



*The Abdus Salam
International Centre for Theoretical Physics*



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**Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced
Reactor Technologies**

19 - 30 May 2008

Neutron Induced Cross Section Measurements.

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Neutron Induced Cross Section Measurements



Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

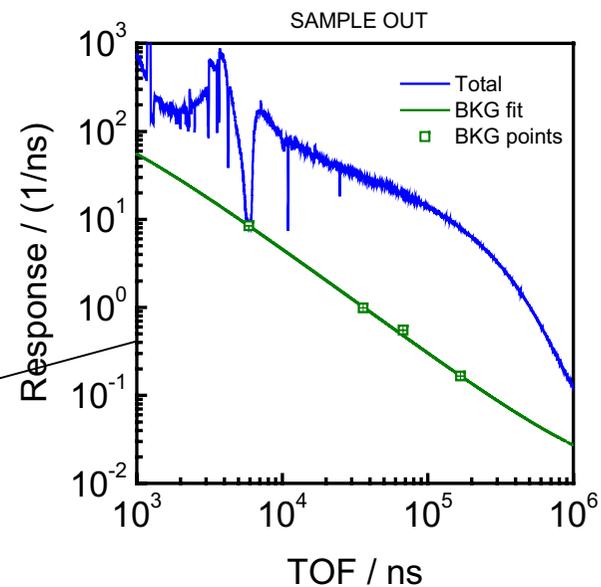
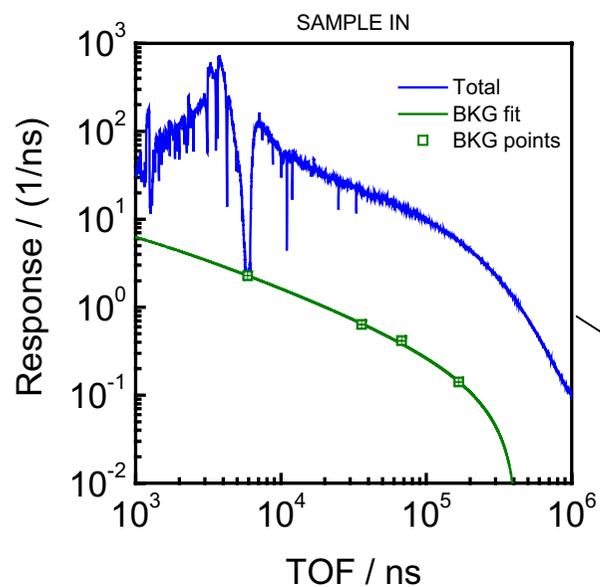
Trieste, Italy, 19 – 30 May 2008

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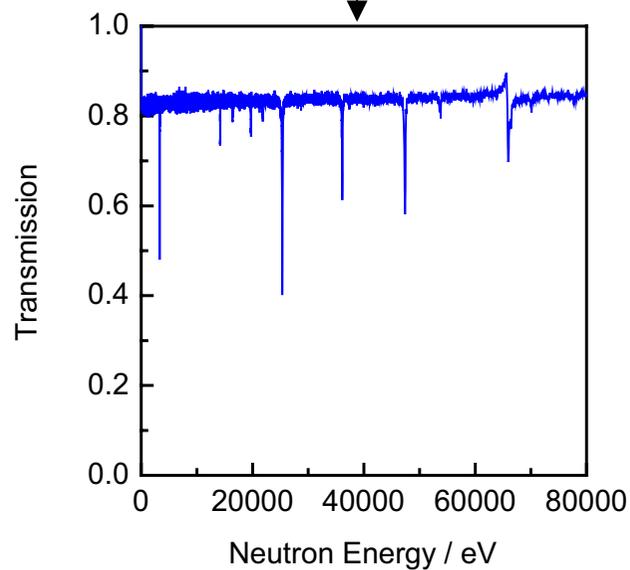
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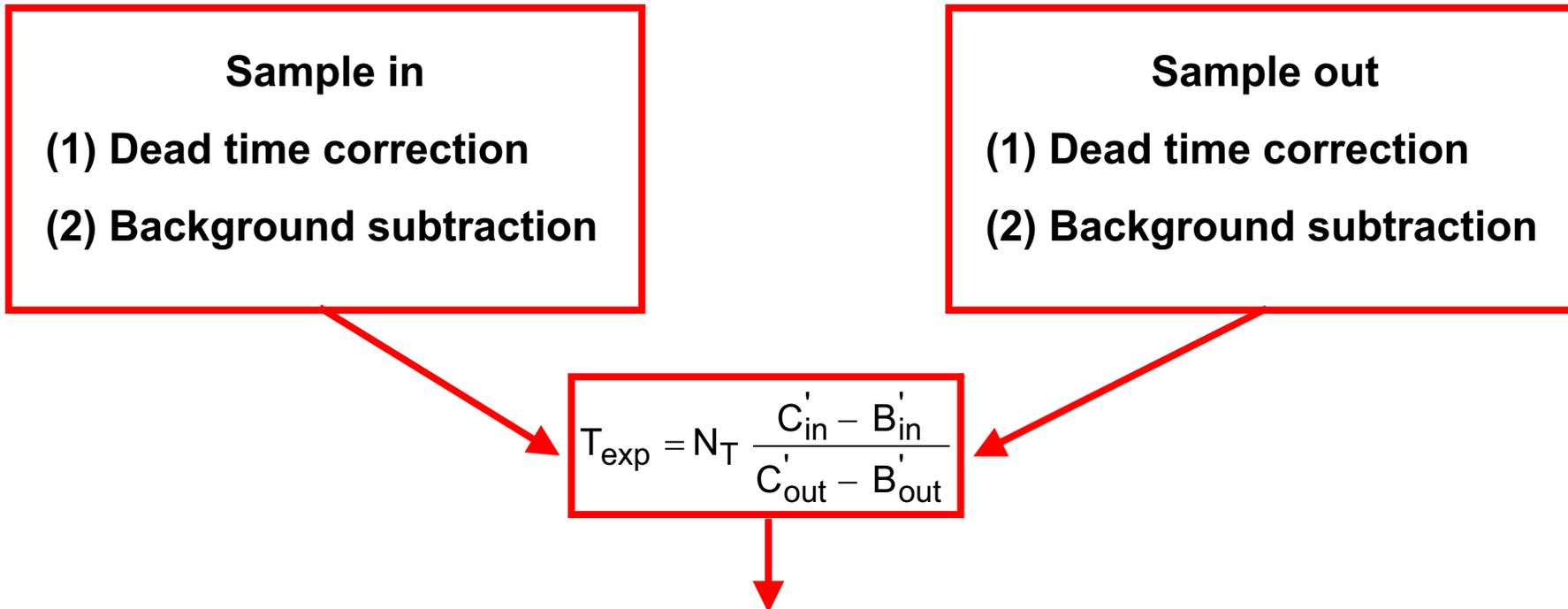
- **Neutron cross section measurements (Part 1)**
- **Data reduction and uncertainties (Part 2)**
 - Experimental observables
 - Definitions and terminology
 - Fitting a mathematical model to experimental data
 - Basic operations
 - AGS
 - Example
 - ISO Guide, “Guide to the expression of uncertainty in measurement”, Geneva, Switzerland, ISO, 1995
 - Mannhart, “A Small Guide to Generating Covariances of Experimental Data”, Juni 1981, PTB-FMRB-84
 - F.H. Fröhner, Nucl. Sci. Eng. 126 (1997) 1 -18

- **Experimental observables**
 - Transmission
 - Reaction yields
- **Definitions and terminology**
- **Fitting a mathematical model to data**
- **Basic operations**
- **AGS**
- **Examples**



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





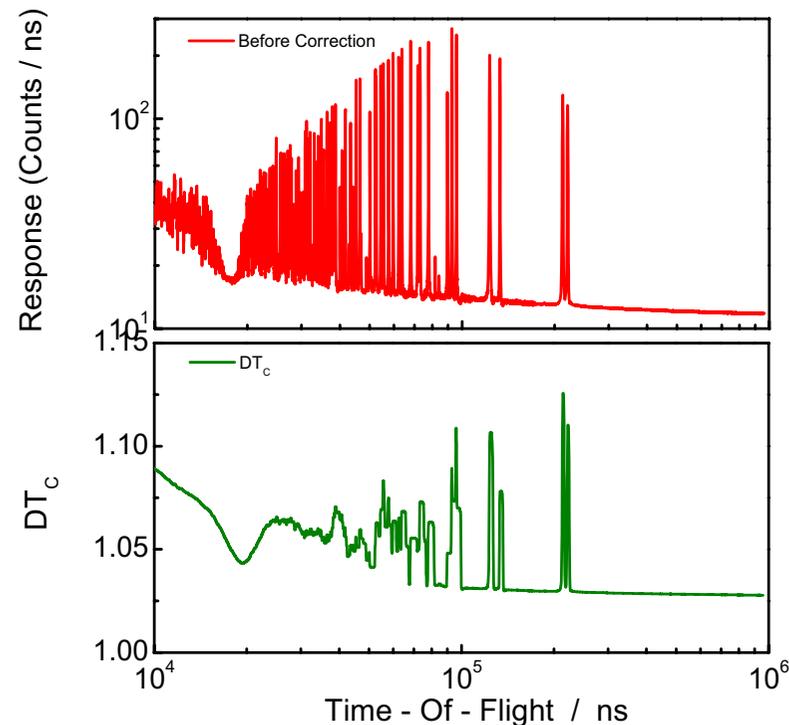
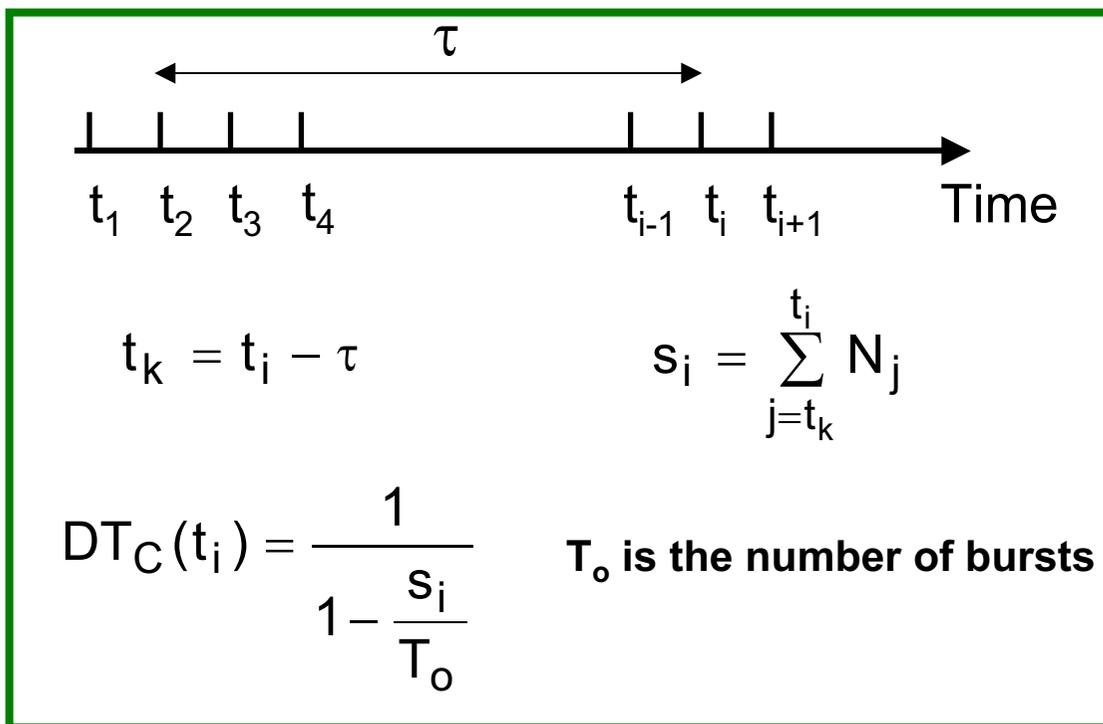
RRR	URR
Resonance shape analysis	Correction for resonance structure
$T_{\text{exp}}(T_n) = \int R_T(T_n, E_n) e^{-\sigma_{\text{tot}}(E_n)} dE_n$	$\langle e^{-n\sigma_{\text{tot}}} \rangle \approx e^{-\langle n\sigma_{\text{tot}} \rangle} \left(1 + \frac{n^2}{2} \text{var } \sigma_{\text{tot}} - \dots \right)$
<u>$T_{\text{exp}}(T_n)$</u>	<u>$\langle T_{\text{exp}} \rangle$</u>

Reaction measurement
(1) Dead time correction
(2) Background subtraction

Flux measurement
(1) Dead time correction
(2) Background subtraction

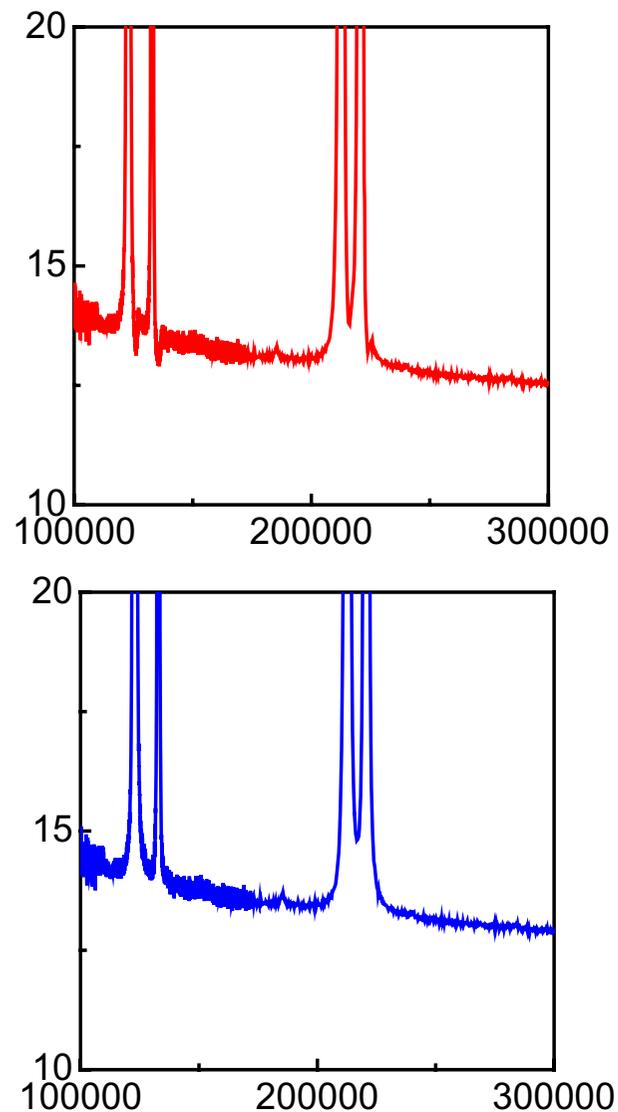
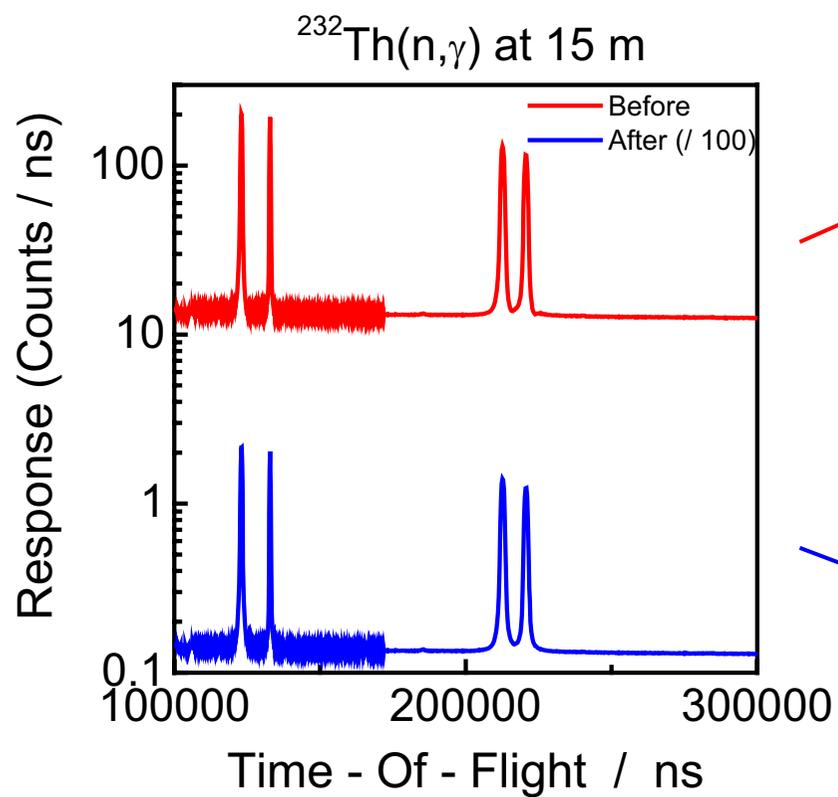
$$Y_{\text{exp}} = N_r \frac{\sigma_{\varphi}}{\varepsilon_r} \frac{C'_r - B'_r}{C'_\varphi - B'_\varphi}$$

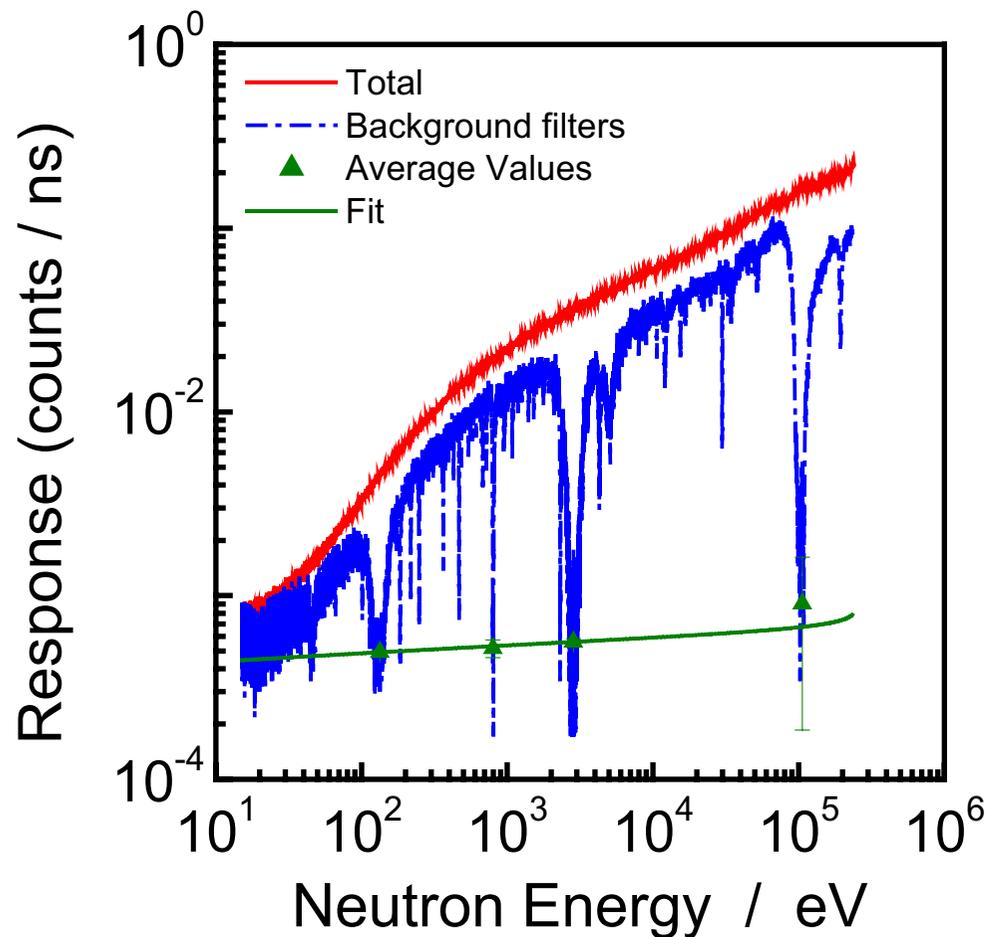
<p>RRR Resonance shape analysis</p> $Y_{\text{exp}}(T_n) = N_r \int R_T(T_n, E_n) \varepsilon_r(E_n) Y_r(E_n) dE_n$	<p>URR Correction for self-shielding and multiple scattering (F_c)</p> $\langle \sigma(n,r) \rangle = F_c \langle Y_{\text{exp}} \rangle$
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System dead time for on-line data processing (time-of-flight + amplitude):

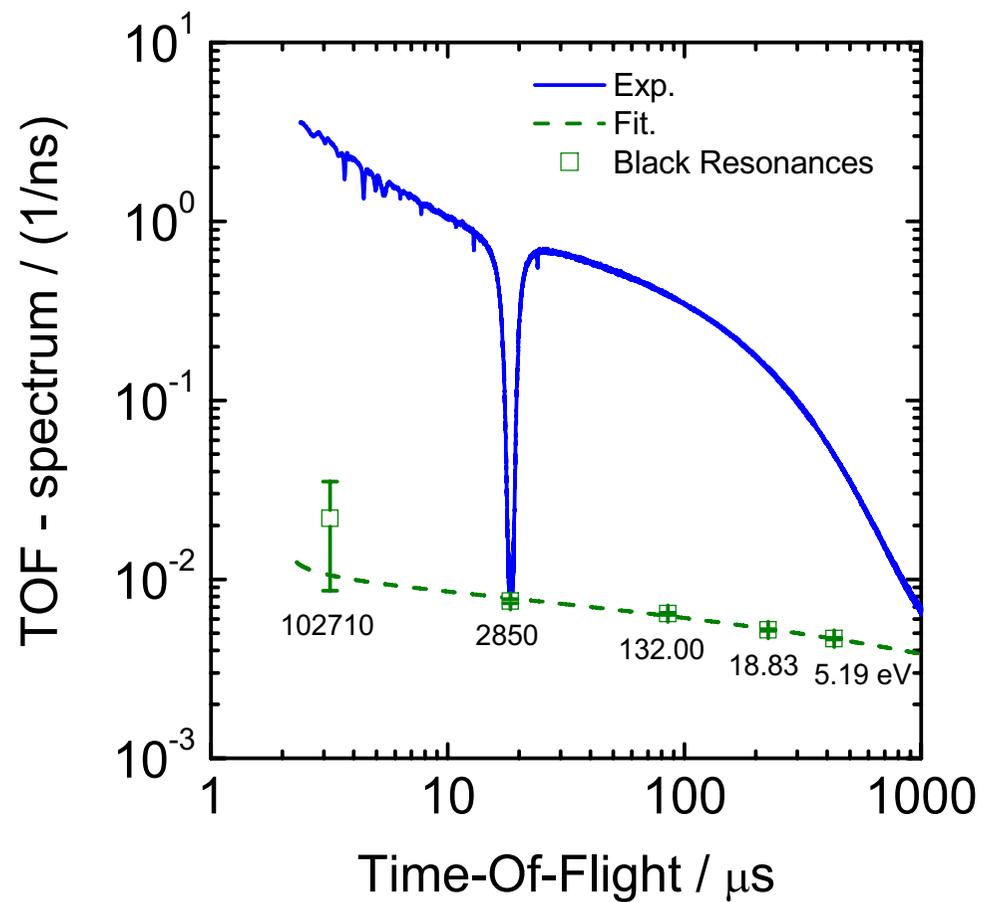
- Acqiris DC282 (digitizer) = 350 ns
- CAEN N1728B (digitizer) = 560 ns
- Conventional system DAQ2000 = 2800 ns (without amplitude similar to digitizers)





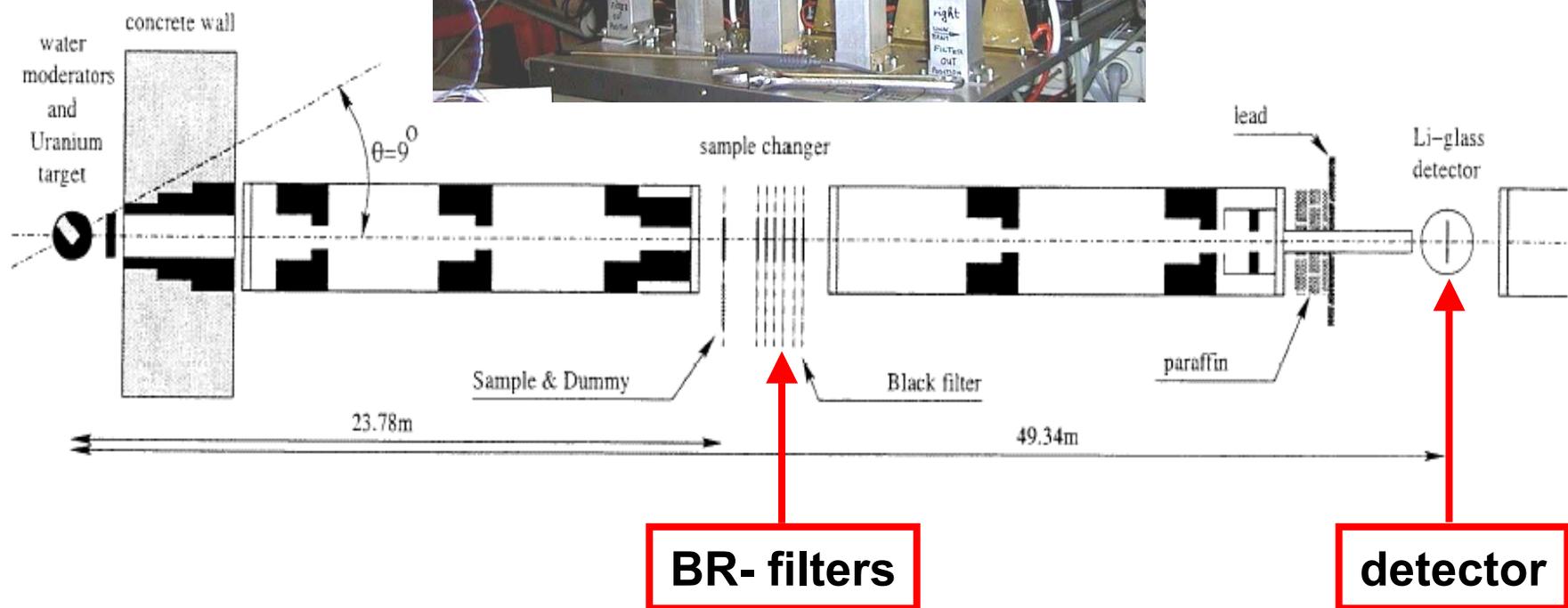
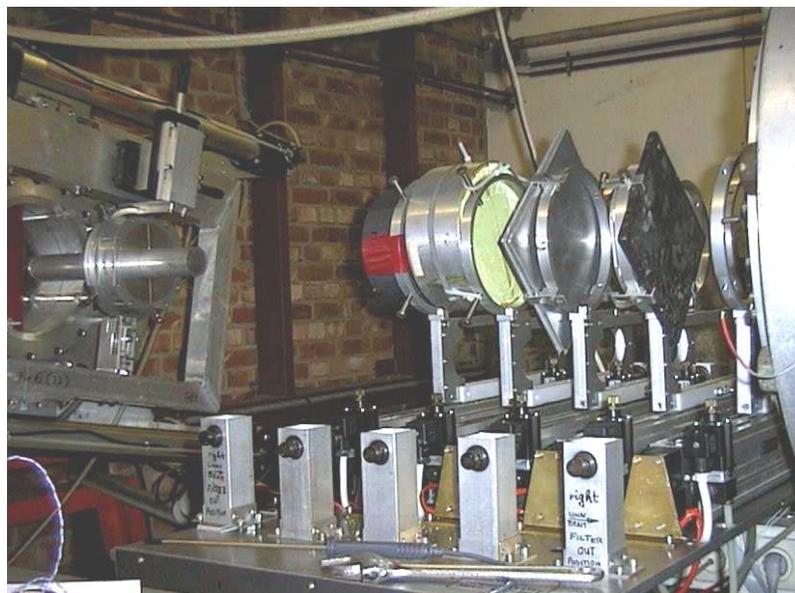
Black Resonance Filters

Element	Energy / eV
Ag	5.19
W	18.83
Co	132.00
Na	2850.00
S	102710.00



Black Resonance Filters

Element	Energy / eV
Ag	5.19
W	18.83
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Na	2850.00
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- **Experimental observables**
- **Definitions and terminology**
 - Probability and statistical quantities
 - Error and Uncertainty
 - Propagation of uncertainties
- **Fitting a mathematical model to data**
- **Basic operations**
- **AGS**
- **Examples**

P(x) theoretical probability density function (PDF) of x

P(x,y) theoretical probability density function of (x,y)

- **Mean** $\mu_x = \langle x \rangle = \int x P(x) dx$

- **Variance** $\sigma_x^2 = \langle (x - \mu_x)^2 \rangle = \int (x - \mu_x)^2 P(x) dx$

- **Covariance** $\sigma_{xy}^2 = \langle (x - \mu_x)(y - \mu_y) \rangle = \int (x - \mu_x)(y - \mu_y) P(x, y) dx dy$

- **Correlation** $\rho(x, y) = \frac{\sigma_{xy}^2}{\sigma_x \sigma_y}$

n observations x_1, \dots, x_n of variable x

m observations $(x_1, y_1) \dots, (x_n, y_n)$ of variable (x, y)

- **Sample mean**
$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$$
- **Sample variance**
$$s_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$$
- **Sample covariance**
$$s_{xy} = \frac{1}{n-1} \sum_{i=1}^n \sum_{j=1}^n (x_i - \bar{x})(y_j - \bar{y})$$
- **Sample correlation**
$$r(x, y) = \frac{s_{xy}}{s_x s_y}$$

n observations x_1, \dots, x_n of variable $x \rightarrow z = f(x_1, \dots, x_n)$

- **Linear function**
$$z = f(x_i) = \sum_{i=1}^k a_i x_i$$

- **Mean**
$$\mu_z = \langle f(x_i) \rangle = \sum_{i=1}^k a_i \mu_i$$

- **Variance**
$$\sigma_z^2 = \langle (f(x_i) - \mu_f)^2 \rangle = \sum_i a_i^2 \sigma_{x_i}^2 + \sum_{i \neq j} a_i a_j \sigma_{x_i x_j}$$

- **Taylor expansion**
(1st order !)

$$z = f(x_i) \cong f(\mu_i) + \sum_i \left. \frac{\partial f}{\partial x_i} \right|_{\mu} (x_i - \mu_i)$$

$$z = f(x_i) \cong f(\mu_i) + \sum_i g_i (x_i - \mu_i) \quad g_i = \left. \frac{\partial f}{\partial x_i} \right|_{\mu}$$

- **Mean**

$$\mu_z = \langle f(x_i) \rangle \cong f(\mu_i)$$

- **Variance**

$$\sigma_z^2 = \langle (f(x_i) - \mu_f)^2 \rangle \cong \sum_i g_i^2 \sigma_{x_i}^2 + \sum_{i \neq j} g_i g_j \sigma_{x_i x_j}$$

- **Linear function**

$$\vec{z} = f(\vec{x}) = \underline{A}\vec{x}$$

$$a_{ik} = \frac{\partial f_i}{\partial x_k}$$

– Mean

$$\vec{\mu}_z = \underline{A} \vec{\mu}_x$$

– Variance

$$\underline{V}_z = \underline{A} \underline{V}_x \underline{A}^T$$

- **Non-linear function
(1st order Taylor !)**

$$\vec{z} = f(\vec{x}) \cong f(\vec{\mu}_x) + \underline{G}_x (\vec{x} - \vec{\mu}_x)$$

$$g_{x,ik} = \frac{\partial f_i}{\partial x_k}$$

– Mean

$$\vec{\mu}_z \cong f(\vec{\mu}_x)$$

sensitivity matrix
design matrix

– Variance

$$\underline{V}_z \cong \underline{G}_x \underline{V}_x \underline{G}_x^T$$

- **Uncertainty (dispersion (or width), always > 0)**

“Uncertainty is a parameter associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand”

- **Error (difference between two quantities, can be + or -)**

“Error is the result of a measurement minus a true value of the measurand”

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

- **Systematic error**

Mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions minus a true value of the measurand.

The expectation value of the error arising from a systematic effect = 0

- **Random error**

Result of a measurement minus the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions.

The expectation value of a random error = 0

- If a systematic error arises from a recognized effect, the effect can be quantified and a correction or correction factor should be applied.
- The uncertainty on the correction factor should not be quoted as a systematic error.
- One should not enlarge the uncertainty to compensate for a systematic effect that is not recognized!

- **Type A evaluation**

- Method of evaluation of uncertainty by the statistical analysis of series of observations
- Is obtained from an **observed** frequency distribution

- **Type B evaluation**

- Method of evaluation of uncertainty by means other than the statistical analysis of series of observations.
- Is obtained from an **assumed** probability density function (subjective probability) .
- The evaluation is based on scientific judgement
 - Theoretical distribution
 - Experience from previous measurement data
 - Data provided in calibration or other certificates

- **Propagation of uncertainties \Rightarrow combined uncertainty**

$$\underline{V}_f \cong \underline{G}_x \underline{V}_x \underline{G}_x^T \quad g_{x,ik} = \frac{\partial f_i}{\partial x_k} \quad \text{non-linear problem : approximation!}$$

- **Type A evaluation**

- Perform repeated measurements and record the number of events in time t
- Calculate the uncertainty from the standard deviation of the observed frequency distribution

$$s_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$$

- **Type B evaluation : Poisson statistics**

- The observed quantity is distributed as a Poisson distribution
- The uncertainty is defined by the standard deviation of a Poisson distribution

$$\sigma_x^2 = \mu_x$$

- **Evaluation of uncertainty components**

- Type A : statistical analysis of repeated measurements
- Type B : scientific judgement

- **All uncertainties are statistical !**

(uncertainty due to counting statistics, uncertainty on the normalization, ...)

(correlated or not-correlated uncertainties)

- **Standard (u_x) or expanded uncertainty**

– Standard uncertainty : $(\bar{x} \pm u_x)$ with $u_x = \frac{s_x}{\sqrt{n}}$ $\lambda_p = 1 \Rightarrow p = 0.68$

– Expanded uncertainty : $\lambda_p > 1$

e.g. $\lambda_p = 1.96 \Rightarrow p = 0.95$

$$P\left(\left|\bar{x} - \mu_x\right| \leq \lambda_p \frac{\sigma}{\sqrt{n}}\right) = p$$

- **Definitions and terminology**
- **Experimental observables**
- **Fitting a mathematical model to data**
 - Least squares – Maximum likelihood
 - Generalized least squares method
- **Basic operations**
- **AGS**
- **Examples**

Central limit theorem:

The sum of a large number of independent and identically-distributed random variables will be approximately normally distributed

If x_1, \dots, x_n are **independent** and **identically** distributed with mean μ_x and variance σ^2 then :

for large n :

the distribution of $\bar{x} = \frac{\sum_i x_i}{n}$ is the normal distribution with parameters $(\mu_x, \frac{\sigma}{\sqrt{n}})$

$$P(\bar{x} | \mu_x, \sigma_x) d\bar{x} = \frac{1}{\sqrt{2\pi\sigma_x}} \exp\left(-\frac{1}{2}\left(\frac{\bar{x} - \mu_x}{\sigma_x}\right)^2\right) d\bar{x} \quad \text{with } \sigma_x = \frac{\sigma}{\sqrt{n}}$$

General: based on maximum entropy principle

Fröhner, Nucl. Sci. Eng. 126 (1997) 1

For observables $\vec{x} = (x_1, \dots, x_n)$ with covariance matrix \underline{V}_x

which are **identically** distributed with mean $\vec{\mu}_x$

$$P(\vec{x} | \vec{\mu}_x, \underline{V}_x) d\vec{x} = \frac{1}{\sqrt{\det(2\pi\underline{V}_x)}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu}_x)^T \underline{V}_x^{-1}(\vec{x} - \vec{\mu}_x)\right) d\vec{x}$$

Problem: n data points $(x_1, z_1), \dots, (x_n, z_n)$ and a model function $\vec{z} = f(\vec{x}, \vec{a})$ that in addition to the variable x also depends on k parameters a_1, \dots, a_k with $n > k$.

Solution:

(1) Least squares : find the vector \vec{a} such that the curve fits best the given data in the least squares sense, that is, the weighed sum of squares is minimized:

$$\chi^2(\vec{a}) = (\vec{z}_{\text{exp}} - f(\vec{x}, \vec{a}))^T \underline{V}_z^{-1} (\vec{z}_{\text{exp}} - f(\vec{x}, \vec{a}))$$

(2) Maximum likelihood: find the vector \vec{a} that maximizes the likelihood function.

When the PDF is the normal distribution :

$$P(\vec{a} | \vec{z}, \underline{V}_z) d\vec{a} \propto \exp\left(-\frac{1}{2} (\vec{z}_{\text{exp}} - f(\vec{x}, \vec{a}))^T \underline{V}_z^{-1} (\vec{z}_{\text{exp}} - f(\vec{x}, \vec{a}))\right) d\vec{a}$$

Least squares method is equivalent to Maximum likelihood

Input from experiment : \mathbf{z}_{exp} and \mathbf{V}_z , \mathbf{x}_{exp} and \mathbf{V}_x

- Linear model

$$\mathbf{z}_m = f(\vec{\mathbf{x}}, \vec{\mathbf{a}}) = \underline{\mathbf{G}}_a \vec{\mathbf{a}} \quad \mathbf{g}_{a,ij} = \frac{\partial f_i}{\partial a_j}$$

$$\underline{\mathbf{V}} = (\underline{\mathbf{V}}_z + \underline{\mathbf{G}}_x \underline{\mathbf{V}}_x \underline{\mathbf{G}}_x^T) \quad \mathbf{g}_{x,ij} = \frac{\partial f_i}{\partial x_j}$$

$$\vec{\mathbf{a}} = (\underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} \underline{\mathbf{G}}_a)^{-1} (\underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} \vec{\mathbf{z}}_{\text{exp}})$$

$$\underline{\mathbf{V}}_a = (\underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} \underline{\mathbf{G}}_a)^{-1}$$

- Non-linear model (1st order Taylor)

$$\mathbf{z}_m = f(\vec{\mathbf{x}}, \vec{\mathbf{a}}) \cong f(\vec{\mathbf{x}}, \vec{\mathbf{a}}_0) + \underline{\mathbf{G}}_a (\vec{\mathbf{a}} - \vec{\mathbf{a}}_0)$$

$$\underline{\mathbf{V}} = (\underline{\mathbf{V}}_z + \underline{\mathbf{G}}_x \underline{\mathbf{V}}_x \underline{\mathbf{G}}_x^T)$$

$$(\vec{\mathbf{a}} - \vec{\mathbf{a}}_0) = (\underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} \underline{\mathbf{G}}_a)^{-1} \underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} (\vec{\mathbf{z}}_{\text{exp}} - f(\vec{\mathbf{x}}, \vec{\mathbf{a}}_0))$$

$$\underline{\mathbf{V}}_{a-a_0} = (\underline{\mathbf{G}}_a^T \underline{\mathbf{V}}^{-1} \underline{\mathbf{G}}_a)^{-1}$$

solved by iteration

- **Definitions and terminology**
- **Fitting a mathematical model to data**
- **Basic operations (+ , - , x , /)**
 - Background
 - Normalization
 - Fit correlated data
- **AGS**
- **Examples**

Example: y vector dimension 2 $\rightarrow z = f(y_1, y_2, b)$

$$\vec{z} = \vec{y} - b$$

V_y uncorrelated uncertainties from counting statistics : $V_y = \begin{bmatrix} \sigma_{y_1}^2 & 0 \\ 0 & \sigma_{y_2}^2 \end{bmatrix}$

V_b uncertainty on background (not correlated with V_y) : $V_b = \sigma_b^2$

$$V_z = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \sigma_{y_1}^2 & 0 & 0 \\ 0 & \sigma_{y_2}^2 & 0 \\ 0 & 0 & \sigma_b^2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix} = \begin{bmatrix} \sigma_{y_1}^2 + \sigma_b^2 & \sigma_b^2 \\ \sigma_b^2 & \sigma_{y_2}^2 + \sigma_b^2 \end{bmatrix}$$

$$\underline{V}_z = \underline{A} \underline{V}_x \underline{A}^T \quad a_{ik} = \frac{\partial f_i}{\partial x_k}$$

$$(y_1 - b, y_2 - b) = (z_1, z_2) \rightarrow (z_1 + z_2, z_1 - z_2)$$

$$V_{(z_1, z_2)} = \begin{bmatrix} \sigma_{y_1}^2 + \sigma_b^2 & \sigma_b^2 \\ \sigma_b^2 & \sigma_{y_2}^2 + \sigma_b^2 \end{bmatrix}$$

$$V_{(z_1 + z_2, z_1 - z_2)} = \begin{bmatrix} \sigma_{y_1}^2 + \sigma_{y_2}^2 + 4\sigma_b^2 & \sigma_{y_1}^2 - \sigma_{y_2}^2 \\ \sigma_{y_1}^2 - \sigma_{y_2}^2 & \sigma_{y_1}^2 + \sigma_{y_2}^2 \end{bmatrix}$$

$$\sigma_{z_1 + z_2}^2 = \sigma_{y_1}^2 + \sigma_{y_2}^2 + 4\sigma_b^2$$

$$\sigma_{z_1 - z_2}^2 = \sigma_{y_1}^2 + \sigma_{y_2}^2$$

$$(y_1 - b, y_2 - b) = (z_1, z_2) \rightarrow (z_1 + z_2, z_1 - z_2)$$

Covariance

$$\sigma_{z_1+z_2}^2 = \sigma_{y_1}^2 + \sigma_{y_2}^2 + 4\sigma_b^2$$

$$\sigma_{z_1-z_2}^2 = \sigma_{y_1}^2 + \sigma_{y_2}^2$$

Only diagonal terms

$$\sigma_{y_1}^2 + \sigma_{y_2}^2 + 2\sigma_b^2$$

$$\sigma_{y_1}^2 + \sigma_{y_2}^2 + 2\sigma_b^2$$

$$(y_1 - b, y_2 - b) = (z_1, z_2) \rightarrow (z_1 + z_2, z_1 - z_2) = (v_1, v_2) \rightarrow (v_1 + v_2) = 2z_1$$

Covariance

$$\sigma_{2z_1}^2 = V_{v_1+v_2} = \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} \sigma_{y_1}^2 + \sigma_{y_2}^2 + 4\sigma_b^2 & \sigma_{y_1}^2 - \sigma_{y_2}^2 \\ \sigma_{y_1}^2 - \sigma_{y_2}^2 & \sigma_{y_1}^2 + \sigma_{y_2}^2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 4(\sigma_{y_1}^2 + \sigma_b^2) = 4\sigma_{z_1}^2$$

Only diagonal terms

$$\sigma_{2z_1}^2 = 2\sigma_{y_1}^2 + 2\sigma_{y_2}^2 + 4\sigma_b^2 = 2\sigma_{z_1}^2 + 2\sigma_{z_2}^2$$

Example: y vector dimension 2 $\rightarrow z = f(y_1, y_2, N)$

$$\vec{z} = N \vec{y}$$

V_y uncorrelated uncertainties from counting statistics : $V_y = \begin{bmatrix} \sigma_{y_1}^2 & 0 \\ 0 & \sigma_{y_2}^2 \end{bmatrix}$

V_N uncertainty on normalization (not correlated with V_y) : $V_N = \sigma_N^2$

$$V_z \approx \begin{bmatrix} N & 0 & y_1 \\ 0 & N & y_2 \end{bmatrix} \begin{bmatrix} \sigma_{y_1}^2 & 0 & 0 \\ 0 & \sigma_{y_2}^2 & 0 \\ 0 & 0 & \sigma_N^2 \end{bmatrix} \begin{bmatrix} N & 0 \\ 0 & N \\ y_1 & y_2 \end{bmatrix} = \begin{bmatrix} N^2 \sigma_{y_1}^2 + y_1^2 \sigma_N^2 & y_1 y_2 \sigma_N^2 \\ y_1 y_2 \sigma_N^2 & N^2 \sigma_{y_2}^2 + y_2^2 \sigma_N^2 \end{bmatrix}$$

not -linear

$$(Ny_1, Ny_2) = (z_1, z_2) \Rightarrow (z_1 z_2, z_1/z_2)$$

$$V_{(z_1, z_2)} = \begin{bmatrix} N^2 \sigma_{y_1}^2 + y_1^2 \sigma_N^2 & y_1 y_2 \sigma_N^2 \\ y_1 y_2 \sigma_N^2 & N^2 \sigma_{y_2}^2 + y_2^2 \sigma_N^2 \end{bmatrix}$$

$$V_{(z_1 z_2, z_1/z_2)} = \begin{bmatrix} N^4 y_2^2 \sigma_{y_1}^2 + N^4 y_1^2 \sigma_{y_2}^2 + 4N^2 y_1^2 y_2^2 \sigma_N^2 & N^2 \sigma_{y_1}^2 - \frac{y_1^2}{y_2^2} N^2 \sigma_{y_2}^2 \\ N^2 \sigma_{y_1}^2 - \frac{y_1^2}{y_2^2} N^2 \sigma_{y_2}^2 & \frac{\sigma_{y_1}^2}{y_2^2} + \frac{y_1^2}{y_2^4} \sigma_{y_2}^2 \end{bmatrix}$$

$$\sigma_{z_1 z_2}^2 = N^4 y_2^2 \sigma_{y_1}^2 + N^4 y_1^2 \sigma_{y_2}^2 + 4N^2 y_1^2 y_2^2 \sigma_N^2$$

$$\sigma_{z_1/z_2}^2 = \frac{\sigma_{y_1}^2}{y_2^2} + \frac{y_1^2}{y_2^4} \sigma_{y_2}^2$$

$$(Ny_1, Ny_2) = (z_1, z_2) \rightarrow (z_1 z_2, z_1/z_2)$$

Covariance

$$\sigma_{z_1 z_2}^2 = N^4 y_2^2 \sigma_{y_1}^2 + N^4 y_1^2 \sigma_{y_2}^2 + 4N^2 y_1^2 y_2^2 \sigma_N^2$$

$$\sigma_{z_1/z_2}^2 = \frac{\sigma_{y_1}^2}{y_2^2} + \frac{y_1^2}{y_2^4} \sigma_{y_2}^2$$

Only diagonal terms

$$N^4 y_2^2 \sigma_{y_1}^2 + N^4 y_1^2 \sigma_{y_2}^2 + 2N^2 y_1^2 y_2^2 \sigma_N^2$$

$$\frac{\sigma_{y_1}^2}{y_2^2} + \frac{y_1^2}{y_2^4} \sigma_{y_2}^2 + 2 \frac{\sigma_N^2}{N^2} \frac{y_1^2}{y_2^2}$$

Fit correlated data: common “offset “ uncertainty

z_1 and z_2 are observables of the same quantity K which are deduced from the experimental data (y_1, y_2) affected by a common “offset error” with uncertainty σ_b and mean =0.

The covariance matrix for $(z_1, z_2) = (y_1 - 0, y_2 - 0)$ is :

$$V_{(z_1, z_2)} = \begin{bmatrix} \sigma_{y_1}^2 + \sigma_b^2 & \sigma_b^2 \\ \sigma_b^2 & \sigma_{y_2}^2 + \sigma_b^2 \end{bmatrix}$$

where σ_{y_1} and σ_{y_2} are the uncorrelated uncertainty components of y_1 and y_2 (e.g. due to counting statistics).

The best value K is obtained by minimizing the expression:

$$\chi^2(k) = (\vec{z}_{\text{exp}} - K)^T V_{(z_1, z_2)}^{-1} (\vec{z}_{\text{exp}} - K)$$

Solution :
$$\chi^2(k) = (\vec{z}_{\text{exp}} - K)^T \underline{V}_{(z_1, z_2)}^{-1} (\vec{z}_{\text{exp}} - K)$$

The best value k:
$$K = \frac{z_1 \sigma_{y_2}^2 + z_2 \sigma_{y_1}^2}{\sigma_{y_1}^2 + \sigma_{y_2}^2} \quad (\text{weighted average})$$

with uncertainty :
$$\sigma_K^2 = \frac{\sigma_{y_1}^2 \sigma_{y_2}^2}{\sigma_{y_1}^2 + \sigma_{y_2}^2} + \sigma_b^2$$

Fit correlated data: common “normalization” uncertainty

z_1 and z_2 are observables of the same quantity K which are deduced from the experimental data (y_1, y_2) affected by a common “normalization” with uncertainty σ_N and mean $N = 1$.

The covariance matrix for $(z_1, z_2) = (N y_1, N y_2)$ with $N = 1$ is :

$$V_{(z_1, z_2)} = \begin{bmatrix} \sigma_{y_1}^2 + y_1^2 \sigma_N^2 & y_1 y_2 \sigma_N^2 \\ y_1 y_2 \sigma_N^2 & \sigma_{y_2}^2 + y_2^2 \sigma_N^2 \end{bmatrix}$$

where σ_{y_1} and σ_{y_2} are the uncorrelated uncertainty components (e.g. due to counting statistics).

The best value k is obtained by minimizing the expression:

$$\chi^2(k) = (\vec{z}_{\text{exp}} - K)^T \underline{V}_{(z_1, z_2)}^{-1} (\vec{z}_{\text{exp}} - K)$$

Solution : $\chi^2(k) = (\vec{z}_{\text{exp}} - Z)^T \underset{-(z_1, z_2)}{V}^{-1} (\vec{z}_{\text{exp}} - Z)$

The best value K:
$$K = \frac{z_1 \sigma_{y_2}^2 + z_2 \sigma_{y_1}^2}{\sigma_{y_1}^2 + \sigma_{y_2}^2 + \underline{(y_1 - y_2)^2 \sigma_N^2}} \quad (\neq \text{weighted average})$$

with uncertainty :
$$\sigma_Z^2 = \frac{\sigma_{y_1}^2 \sigma_{y_2}^2 + (y_1^2 \sigma_{y_2}^2 + y_2^2 \sigma_{y_1}^2) \sigma_N^2}{\sigma_{y_1}^2 + \sigma_{y_2}^2 + (y_1 - y_2)^2 \sigma_N^2}$$

Only in case $(y_1 - y_2)^2 \sigma_N^2$ is small K approaches the weighted average.

⇒ Known as : “Peelle’s Pertinent Puzzle”, see Fröhner NSE 126 (1997) 1

⇒ Due to “non-linearities”

Solution : treat the normalization as a separate observable

Observables: $(N'_{\text{exp}}, y_1, y_2)$ with covariance matrix $V_{(N', y_1, y_2)}$

The function is : $(N'_{\text{exp}}, y_1, y_2) = (N', KN', KN') = f(N', K)$ (note $N' = 1/N$)

$$V_{(N', y_1, y_2)} = \begin{bmatrix} \sigma_{N'}^2 & 0 & 0 \\ 0 & \sigma_{y_1}^2 & 0 \\ 0 & 0 & \sigma_{y_2}^2 \end{bmatrix}$$

(N', K) are determined by minimizing:

$$\chi^2(N', K) = ((N'_{\text{exp}}, y_1, y_2) - (N', N'K, N'K))^T \underline{V}_{(N', y_1, y_2)}^{-1} ((N'_{\text{exp}}, y_1, y_2) - (N', N'K, N'K))$$

Two measurements (z_1, z_2) of variable Z each with 10% uncorrelated uncertainty and 20% uncertainty on the calibration factor N :

$$z_1 = 1.5$$

$$z_2 = 1.0$$

$$V_{z_1, z_2} = \begin{bmatrix} 0.15^2 + (1.15 \times 0.20)^2 & 1.0 \times 1.5 \times 0.20^2 \\ 1.0 \times 1.5 \times 0.20^2 & 0.10^2 + (1.0 \times 0.20)^2 \end{bmatrix}$$

$$= \begin{bmatrix} 0.1125 & 0.06 \\ 0.06 & 0.05 \end{bmatrix}$$

Best value for Z ?

Weighted average (only uncorrelated terms) : 1.154 ± 0.083

Least square without covariance : 1.154 ± 0.083

Least squares with covariance : 0.882 ± 0.218

Least squares with calibration factor as parameter : 1.154 ± 0.254

Least squares without covariance + adding u_N afterwards : 1.154 ± 0.245

- **Uncertainties**

- V_C : diagonal, uncorrelated uncertainties due do counting statistics
Poisson (Type B), or preferably by repeated measurements (Type A)
- B : background subtraction → introduces correlated uncertainties
- N : normalization → introduces correlated uncertainties

- **N and B can be considered as due to systematic effects. The value for B and N are the systematic corrections. These corrections have their uncertainties (or better covariance matrix)**

- **Not correcting for N and/or B implies that the value Z can not be quoted !**

- **Be careful with large uncertainties on the normalization.**
- **Quote all the components involved in the data reduction process**
- **Separate as much as possible the components which create correlated uncertainties**
- **Include the normalization in the model**

- x_i : \underline{V}_x only uncorrelated uncertainties (counting statistics)
- c_i : \underline{V}_c correlated uncertainties (normalization, background, ...)

$$\vec{Y} = \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \\ c_1 \\ \cdot \\ \cdot \\ \cdot \\ c_m \end{bmatrix}$$

$$\underline{V}_Y = \begin{bmatrix} \sigma_{x_1}^2 & 0 & \dots & 0 & 0 \\ 0 & \sigma_{x_2}^2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \sigma_{x_n}^2 & 0 \\ \hline 0 & 0 & \dots & 0 & \underline{V}_c \end{bmatrix}$$

$$g_{ik} = \frac{\partial f_i}{\partial Y_k}$$

$$\Rightarrow \underline{V}_Z \cong \underline{G}_Y^T \underline{V}_Y \underline{G}_Y$$

$$T = f(N_T, \tau_d, C_{in}, B_{in}, C_{out}, B_{out})$$

$$Y_r = f(N_r, \varepsilon_r, \tau_d, C_r, B_r, C_\varphi, B_\varphi)$$

- **C** counting statistics (not correlated)
- τ_d u_{τ_d} from least square fit of time interval distribution
- **B** least square fit (correlated uncertainties)
- N_T $u_{N_T} \approx 0.5 \%$ (alternating sequences of “in-out” measurements)
Borella et al., Phys. Rev. C 76 (2007) 014605
- ε_r depends on method
- N_r depends on method (related to ε_r)

(n, γ) for total energy principle with PHWT $u_{N_r} \approx 2\%$
Borella et al. Nucl. Instr. Meth. A577, (2007) 626

Reaction yield

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

C' dead time corrected counts
 B' background contribution
 N normalization factor

Transmission

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

Histogram operations + Covariance information (AGS)

$Y_{\text{exp}} + \text{covariance}$
 $T_{\text{exp}} + \text{covariance}$

input

Reaction models : Resonance parameters + covariances
 Cross sections + covariances

Z : function of vectors **Z**₁, **Z**₂, and parameter vector **b**:

$$\mathbf{Z} = F(\mathbf{b}, \mathbf{Z}_1, \mathbf{Z}_2)$$
 Uncertainty propagation results in:

$$V_Z = \left(\frac{\partial F}{\partial \mathbf{b}} \right) V_b \left(\frac{\partial F}{\partial \mathbf{b}} \right)^T + \left(\frac{\partial F}{\partial \mathbf{Z}_1} \right) V_{Z_1} \left(\frac{\partial F}{\partial \mathbf{Z}_1} \right)^T + \left(\frac{\partial F}{\partial \mathbf{Z}_2} \right) V_{Z_2} \left(\frac{\partial F}{\partial \mathbf{Z}_2} \right)^T + \dots$$

AGS

⇒

$$V_Z = S_Z S_Z^T + D_Z$$

correlated part
 dimension: n x k

uncorrelated part
 diagonal : n values

n : length of vector **Z**

k : number of common sources of uncertainties

Uncertainty in AGS : $Z_1 = F(a_1, Y_1)$

$$Z_1 = F(a_1, Y_1)$$

Z_1, Y_1 : dimension n
 a_1 : dimension k_1

$$V_{Z_1} = \left(\frac{\partial F}{\partial a_1} \right) V_{a_1} \left(\frac{\partial F}{\partial a_1} \right)^T + \left(\frac{\partial F}{\partial Y_1} \right) V_{Y_1} \left(\frac{\partial F}{\partial Y_1} \right)^T$$

V_{a_1} covariance matrix
 (symmetric & positive definite)

V_{Y_1} only diagonal terms : $D_{Y_1} = V_{Y_1}$

$V_{a_1} = L_{a_1} L_{a_1}^T$ (Cholesky decomposition)
 L_a : lower triangular matrix

$\left(\frac{\partial F}{\partial Y_1} \right)$ only diagonal terms

$$S_{a_1} = \left(\frac{\partial F}{\partial a_1} \right) L_{a_1}$$

$$D_{Z_1} = \left(\frac{\partial F}{\partial Y_1} \right) D_{Y_1} \left(\frac{\partial F}{\partial Y_1} \right)^T$$

$\sigma^2_{Y_1 u}$

$$V_{Z_1} = S_{a_1} S_{a_1}^T + D_{Z_1}$$

dimension: $n \times k_1$

n values (diagonal)

Example : $Z = a Y$

$$Z = a Y$$

Z, Y : dimension n
 a : dimension 1

$$V_Z = \left(\frac{\partial F}{\partial a} \right) V_a \left(\frac{\partial F}{\partial a} \right)^T + \left(\frac{\partial F}{\partial Y} \right) V_Y \left(\frac{\partial F}{\partial Y} \right)^T$$

$$V_a = \sigma_a \sigma_a$$

V_Y only diagonal terms : $D_Y = V_Y$

$$\frac{\partial F}{\partial a} = Y$$

$\left(\frac{\partial Z}{\partial Y} \right)$ only diagonal terms

$$S_a = Y \sigma_a$$

$$D_Z = a^2 D_Y \rightarrow a^2 \sigma_{Y u}^2$$

$$V_Z = S_a S_a^T + D_Z$$

dimension: $n \times 1$

n values (diagonal)

$$Z = F(b, Z_1, Z_2)$$

Z, Z_1, Z_2 : dimension n
 b : dimension k_b

$$V_b = L_b L_b^T$$

$$S_b = \left(\frac{\partial Z}{\partial b} \right) L_b$$

$$V_{Z_1} = S_{a_1} S_{a_1}^T + D_{Z_1}$$

$\dim S_{a_1} = n \times k_1$

$$V_{Z_2} = S_{a_2} S_{a_2}^T + D_{Z_2}$$

$\dim S_{a_2} = n \times k_2$

$$V_Z = \left(\frac{\partial F}{\partial b} \right) V_b \left(\frac{\partial F}{\partial b} \right)^T + \left(\frac{\partial F}{\partial Z_1} \right) V_{Z_1} \left(\frac{\partial F}{\partial Z_1} \right)^T + \left(\frac{\partial F}{\partial Z_2} \right) V_{Z_2} \left(\frac{\partial F}{\partial Z_2} \right)^T$$

$$V_Z = S_b S_b^T + \left(\frac{\partial F}{\partial Z_1} \right) S_{a_1} S_{a_1}^T \left(\frac{\partial F}{\partial Z_1} \right)^T + \left(\frac{\partial F}{\partial Z_2} \right) S_{a_2} S_{a_2}^T \left(\frac{\partial F}{\partial Z_2} \right)^T + \left(\frac{\partial F}{\partial Z_1} \right) D_{Z_1} \left(\frac{\partial F}{\partial Z_1} \right)^T + \left(\frac{\partial F}{\partial Z_2} \right) D_{Z_2} \left(\frac{\partial F}{\partial Z_2} \right)^T$$

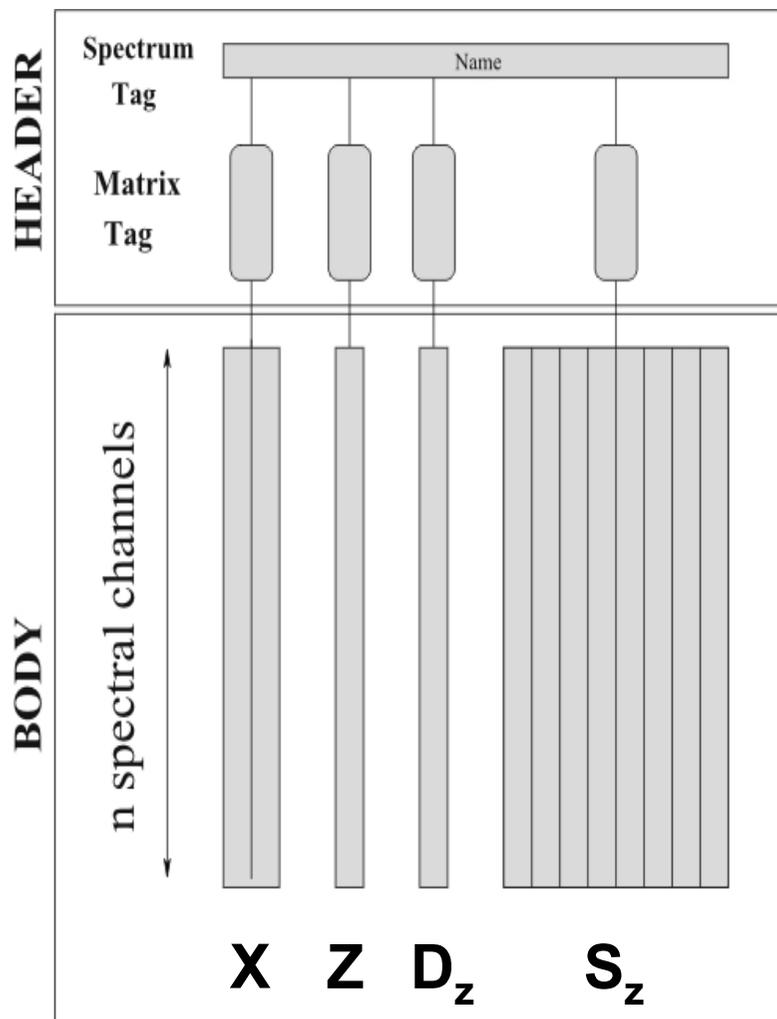
$$S_Z = \left(S_b \quad \left(\frac{\partial F}{\partial Z_1} \right) S_{a_1} \quad \left(\frac{\partial F}{\partial Z_2} \right) S_{a_2} \right)$$

$$D_Z = \left(\frac{\partial F}{\partial Z_1} \right) D_{Z_1} \left(\frac{\partial F}{\partial Z_1} \right)^T + \left(\frac{\partial F}{\partial Z_2} \right) D_{Z_2} \left(\frac{\partial F}{\partial Z_2} \right)^T$$

$$V_Z = S_Z S_Z^T + D_Z$$

dimension: $n \times k$
 $k = k_b + k_1 + k_2$

n values (diagonal)



Storage and calculus

Covariance matrix

n^2 elements (e.g. 32k x 8 bytes)
 $2n^2$ mult. & sum. /step (20 steps)

→ 8 Gb !
 → 8×10^{10} flops!

AGS representation

$n(k+1)$ elements (32k, 20 corr.)
 $n(k+1)$ mult. & sum./step (20 steps)

→ 5 Mb
 → 7×10^3 flops

<i>Write only commands</i>	
ags_mpty	Create an empty AGS file
ags_getA	Import spectra from another AGS file
ags_getE	Import/interpolate evaluated data from an ENDF file
ags_getXY	Import histogram data from an ASCII file
<i>Read/Write commands : Operations on spectra</i>	
ags_addval	Add a constant value to all Y-values of a spectrum
ags_avgr	Average Y values per channel
ags_func	Calculates the Y values for a special function
ags_idtc	Determine the dead time correction of a TOF-spectrum
ags_divi	Divide a spectrum by another
ags_mult	Multiply a spectrum with another
ags_lico	Linear combination of n spectra with n constants
ags_ener	Build energy from TOF X-vector
ags_fit	Non-linear fit of spectra
ags_fxyp	User-programmed function
<i>Read Only commands</i>	
ags_edit	Edit constants and scalers attached to a spectrum
ags_list	List Y values of spectra with common X values
ags_putX	Export final result to an ASCII file
ags_scan	Scan the contents of an AGS file

```
# create ags-file
ags_mpty TRFAK

# read sample out
scaler=TOout,CMout
ags_getXY TRFAK /SCALER=$scaler /FROM=spout.his /ALIAS=SOUT

# read sample in
scaler=TOin,CMin
ags_getXY TRFAK /SCALER=$scaler /FROM=spin.his /ALIAS=SIN /LIKE=A01SOUT

# dead time correction
dtcoef=DTCOEF
ags_idtc TRFAK,A01SOUT /DTIME=$dtcoef /LPSC=1
ags_idtc TRFAK,B01SIN /DTIME=$dtcoef /LPSC=1

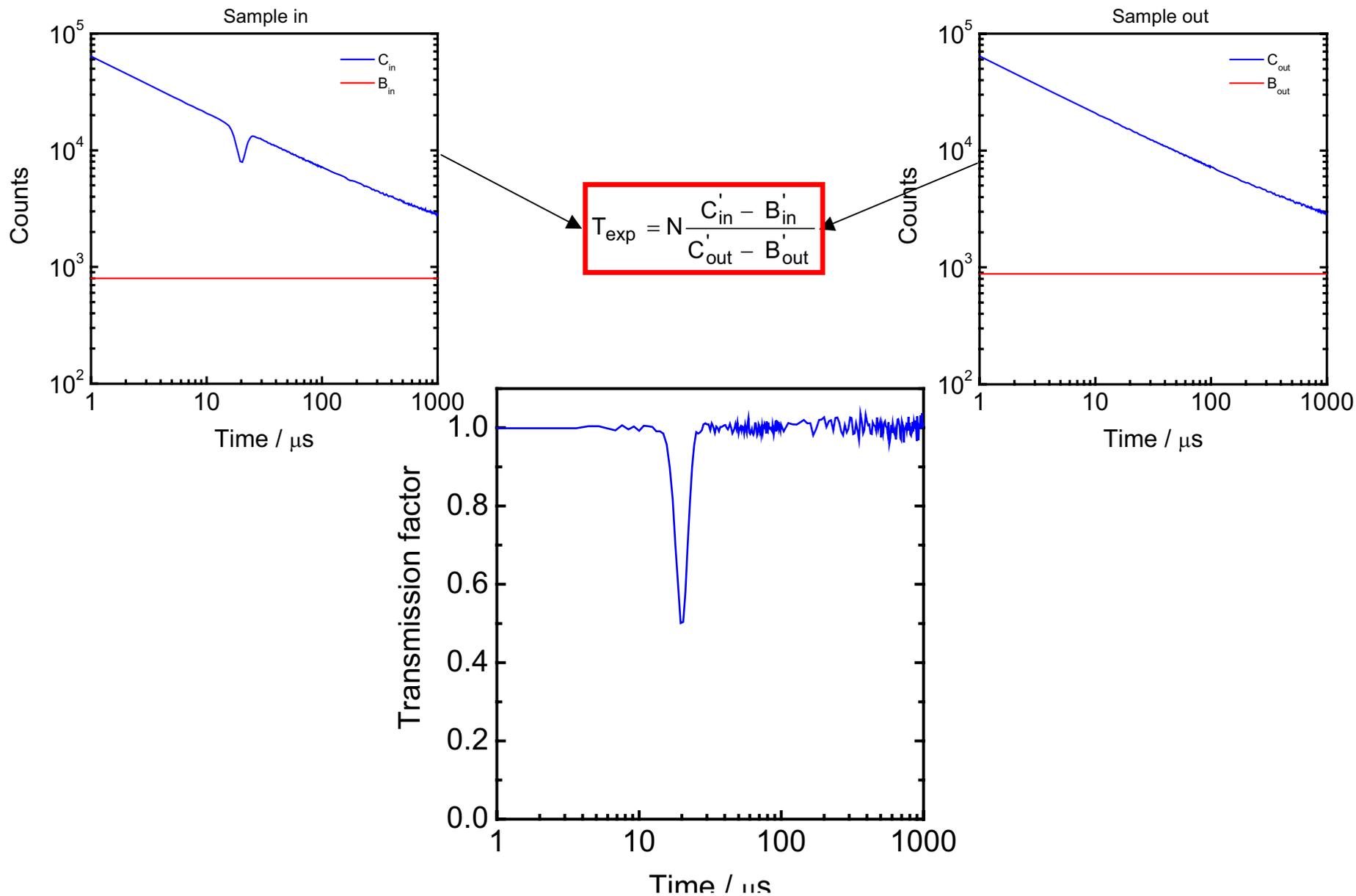
# normalize to central monitor and divide by bin width
ags_avgr TRFAK,C01SOUT /CMSC=2
ags_avgr TRFAK,D01SIN /CMSC=2

#calculate background contribution
ags_func TRFAK /FUN=f01 /PARFILE=PAROUT /ALIAS=SBOUT /LIKE=A01SOUT
ags_func TRFAK /FUN=f01 /PARFILE=PARIN /ALIAS=SBIN /LIKE=A01SOUT

#subtract background
ags_lico TRFAK,E01SOUT,G01SBOUT /ALIAS=SOUTNET /PAR=1.0,-1.0
ags_lico TRFAK,F01SIN,H01SBIN /ALIAS=SINNET /PAR=1.0,-1.0

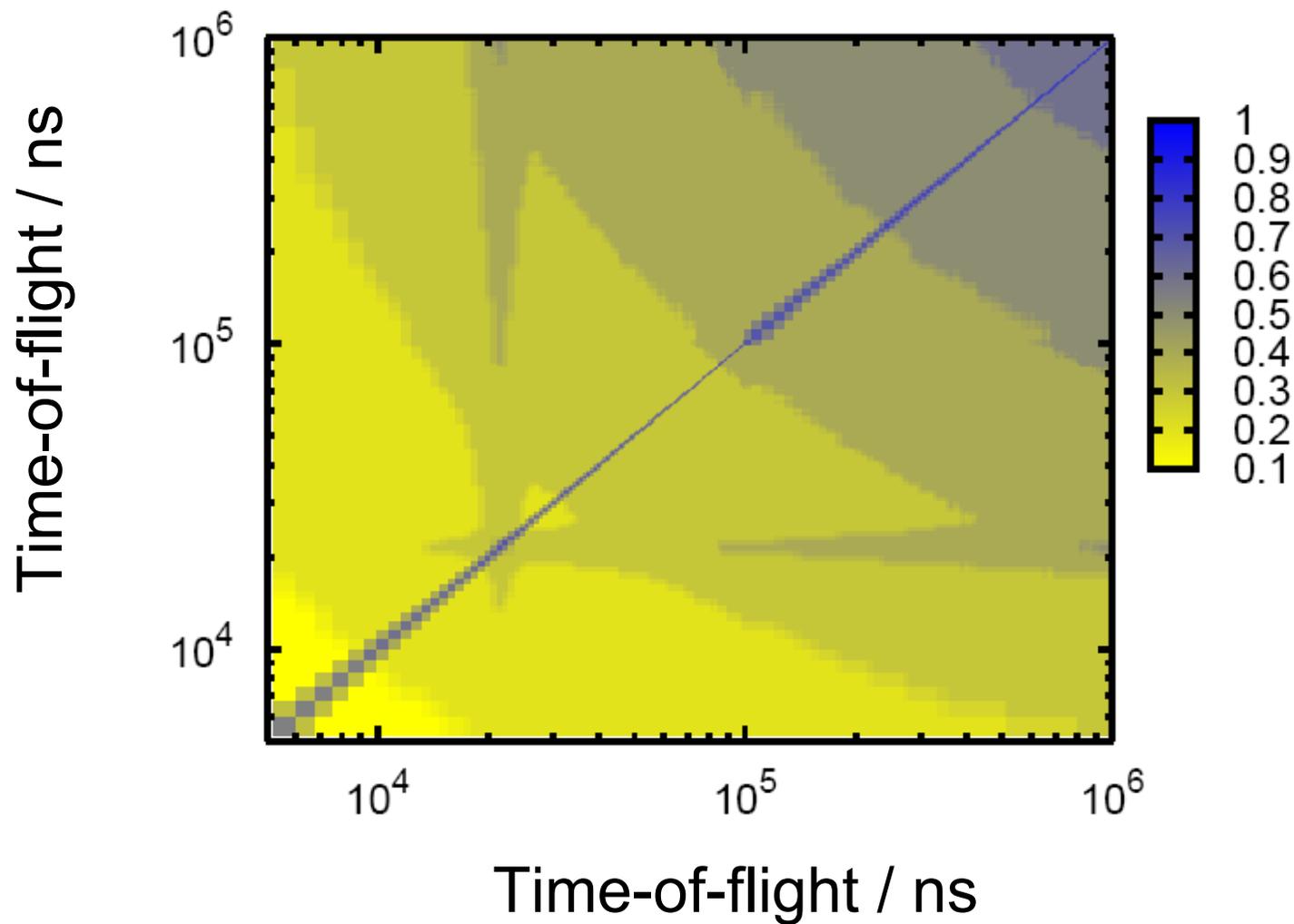
#create transmission factor
ags_divi TRFAK,I01SOUTNET,J01SINNET /ALIAS=TRFAK
```

$$T = \frac{C'_{in} - B'_{in}}{C'_{out} - B'_{out}}$$

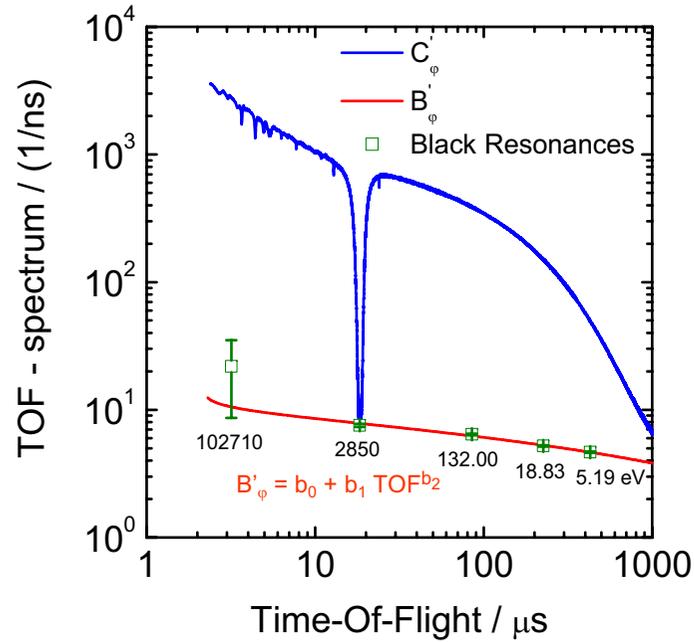


$\delta B_{in} / B_{in} : 10.0 \%$
 $\delta B_{out} / B_{out} : 5.0 \%$
 $\delta N / N : 0.5 \%$

X _L	X _H	Z	δZ	δZ_u	$V_Z = D_Z + S S^T$			
					D _Z	S		N
					δZ_u^2	B _{in}	B _{out}	N
800	1600	0.999	0.79E-2	0.59E-2	0.35E-4	0.14E-2	-0.08E-2	0.50E-2
1600	2400	0.999	0.86E-2	0.67E-2	0.45E-4	0.18E-2	-0.10E-2	0.50E-2
2400	3200	0.999	0.92E-2	0.73E-2	0.54E-4	0.21E-2	-0.12E-2	0.50E-2
3200	4000	0.999	0.97E-2	0.78E-2	0.61E-4	0.24E-2	-0.13E-2	0.50E-2
.
.
.
16000	16800	0.899	1.30E-2	1.07E-2	1.15E-4	0.51E-2	-0.25E-2	0.45E-2
16800	17600	0.818	1.24E-2	1.02E-2	1.04E-4	0.53E-2	-0.24E-2	0.41E-2
17600	18400	0.701	1.15E-2	0.93E-2	0.86E-4	0.54E-2	-0.21E-2	0.35E-2
18400	19200	0.594	1.06E-2	0.84E-2	0.71E-4	0.55E-2	-0.18E-2	0.30E-2
19200	20000	0.501	0.98E-2	0.76E-2	0.57E-4	0.56E-2	-0.15E-2	0.25E-2
20000	20800	0.504	1.00E-2	0.77E-2	0.59E-4	0.57E-2	-0.16E-2	0.25E-2
20800	21600	0.581	1.09E-2	0.85E-2	0.73E-4	0.58E-2	-0.19E-2	0.29E-2
21600	22400	0.707	1.22E-2	0.98E-2	0.97E-4	0.60E-2	-0.23E-2	0.35E-2
.
.
.
964000	972000	0.999	5.91E-2	3.75E-2	14.06E-4	3.98E-2	-2.18E-2	0.50E-2
972000	980000	1.037	6.09E-2	3.89E-2	15.13E-4	4.04E-2	-2.31E-2	0.52E-2
980000	988000	1.001	6.01E-2	3.80E-2	14.46E-4	4.05E-2	-2.23E-2	0.50E-2
988000	996000	1.010	5.92E-2	3.77E-2	14.23E-4	3.96E-2	-2.20E-2	0.50E-2



Example : $^{232}\text{Th}(n,\gamma)$ in URR CRP IAEA "Th-U fuel cycle"

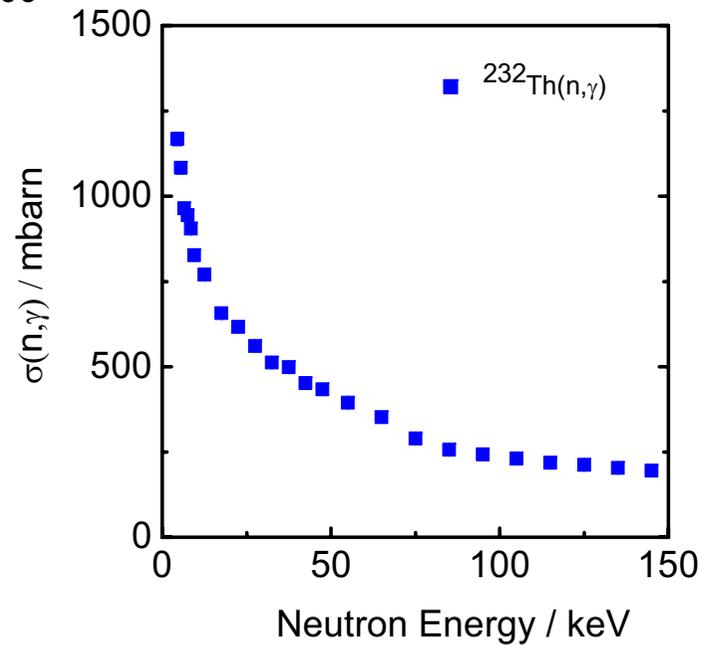
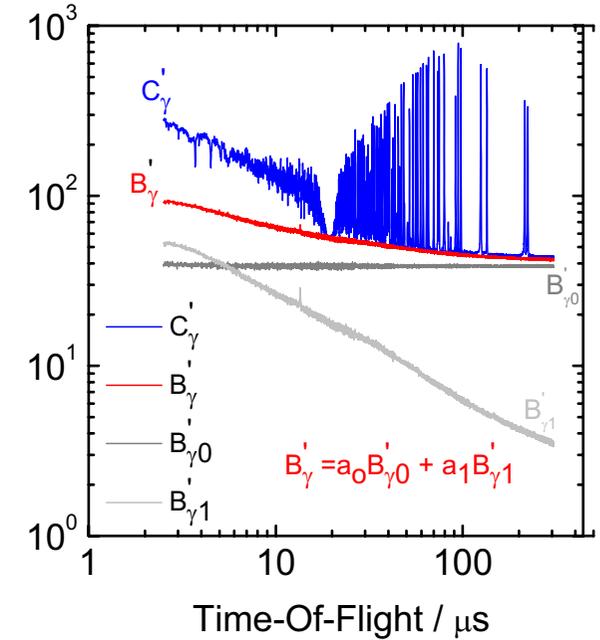


A. Borella et al. NSE 152 (2006) 1-14

$$Y_{\gamma,\text{exp}} = N \frac{1}{\varepsilon_r} \frac{C'_\gamma - B_\gamma}{\phi}$$

$$Y_{\gamma,\text{exp}} = N \frac{\sigma_\phi}{\varepsilon_r} \frac{C'_\gamma - B_\gamma}{C'_\phi - B_\phi}$$

$$\sigma(n,\gamma) = F_c Y_{\gamma,\text{exp}}$$



Correlated uncertainties due to background in capture data

E_{\min}	E_{\max}	σ_{γ}	$\delta\sigma_{\gamma}$	$\delta\sigma_{\gamma,u}$	ρ
keV	keV	mb	(%)	(%)	
4	6	1107.9	0.49	0.17	1.00 0.60 0.57 0.58 0.55 0.53 0.62 0.58 0.56 0.61 0.58 0.54 0.51
6	8	934.2	0.44	0.19	1.00 0.55 0.56 0.53 0.51 0.60 0.57 0.55 0.60 0.56 0.53 0.49
8	10	845.1	0.43	0.21	1.00 0.54 0.51 0.49 0.58 0.55 0.52 0.57 0.54 0.51 0.47
10	15	749.1	0.38	0.15	1.00 0.52 0.50 0.59 0.56 0.54 0.59 0.55 0.52 0.49
15	20	638.7	0.39	0.18	1.00 0.48 0.57 0.54 0.52 0.56 0.53 0.50 0.47
20	30	571.3	0.36	0.14	1.00 0.55 0.52 0.50 0.54 0.51 0.48 0.45
30	40	490.3	0.32	0.18	1.00 0.61 0.59 0.64 0.61 0.57 0.54
40	50	429.6	0.31	0.19	1.00 0.56 0.61 0.58 0.54 0.51
50	60	382.9	0.33	0.22	1.00 0.59 0.56 0.52 0.49
60	80	311.4	0.30	0.18	1.00 0.61 0.57 0.54
80	100	242.5	0.33	0.22	1.00 0.54 0.51
100	120	217.8	0.33	0.23	1.00 0.48
120	140	201.6	0.33	0.24	1.00

dead time, background + normalization (1.5%)

E_{\min}	E_{\max}	σ_{γ}	$\delta\sigma_{\gamma}$	$\delta\sigma_{\gamma,u}$	ρ													
keV	keV	mb	(%)	(%)														
4	6	1107.9	1.70	0.17	1.00	0.85	0.85	0.86	0.86	0.87	0.88	0.88	0.88	0.89	0.89	0.88	0.88	
6	8	934.2	1.64	0.19		1.00	0.88	0.89	0.89	0.89	0.91	0.91	0.91	0.92	0.92	0.91	0.91	
8	10	845.1	1.63	0.21			1.00	0.89	0.89	0.90	0.91	0.91	0.91	0.92	0.92	0.91	0.91	
10	15	749.1	1.61	0.15				1.00	0.90	0.91	0.93	0.92	0.93	0.93	0.93	0.93	0.92	
15	20	638.7	1.61	0.18					1.00	0.91	0.92	0.92	0.93	0.93	0.93	0.93	0.92	
20	30	571.3	1.59	0.14						1.00	0.93	0.93	0.93	0.94	0.93	0.93	0.93	
30	40	490.3	1.56	0.18							1.00	0.95	0.95	0.96	0.95	0.95	0.95	
40	50	429.6	1.56	0.19								1.00	0.95	0.96	0.95	0.95	0.95	
50	60	382.9	1.55	0.22									1.00	0.96	0.96	0.95	0.95	
60	80	311.4	1.55	0.18										1.00	0.96	0.96	0.96	
80	100	242.5	1.56	0.22											1.00	0.96	0.95	
100	120	217.8	1.55	0.23												1.00	0.95	
120	140	201.6	1.55	0.24														1.00

Application of reaction model to deduce model parameters:

REFIT, SAMMY	⇒	resolved resonance parameters
FITACS	⇒	average resonance parameters

Minimize χ^2 as a function of parameters \vec{a} (resonance parameters)

$$\chi^2(\vec{a}) = (\vec{z}_{\text{exp}} - \vec{z}_M(\vec{a}))^T \underline{V}_{z,\text{exp}}^{-1} (\vec{z}_{\text{exp}} - \vec{z}_M(\vec{a}))$$

Covariance of parameters \vec{a}

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

Covariance of calculated \underline{Z}_M

$$\underline{V}_{z,M} = \underline{G}_a \underline{V}_a \underline{G}_a^T$$

Z_{exp} : $\langle \sigma_{\gamma} \rangle$ average capture cross section
 Model : Generalized SLBW in URR
 \vec{a} : Γ_0 and Γ_1 average radiation width for $\ell = 0, 1$

	$\delta Z_{\text{exp}} = 1.6\%$ and $\rho = 0.0$			$\delta Z_{\text{exp}} = 1.6\%$ and $\rho = 0.9$		
	$\delta Z_u = 1.6\%$ $\delta Z_c = 0.0\%$			$\delta Z_u = 0.5\%$ $\delta Z_c = 1.5\%$		
Γ_0	1.18 %	1.00	- 0.74	1.81 %	1.00	0.88
Γ_1	0.95 %		1.00	0.97 %		1.00
E_n / keV	$\delta \sigma_{\gamma, M} (\%)$			$\delta \sigma_{\gamma, M} (\%)$		
5	0.48			0.88		
50	0.33			0.80		
100	0.35			0.97		

- **Error \neq uncertainty**
 - Random error : expectation value = 0
 - Systematic error (correction factor) : expectation value = 0
- **All uncertainties are statistical**
- **Evaluation of uncertainties**
 - Type A : statistical analysis of repeated measurements
 - Type B : scientific judgment
- **Importance of covariance information**
- **Quote all components involved in the data reduction process which create correlated uncertainties**
- **AGS, reduction of TOF-data with propagation of correlated and uncorrelated uncertainties including full reporting of the reduction process**