.140	1.00	0.50	0.36	0.59	0.02	0.00	-0.31
Γ_γ / meV	-	113.5	± 0.36		1.00	0.45	0.17	0.04	-0.02	-0.63
Γ_n / meV	-	0.640	± 0.0040			1.00	0.15	-0.80	0.04	-0.47
L / m	0.006	26.4439	± 0.006				1.00	0.02	-0.04	-0.05
n / (at/b)	0.5 %	$1.360\ 10^{-4}$	± 0.5 %					1.00	-0.04	-0.04
T_D / meV	0.5 %	25.46	± 0.5 %						1.00	-0.03
N (norm)	0.005	1.000	± 0.0013							1.00

^{113}Cd : Monte Carlo simulations

(full transformation of variables)



Case studies : experimental data base created

- **Resonance parameters**
- T_{exp} = 0.1, 0.5 and 0.9
  Y_{exp} = 10^{-4}, 0.3 and 0.9
- **counting statistics uncertainty**
  - 0.1, 1.0, 10% in peak (or baseline)
- **Experimental parameters**
  - Data reduction (GELINA)
    - Dead time
    - Background
  - Data analysis
    - normalization
    - $\Delta n/n$ = 0.2%
    - ΔT_{eff} = 5 K
    - Response function

E / eV	Γ_γ / meV	Γ_n / meV
10	10	10
1	100	100
100	1	100

With:

$(\Delta_D + \Delta_R) < \Gamma$

$(\Delta_D + \Delta_R) > \Gamma$