
Evaluation of experimental data in the resolved resonance region

Contribution of the Nuclear Data Group of Cadarache

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Outlines

Neutron Resonance Shape Analysis Codes

⇒ SAMMY (ORNL) and CONRAD (CEA/Cadarache)

Implicit Data Covariance Matrix with the AGS methodology

⇒ ^{235}U fission cross section

Use IDC matrix in the Neutron Resonance Shape Analysis codes

⇒ Data Covariance Matrix for ^{127}I transmission data

Time resolution of the facility

⇒ Analytic/Monte-Carlo descriptions of the resolution function

Generalization of the IDC methodology to Resonance-Parameter Covariance Matrix

⇒ CONRAD Marginalization

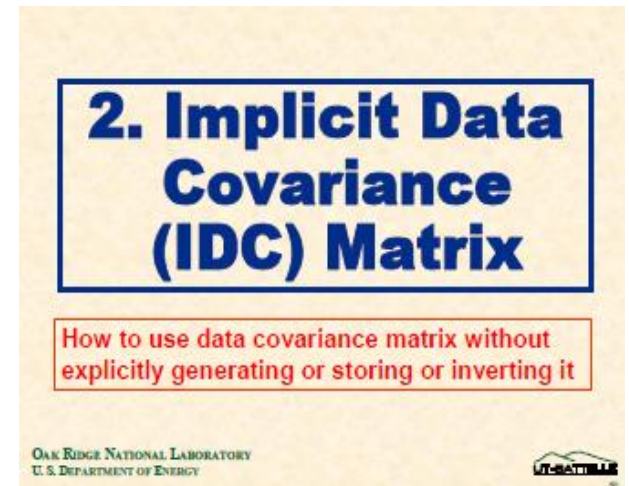
Neutron Resonance Shape Analysis codes

SAMMY: the option “**USER-SUPPLIED IMPLICIT DATA COVARIANCE MATRIX**” was implemented in 2002 to read AGS covariance files (Test Case Tr140, I129 transmission data).

Practical Alternatives to Explicitly Generating and Inverting Data Covariance Matrices, N. M. Larson, Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew, Gatlinburg, Tennessee, April 6-11, 2003

Some Thoughts on the Data Analysis Process, N.M Larson, Second Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements 13-17 October 2003 NIST, Gaithersburg, MD, USA

Use of Covariance Matrices in SAMMY, N.M. Larson, Wonder 2006, 9-11 October, 2006 Chateau de Cadarache, France



CONRAD: by default, CONRAD uses the IDC methodology to read AGS covariance files.

Estimation des incertitudes dans l'évaluation des sections efficaces de réactions nucléaires, Benoit Habert, PhD Thesis, Université de Grenoble, 2009.

A Concise Method for Storing and Communicating the Data Covariance Matrix

N.M. Larson, ORNL/TM-2008/104, August 2008.

The covariance matrix associated with experimental data (cross section, transmission, or other) consists of several components. Statistical uncertainties on the measured quantity (counts) provide a diagonal contribution. Off-diagonal components arise from uncertainties on the parameters (such as normalization or background) that figure into the data reduction process; these are denoted systematic or “common” uncertainties, since they are common to many data points.

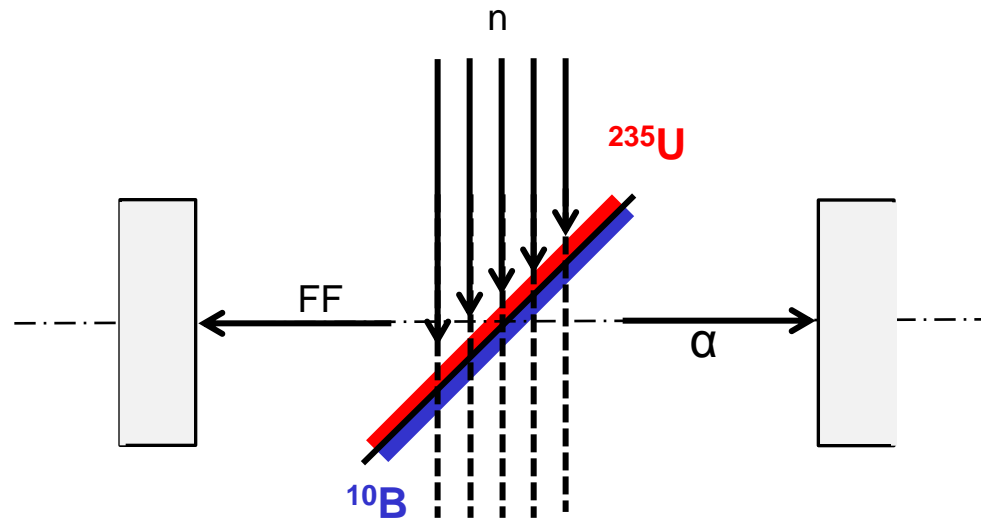
The full off-diagonal **Data Covariance Matrix** (DCM) can be extremely large, since the size is the square of the number of data points. Fortunately, it is not necessary to explicitly calculate, store, or invert the DCM. Likewise, it is not necessary to explicitly calculate, store, or use the inverse of the DCM. Instead, **it is more efficient to accomplish the same results using only the various component matrices that appear in the definition of the DCM.** Those component matrices are either diagonal or small (the number of data points times the number of data-reduction parameters); hence, this “**Implicit Data Covariance**” (IDC) **method requires far less array storage and far fewer computations while producing more accurate results.**

The purpose of this report is to encourage experimentalists to report all information necessary for the creation of the DCM without actually creating the full DCM. Data repositories can then readily store the needed information and communicate it to analysts and evaluators.

Implicit Data Covariance Matrix with AGS methodology

How to generate cross-correlations between different reduced data ?

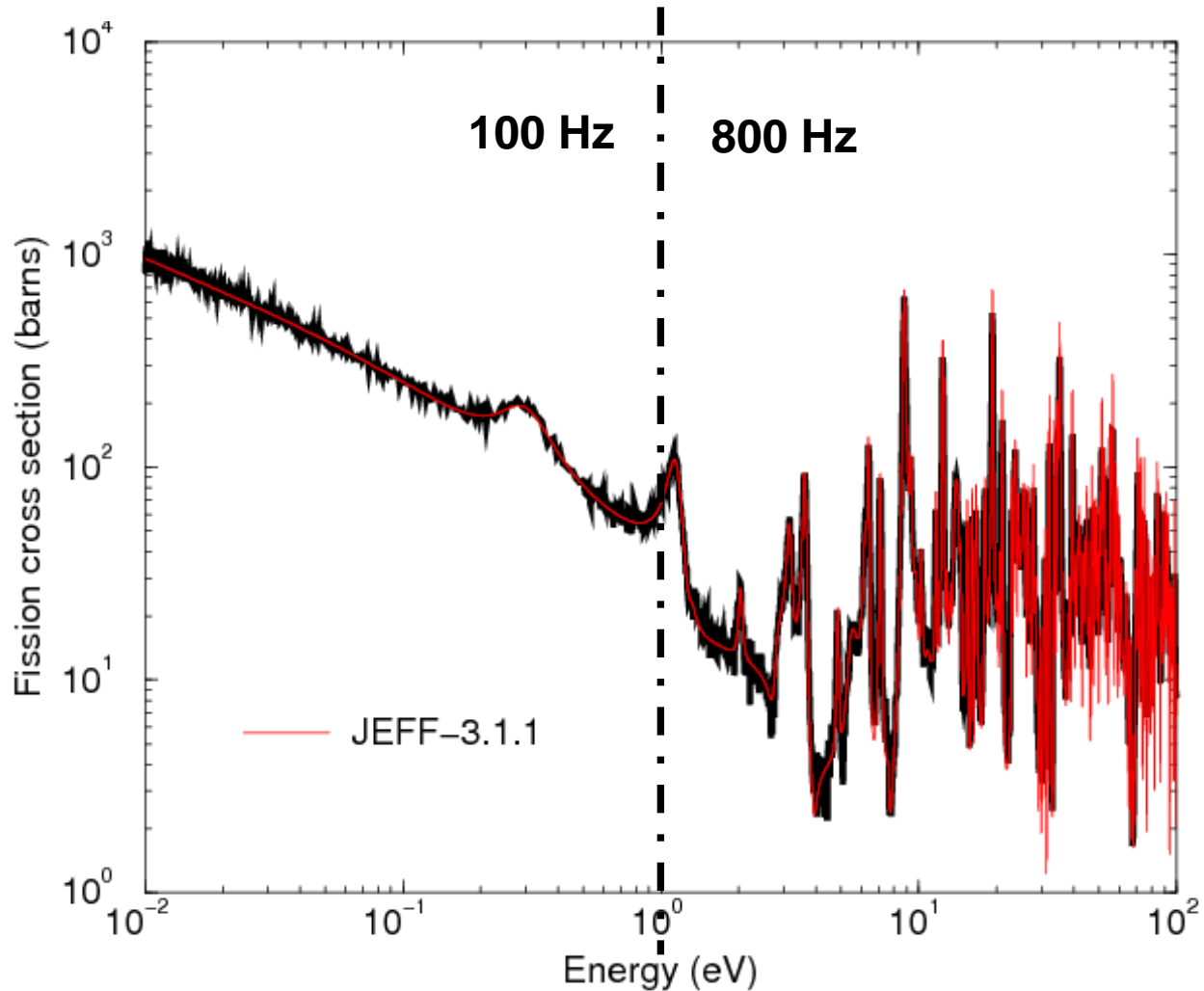
Data Covariance Matrix for fission measurements*



$$\sigma_f(t) = N \frac{a(t)Y_U(t) - B_U(t)}{a(t)Y_B(t) - B_B(t)} \sigma_B(t)$$

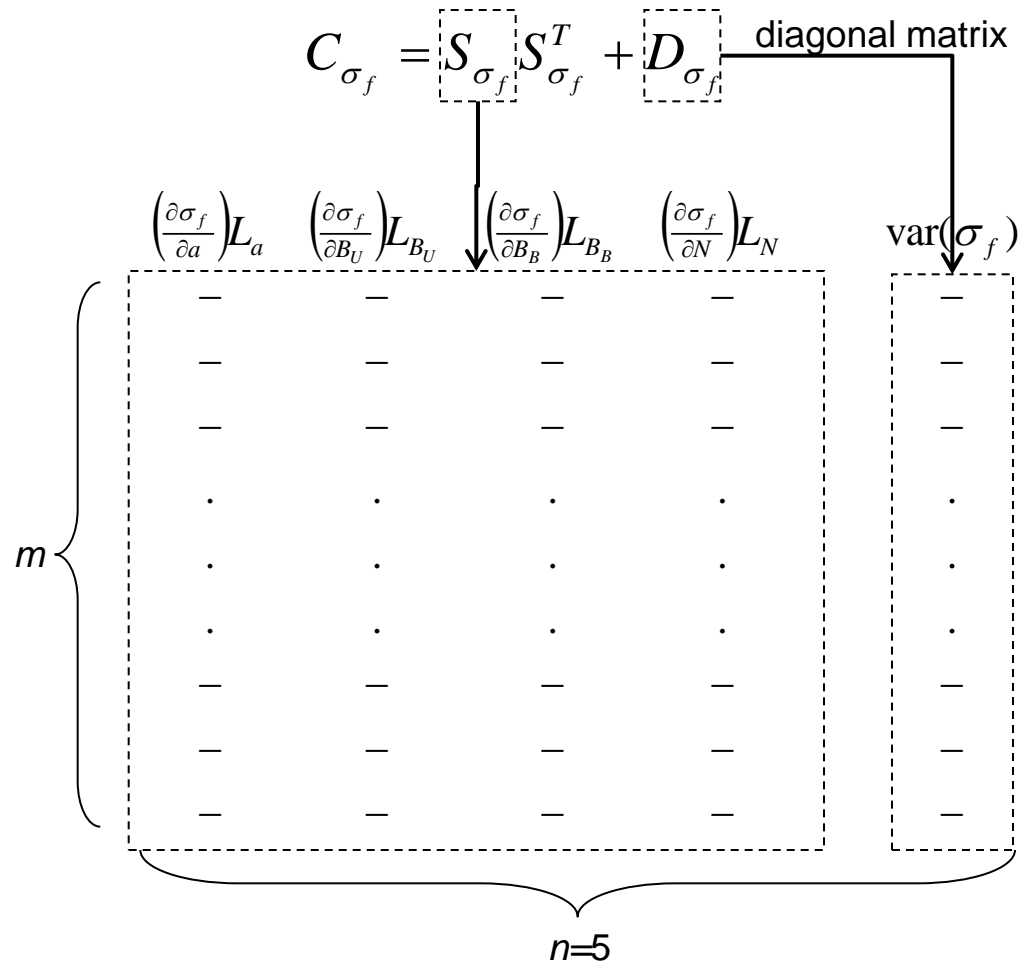
Implicit Data Covariance Matrix with AGS methodology

$^{235}\text{U}(n,f)$ measured at the GELINA facility*, L=10 m, 100Hz, 800Hz

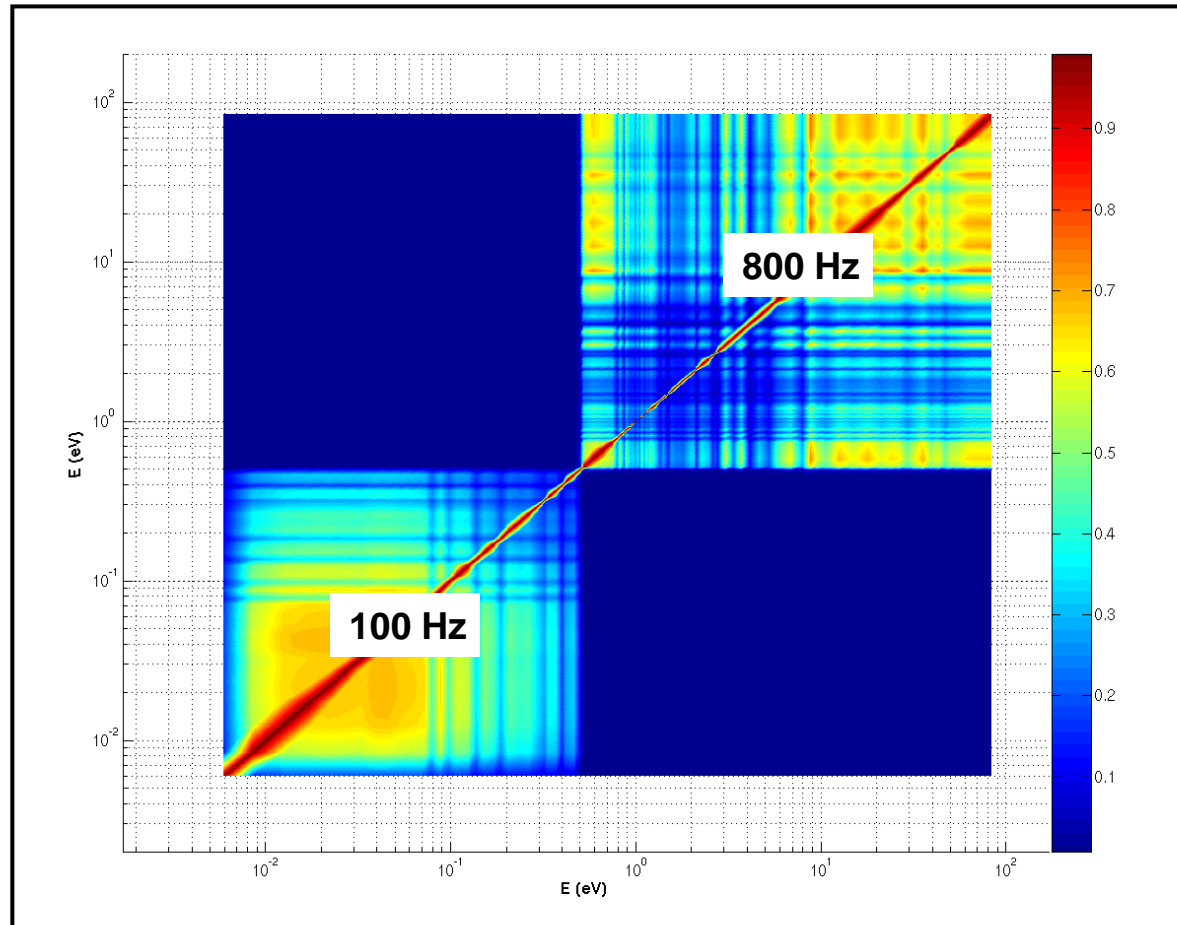


Implicit Data Covariance Matrix with AGS methodology

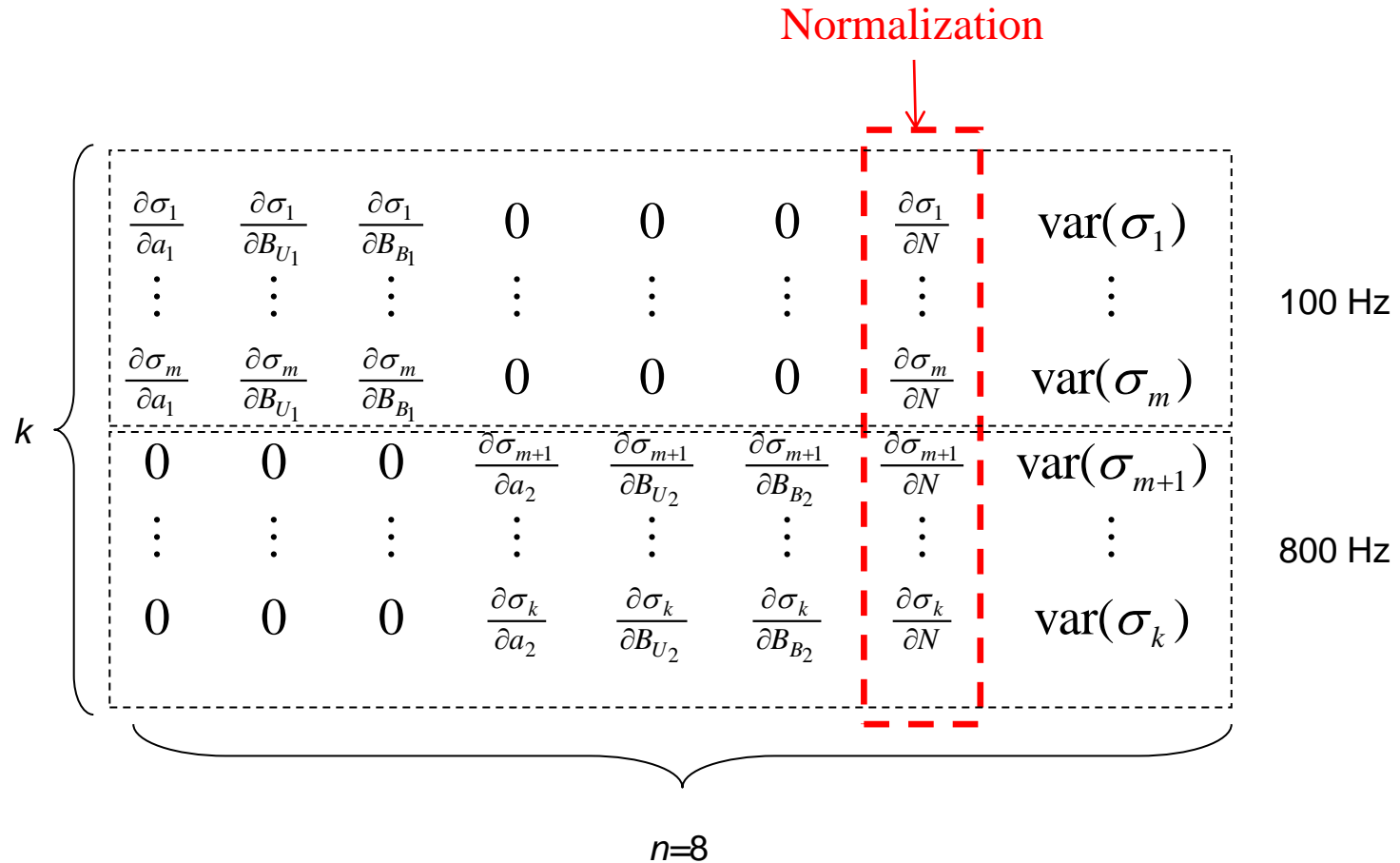
$$\sigma_f(t) = N \frac{a(t)Y_U(t) - B_U(t)}{a(t)Y_B(t) - B_B(t)} \sigma_B(t)$$



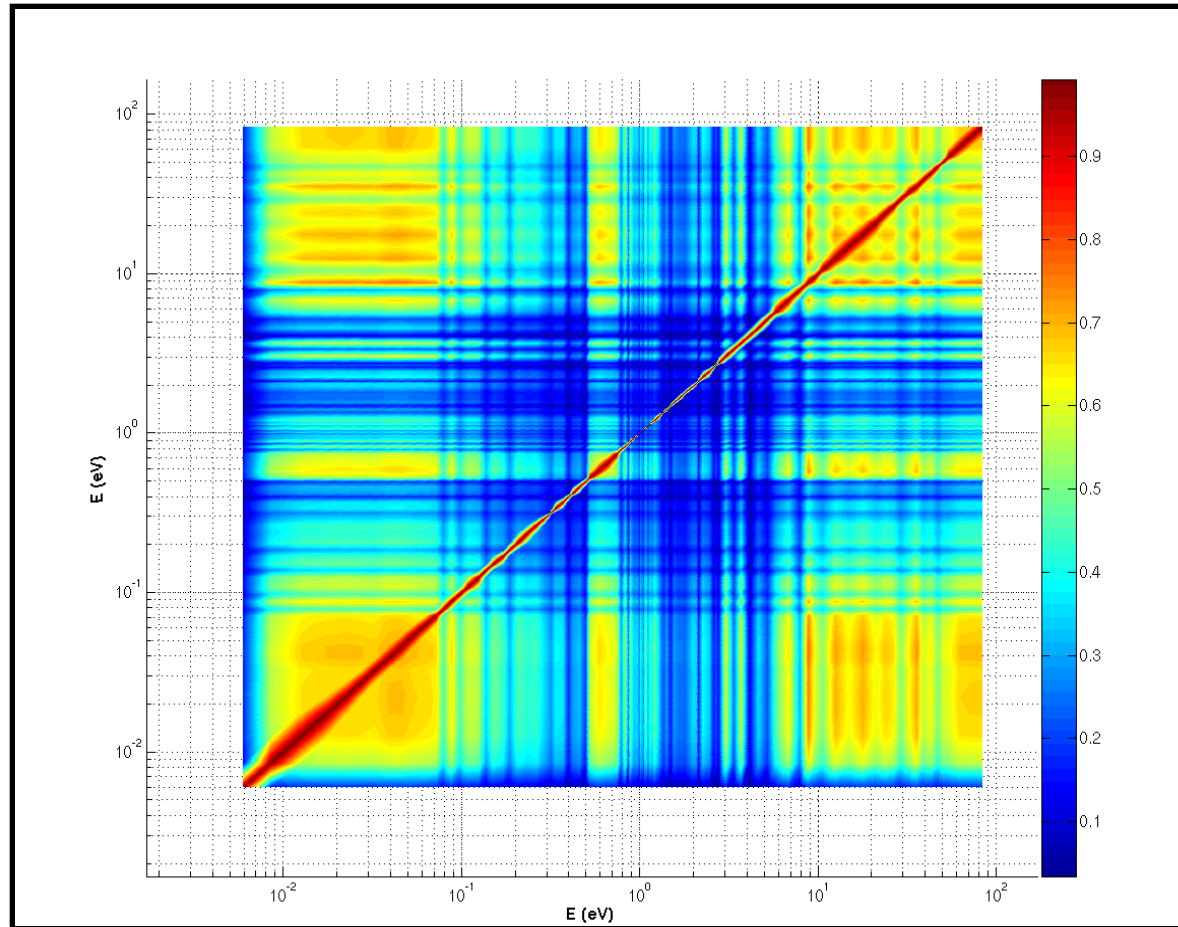
Implicit Data Covariance Matrix with AGS methodology



Implicit Data Covariance Matrix with AGS methodology



Implicit Data Covariance Matrix with AGS methodology



Use Implicit Data Covariance Matrix

What can happen when off-diagonal data covariance matrix elements are used to fit reduced data ?

Linear least-squares \Rightarrow the « best » estimate of the parameters are found iteratively by solving the following equations

$$M_{x_1}^{-1} = M_{x_0}^{-1} + G_x^T C^{-1} G_x$$

$$X_1 = X_0 + M_{x_1}^{-1} G_{x_0}^T C^{-1} (Y_{\text{exp}} - Y_{\text{th}}(x_0))$$

With

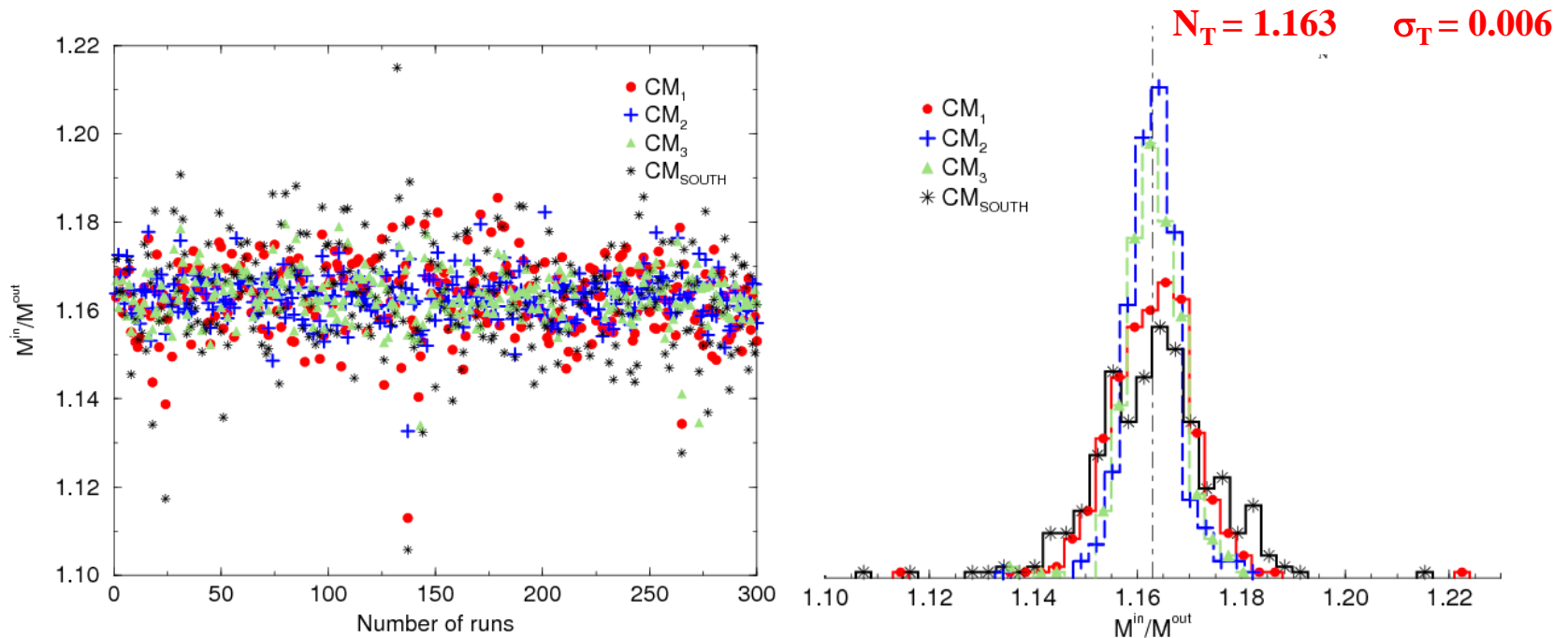
$$C = SS^T + D$$

Use Implicit Data Covariance Matrix

Data Covariance Matrix for transmission

$$T(t) = \frac{1}{N_T} \frac{a_{in}(t)N_{in}(t) - B_{in}}{a_{out}(t)N_{out}(t) - B_{out}}$$

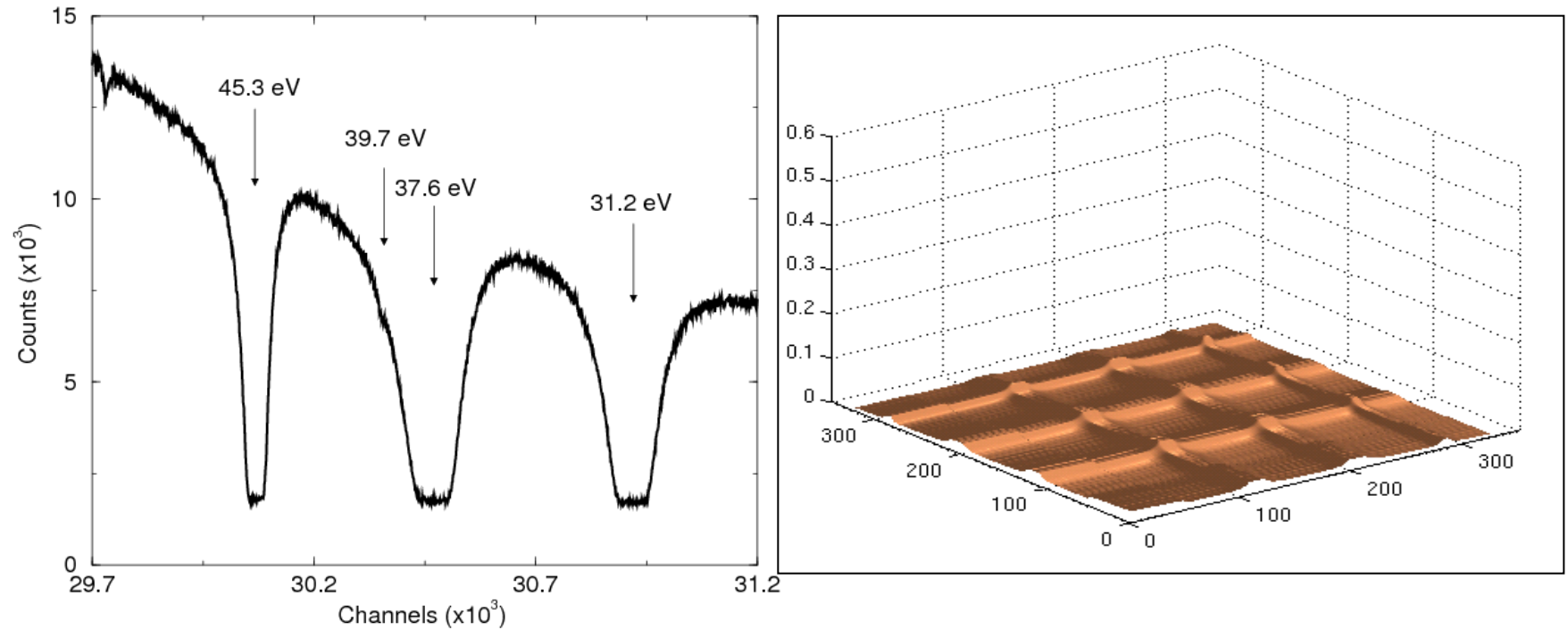
The normalisation of the transmission data is provided by four boron trifluoride (BF_3) detectors placed in the concrete wall above the uranium target



Use Implicit Data Covariance Matrix

Raw transmission data (thick PbI_2 sample) measured at the GELINA facility
L=50m, 800 Hz, FP4

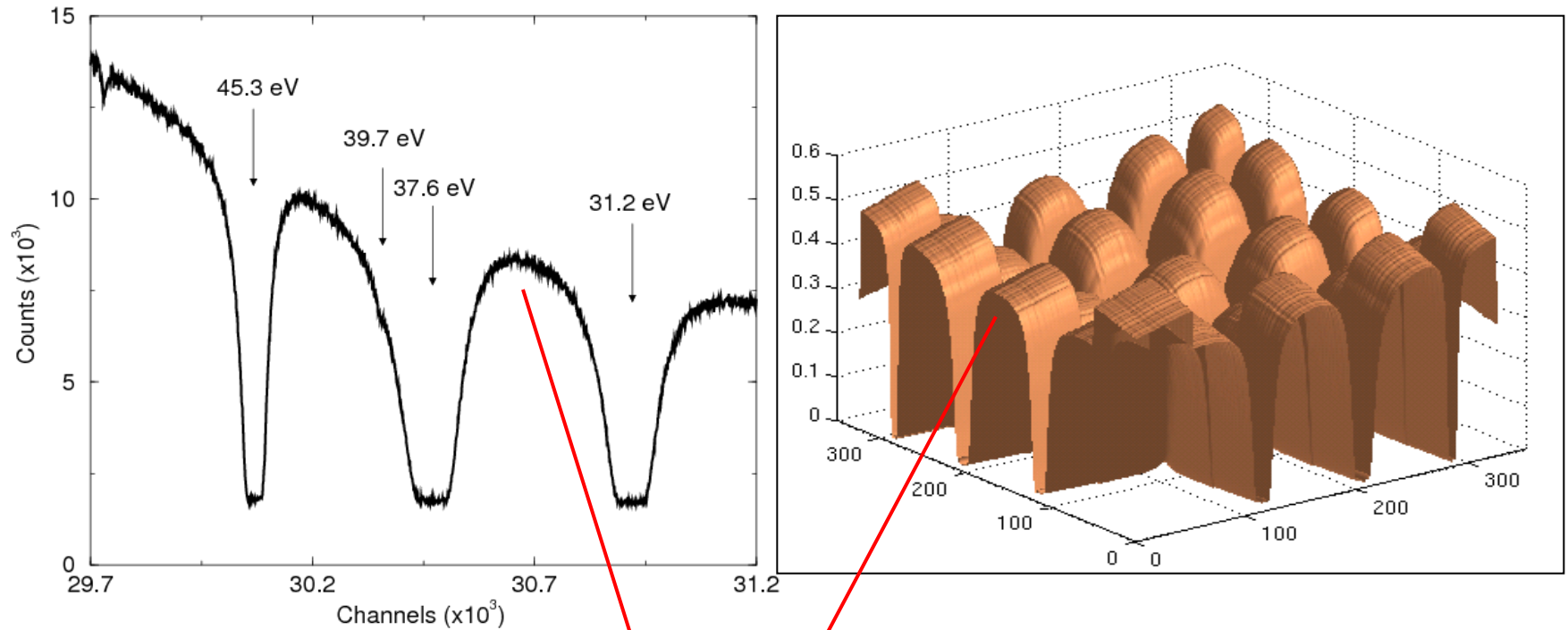
$$N_T = 1.163 \pm 0.0$$



Use Implicit Data Covariance Matrix

Raw transmission data (thick PbI_2 sample) measured at the GELINA facility, $L=50\text{m}$, 800 Hz , FP4

$N_T = 1.163 \pm 0.006$ (0.5%)

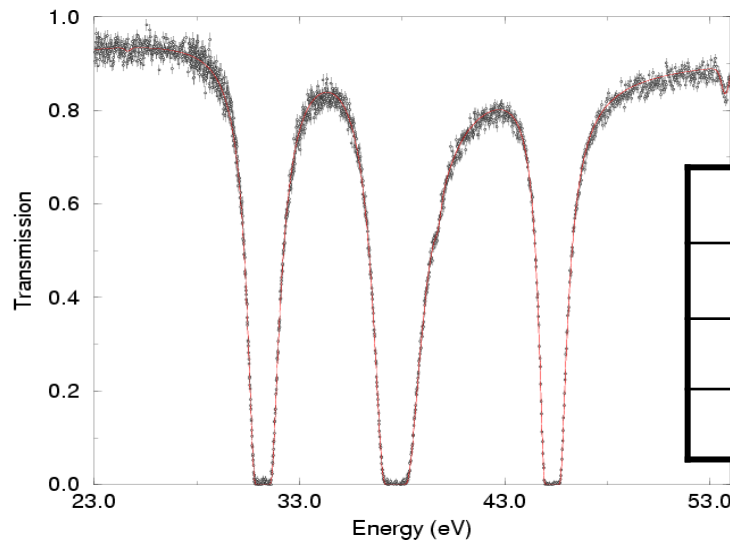


$$\sigma_p = 4\pi R'^2 \Rightarrow \text{potential scattering radius } R'$$

Use Implicit Data Covariance Matrix

Transmission, PbI_2 sample : Least-squares fit of R' with SAMMY and CONRAD. The Implicit Data Covariance matrix $C=SS^T+D$ takes into account the uncertainty on the normalization:

$$N_T=1.163 \pm 0.006 (0.5\%)$$



SAMMY+IDC	$R' = 6.690 \pm 0.001$ fm
CONRAC+IDC	$R' = 6.697 \pm 0.001$ fm
CONRAD+Marginalization	$R' = 6.68 \pm 0.16$ fm
Direct perturbation	$\Delta R' \approx 0.14$ fm

The « unexpected » consequences of IDC can be solved by using the **marginalization** procedure of CONRAD and the **PUP** methodology of SAMMY*

Generalization of the IDC methodology

IDC : a solution to store large Resonance-Parameter Covariance Matrix ?

$M_x \Rightarrow$ Resonance-Parameter Covariance Matrix (RPCM) provided by the fitting model

$M_\theta \Rightarrow$ Covariance matrix between the auxiliary parameters (nuisance or latent parameters)

The covariance matrix can be partitioned as follow :

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \quad \begin{cases} \Sigma_{11} = M_x + M_x^\theta \\ \Sigma_{22} = M_\theta \\ \Sigma_{12} = M_{x,\theta} \end{cases}$$

However, at the end of the fitting procedure, the covariance matrix between the parameters is given by:

$$M = \begin{pmatrix} M_x & 0 \\ 0 & M_\theta \end{pmatrix}$$

Under this fitting model, the cross-covariance matrix $M_{x,\theta}$ between x and θ contained only zeros

Generalization of the IDC methodology

« Zero variance penalty » condition

Non-zero elements can be calculated through the use of a particular case that consists in determining M_x^θ and $M_{x,\theta}$ such that:

$$\text{var}(y) = G_x M_x G_x^T$$

$$\text{var}(y) = G \Sigma G^T$$

For a vector quantity y of general dimension k , the derivative matrix G of the quantity y to the parameters x and θ is defined as:

$$G = (G_x, G_\theta)$$

Where

$$G_x = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_k}{\partial x_1} & \cdots & \frac{\partial y_k}{\partial x_n} \end{pmatrix} \quad G_\theta = \begin{pmatrix} \frac{\partial y_1}{\partial \theta_1} & \cdots & \frac{\partial y_1}{\partial \theta_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_k}{\partial \theta_1} & \cdots & \frac{\partial y_k}{\partial \theta_m} \end{pmatrix}$$

Generalization of the IDC methodology

By using the partitioned form of G , we have

$$\text{var}(y) = G_x M_x G_x^T$$

$$\text{var}(y) = G \Sigma G^T = G_x M_x G_x^T + \underbrace{G_x M_x^\theta G_x^T + G_x M_{x,\theta} G_\theta^T + (G_x M_{x,\theta} G_\theta^T)^T + G_\theta M_\theta G_\theta^T}_{= 0}$$

This condition lead to the following results

$$G_x M_{x,\theta} G_\theta^T + (G_x M_{x,\theta} G_\theta^T)^T = -G_x M_x^\theta G_x^T - G_\theta M_\theta G_\theta^T$$

By definition, $G_\theta M_\theta G_\theta^T$ is a symmetric positive-definite matrix whose the number of rows and columns is equal to the size of y :

$$G_\theta M_\theta G_\theta^T = (G_\theta M_\theta G_\theta^T)^T$$

Therefore :

$$G_x M_{x,\theta} G_\theta^T + (G_x M_{x,\theta} G_\theta^T)^T = -G_x M_x^\theta G_x^T - (G_\theta M_\theta G_\theta^T)^T$$

Generalization of the IDC methodology

$$G_x M_{x,\theta} G_\theta^T + (G_x M_{x,\theta} G_\theta^T)^T = -G_x M_x^\theta G_x^T - (G_\theta M_\theta G_\theta^T)^T$$

This equality is satisfied if we choose M_x^θ and $M_{x,\theta}$ such that:

$$G_x M_{x,\theta} G_\theta^T = -G_\theta M_\theta G_\theta^T \quad (\text{a})$$

$$G_x M_x^\theta G_x^T = G_\theta M_\theta G_\theta^T \quad (\text{b})$$

By multiplying the left and right hand sides of (a) by G_x^T and G_θ , one obtains:

$$M_{x,\theta} = -(G_x^T G_x)^{-1} G_x^T G_\theta M_\theta$$

The covariance matrix M_x^θ can be directly deduced by multiplying the left and right hand sides of equation (b) by G_x^T and G_x :

$$M_x^\theta = (G_x^T G_x)^{-1} G_x^T G_\theta M_\theta G_\theta^T G_x (G_x^T G_x)^{-1}$$

Link with AGS formalism

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \quad \left\{ \begin{array}{l} \Sigma_{11} = M_x + (G_x^T G_x)^{-1} G_x^T G_\theta M_\theta G_\theta^T G_x (G_x^T G_x)^{-1} \\ \Sigma_{12} = -(G_x^T G_x)^{-1} G_x^T G_\theta M_\theta \\ \Sigma_{22} = M_\theta \end{array} \right.$$

Cholesky decomposition of the positive-definite matrix M_x^θ into the product of a lower triangular matrix and its conjugate transpose lead to:

$$\Sigma_{11} = M_x + SS^T$$

If the contribution of the « statistical » uncertainties (from the fit) are negligible compared to the « systematic » uncertainties

$$M_x \approx \text{diag}(\text{var}(x_1) \dots \text{var}(x_n))$$

Generalization of the IDC methodology

Link with AGS formalism:

Simple example with the normalization $N \pm \Delta N$ and the background $B \pm \Delta B$

$$\Sigma_{11} = M_x + SS^T$$

The matrix M_x contains the variance of the resonance parameters given by the fit

$$M_x \approx \text{diag}(\text{var}(E_1), \text{var}(\Gamma\gamma_1), \text{var}(\Gamma n_1) \dots \text{var}(E_n), \text{var}(\Gamma\gamma_n), \text{var}(\Gamma n_n))$$

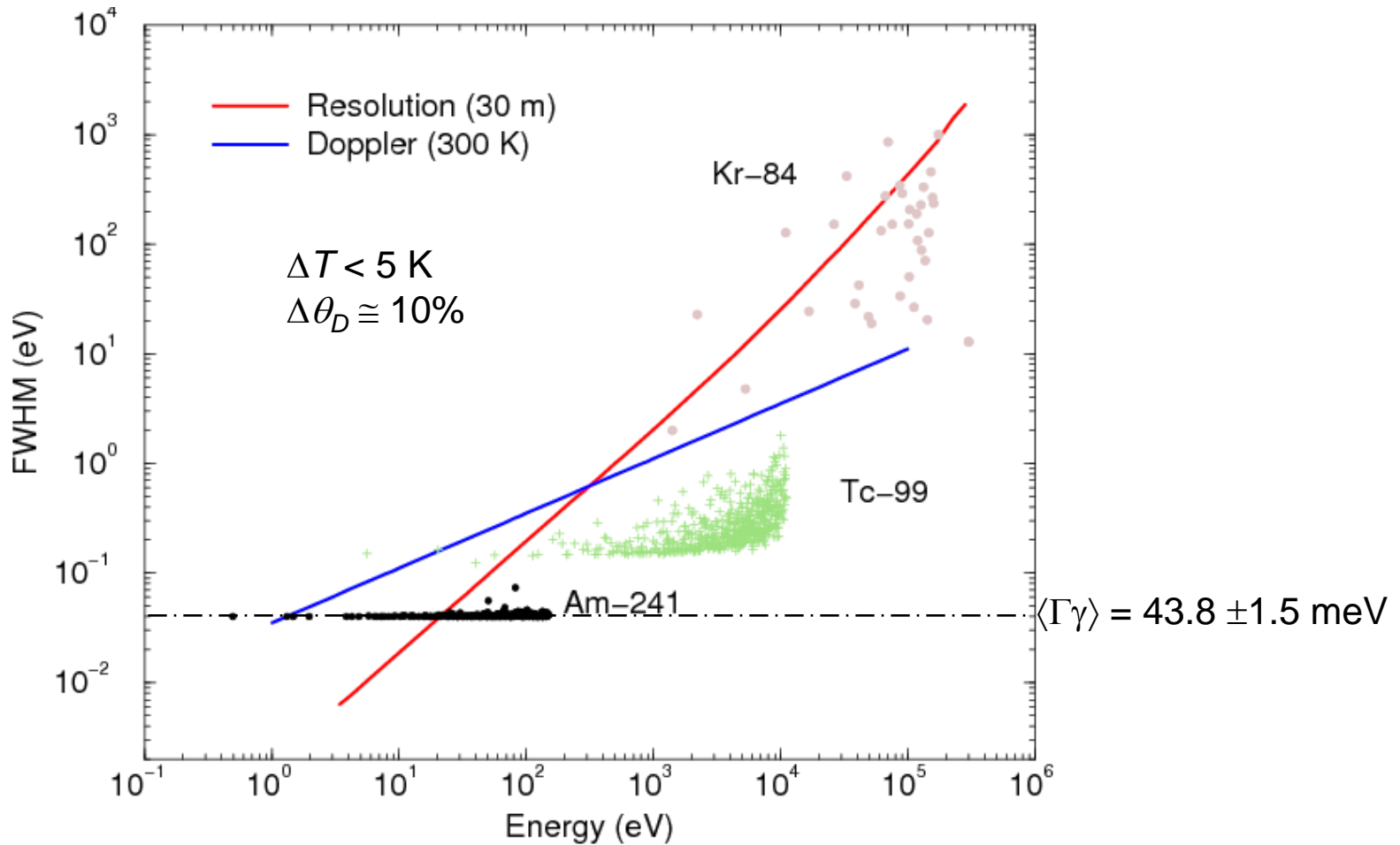
If N and B are independent, the matrix S can be written as follows:

$$S^T = \begin{pmatrix} \frac{\partial E_1}{\partial N} \Delta N, \frac{\partial \Gamma\gamma_1}{\partial N} \Delta N, \frac{\partial \Gamma n_1}{\partial N} \Delta N \dots \frac{\partial E_n}{\partial N} \Delta N, \frac{\partial \Gamma\gamma_n}{\partial N} \Delta N, \frac{\partial \Gamma n_n}{\partial N} \Delta N \\ \frac{\partial E_1}{\partial B} \Delta B, \frac{\partial \Gamma\gamma_1}{\partial B} \Delta B, \frac{\partial \Gamma n_1}{\partial B} \Delta B \dots \frac{\partial E_n}{\partial B} \Delta B, \frac{\partial \Gamma\gamma_n}{\partial B} \Delta B, \frac{\partial \Gamma n_n}{\partial B} \Delta B \end{pmatrix}$$

NB: the positive definiteness requirement will be satisfied if the Resonance-Parameter Covariance Matrices are stored in EXFOR and ENDF-6 format with the IDC methodology.

Time resolution of the facility

How to store Resolution Function in EXFOR ?



Time resolution of the facility

Analytic description of the experimental resolution

Contribution of the neutron source (uranium target, ...)

$$I_t(t) \approx \frac{\ln(2)}{\tau(E)} (k_1 + k_2 E^{k_3}) e^{-\frac{\ln(2)}{\tau(E)} t} \quad \tau(E) = \lambda_\tau \frac{72.298}{\sqrt{E}}$$

Contribution of the water moderator

$$I_m(t) = \frac{1}{2} \left(\frac{\sqrt{E}}{72.298 \Lambda} \right)^3 t^2 e^{-\frac{\sqrt{E}}{72.298 \Lambda} t} \quad \Lambda(E) = \frac{\lambda_0}{\lambda(1eV)} \lambda(E)$$

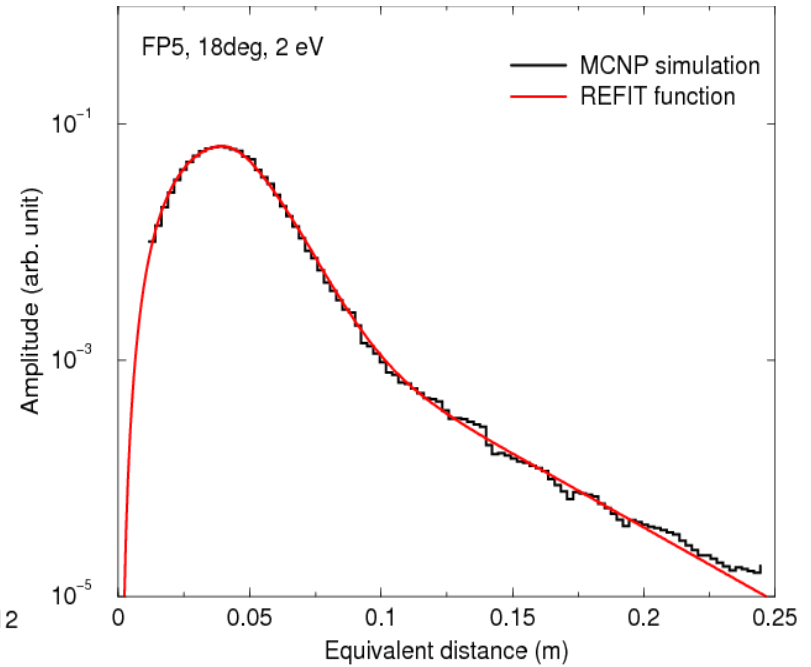
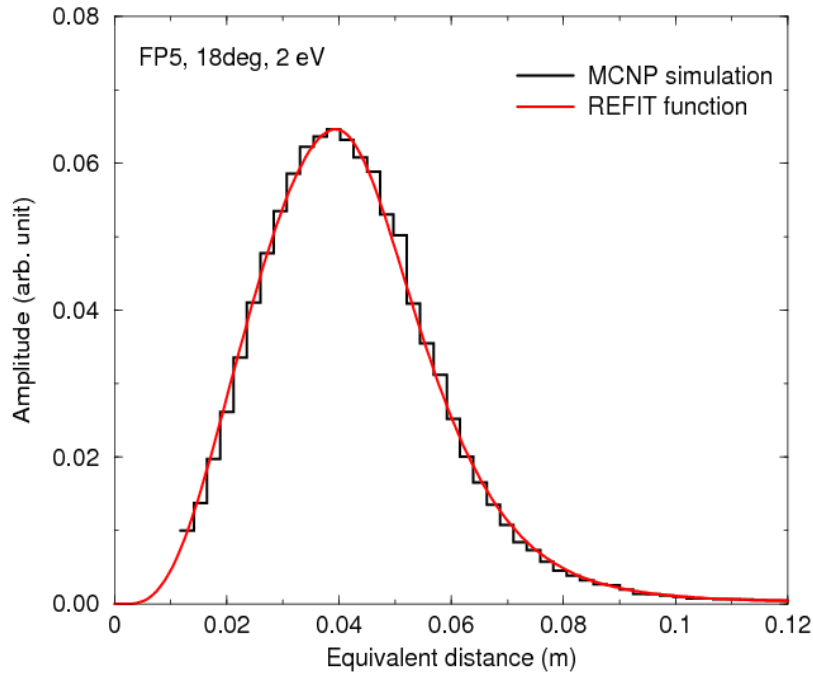
Contribution of the flight path angle

$$I_\theta(t) \propto \sqrt{T_m^2 + (T_m - 2t)^2} \quad T_m = \frac{72.298 D_c \tan(\theta)}{\sqrt{E}}$$

⇒ nuisance parameters of interest are $k_1, k_2, k_3, \lambda_\tau, \lambda_0$ and D_c

Time resolution of the facility

Analytic description of the experimental resolution



Order of magnitude of the parameters :

$$\lambda_0 = 7 \pm 2 \text{ mm}$$
$$\lambda_\tau = 24 \pm 5 \text{ mm}$$
$$D_c = 10 \pm 2 \text{ cm}$$