Joint Research Centre (JRC)

Uncertainty propagation in Time-of-Flight Data

IRMM - Institute for Reference Materials and Measurements

Geel - Belgium

http://irmm.jrc.ec.europa.eu/

http://www.jrc.ec.europa.eu/

- **Definitions**
- **Importance of Covariance Matrix**
- **How to store the matrix**

Definitions

Mean $$\mu_x = \langle x \rangle \qquad \mu_y = \langle y \rangle$$

Variance $$\sigma_x^2 = \langle (x-\mu_x)^2 \rangle = \mathrm{cov}(x,x)$$

Covariance $$\mathrm{cov}(x,y) = \langle (x-\mu_x)(y-\mu_y) \rangle$$

Correlation $$\rho(x,y) = \frac{\mathrm{cov}(x,y)}{\sigma_x \, \sigma_y}$$

Definitions

Linear function

$$f(x_i) = \sum_{i=1}^{k} a_i\, x_i$$

Mean

$$\mu_f = \langle f(x_i) \rangle = \sum_{i=1}^{k} a_i\, \mu_i$$

Variance

$$\sigma_f^2 = \left\langle \left(f(x_i) - \mu_f \right)^2 \right\rangle = \sum_i \sum_j a_i\, a_j \operatorname{cov}(x_i, x_j)$$

Taylor expansion

(1st order)

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

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

Mean

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

Variance

$$\sigma_f^2 = \left\langle \left(f(x_i) - \mu_f \right)^2 \right\rangle \cong \sum_i \sum_j g_i \, g_j \, \mathrm{cov}(x_i, x_j)$$

Matrix Notation

Linear function

$$f(\vec{x}) = \underline{A}\vec{x} \qquad a_{ik} = \frac{\partial f_i}{\partial x_k}$$

Mean

$$\vec{\mu}_f = \underline{A}\,\vec{\mu}_x$$

Variance

$$\underline{V}_f = \underline{A}\,\underline{V}_x\,\underline{A}^T \qquad V_x = \begin{pmatrix} \mathrm{cov}(x_1,x_1) & \mathrm{cov}(x_1,x_2) \\ \mathrm{cov}(x_2,x_1) & \mathrm{cov}(x_2,x_2) \end{pmatrix}$$

Non-linear function (1st order Taylor)

$$f(\vec{x}) \cong f(\vec{\mu}_x) + \underline{G}_x(\vec{x} - \vec{\mu}_x) \qquad g_{x,ik} = \frac{\partial f_i}{\partial x_k}$$

sensitivity matrix
design matrix

Mean

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

Variance

$$\underline{V}_f \cong \underline{G}_x\,\underline{V}_x\,\underline{G}_x^T$$

Propagation of uncertainties : $z = y - b$

Experiment

Independent observables : $(y_1 \pm \sigma_{y_1}) \qquad (y_2 \pm \sigma_{y_2})$

Common background component: $(b \pm \sigma_b)$

Data reduction : $z = y - b$

Average of (y_1, y_2) : $<y> = \dfrac{y_1 + y_2}{2} \qquad \sigma^2_{<y>} = \dfrac{\sigma^2_{y_1} + \sigma^2_{y_1}}{4}$

Background subtraction : $<z> = <y> - b \qquad \sigma^2_{<z>} = \dfrac{\sigma^2_{y_1} + \sigma^2_{y_1}}{4} + \sigma^2_b$

Propagation of uncertainties : z = y – b

$$(y_1, y_2, b) \rightarrow (z_1, z_2) = (y_1 - b, y_2 - b) \rightarrow \langle z \rangle = \frac{z_1 + z_2}{2}$$

uncertainties on y_1 and y_2 not correlated **:** $\underline{V}_y = \begin{bmatrix} \sigma_{y_1}^2 & 0 \\ 0 & \sigma_{y_2}^2 \end{bmatrix}$
e.g. due to counting statistics

uncertainty on background **:** $V_b = \sigma_b^2$
(b not correlated with y_1 and y_2)

$$(z_1, z_2) \quad \Rightarrow \quad < z >$$

Propagation of uncertainties : z = y – b

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

uncorrelated uncertainties due to counting statistics : $\underline{V}_y = \begin{bmatrix} \sigma^2_{y_1} & 0 \\ 0 & \sigma^2_{y_2} \end{bmatrix}$

uncertainty on background (b not correlated with y_1 and y_2): $V_b = \sigma^2_b$

$$\underline{V}_z = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \sigma^2_{y_1} & 0 & 0 \\ 0 & \sigma^2_{y_2} & 0 \\ 0 & 0 & \sigma^2_b \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix} = \begin{bmatrix} \sigma^2_{y_1} + \sigma^2_b & \sigma^2_b \\ \sigma^2_b & \sigma^2_{y_2} + \sigma^2_b \end{bmatrix}$$

$$\underline{V}_z = \underline{A}\, \underline{V}_{y_1, y_2, b}\, \underline{A}^T$$

Propagation of uncertainties : z = y – b

$$(z_1, z_2) \rightarrow \langle z \rangle = \frac{z_1 + z_2}{2}$$

$$V_{\langle z \rangle} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \sigma_{y_1}^2 + \sigma_b^2 & \sigma_b^2 \\ \sigma_b^2 & \sigma_{y_2}^2 + \sigma_b^2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{\sigma_{y_1}^2 + \sigma_{y_2}^2}{4} + \sigma_b^2 \end{bmatrix}$$

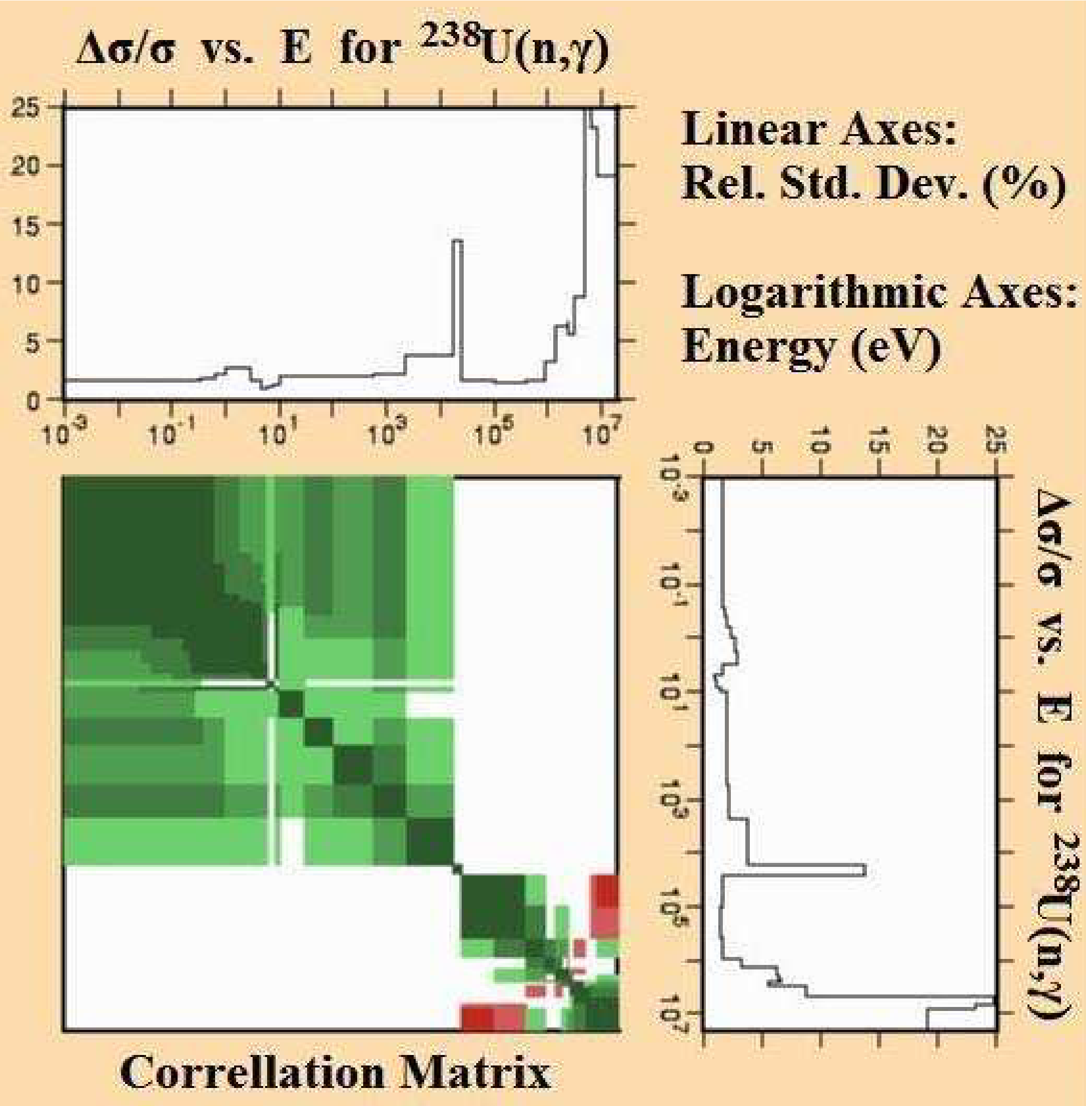
$$\underline{V}_{\langle z \rangle} = \underline{A}\, \underline{V}_{z_1,z_2}\, \underline{A}^T$$

Full covariance $\sigma_{\langle z \rangle}^2 = \frac{\sigma_{y_1}^2 + \sigma_{y_2}^2}{4} + \sigma_b^2$

Only diagonal terms $\sigma_{\langle z \rangle}^2 = \frac{\sigma_{y_1}^2 + \sigma_{y_2}^2}{4} + \frac{\sigma_b^2}{2}$

$\Rightarrow$ Covariance matrix contains information about experiment and data reduction

Examples



Covariance Files in Evaluated Data Files

Produced:
During evaluation from data

Retrospective (model)

L.C. Leal et al., Nucl. Data Sheets 109, 2868 (2008)

Retrospective calculation of C_θ

^{206}Pb + n

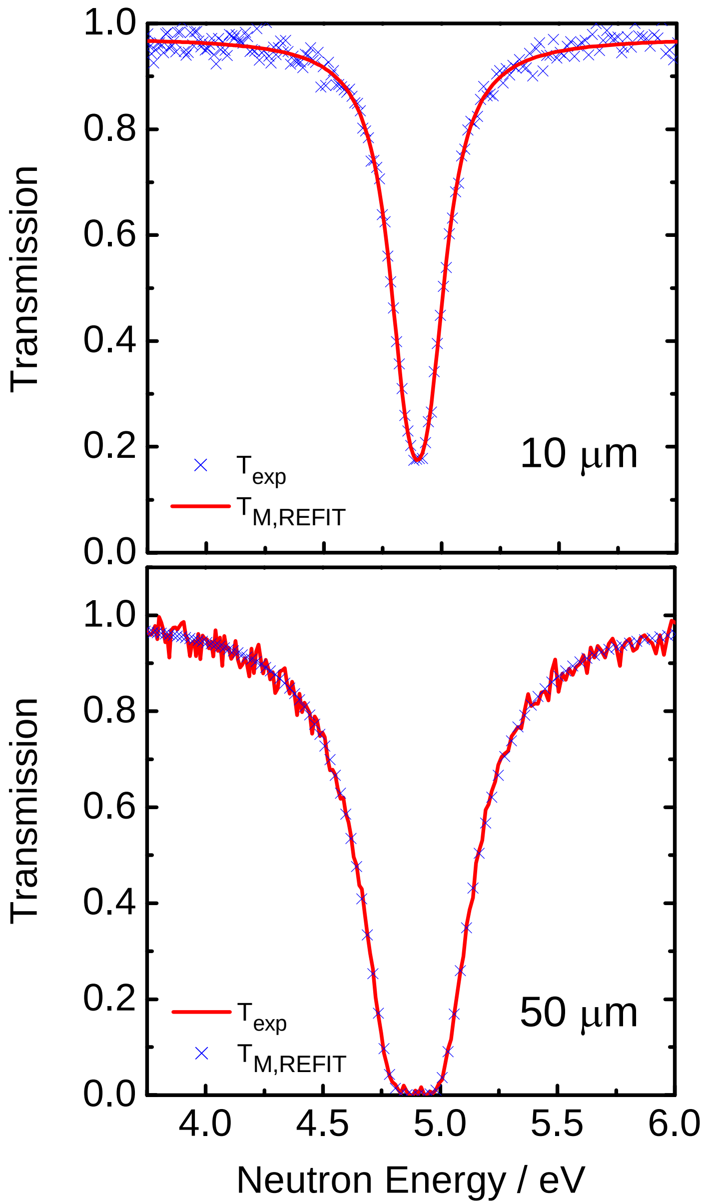
$$C_\theta = (D_\theta^T C_{Y,exp}^{-1} D_\theta)^{-1}$$

GELINA (transmission + capture) + ORELA (transmission)
Borella et al. PRC 76 (2007) 014605 and Horen et al. PRC 20 (1979) 478

RETROSPECTIVE
Rochman and Koning
NIM A589 (2008) 85

E_R	$g\Gamma_n$ / eV	$g\Gamma_\gamma$ / eV	$g\Gamma_n\Gamma_\gamma/(\Gamma_n+\Gamma_\gamma)$ / eV	$\rho(\Gamma_n, \Gamma_\gamma)$	RETROSPECTIVE $\rho(\Gamma_n, \Gamma_\gamma)$
3.36	0.570 ± 0.004	0.146 ± 0.001	0.116 ± 0.001	- 0.15	- 0.16
42.07	1.966 ± 0.163	1.171 ± 0.082	0.734 ± 0.014	- 0.92	- 0.51
66.00	82.210 ± 0.414	1.398 ± 0.018	1.375 ± 0.017	0.03	- 0.00
92.61	32.0 ± 4.0	1.503 ± 0.017	1.436 ± 0.016	- 0.10	- 0.77

C_θ : 4.9 eV resonance for ^{197}Au+n (1/3)



$C_{T,exp}$: only uncorrelated uncertainties due to counting statistics

$\Rightarrow$

Γ_n = (15.06 ± 0.08) meV

Γ_γ = (121.7 ± 1.3) meV

$\rho(\Gamma_n, \Gamma_\gamma)$ = 0.55

$\Rightarrow$

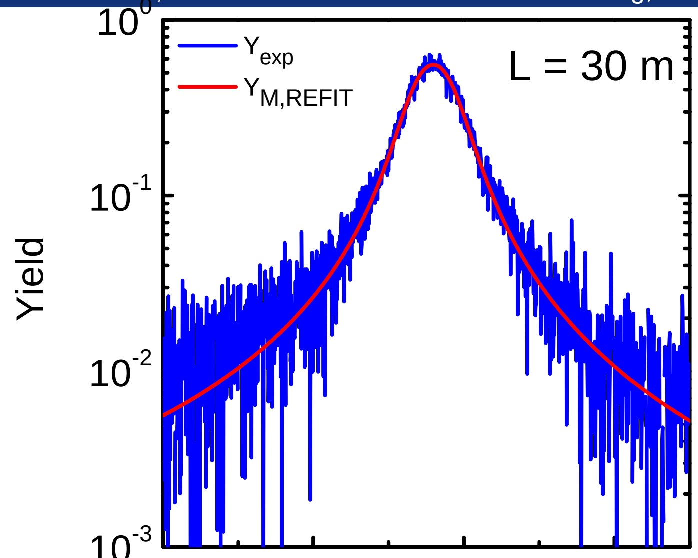
Γ_n = (14.66 ± 0.30) meV

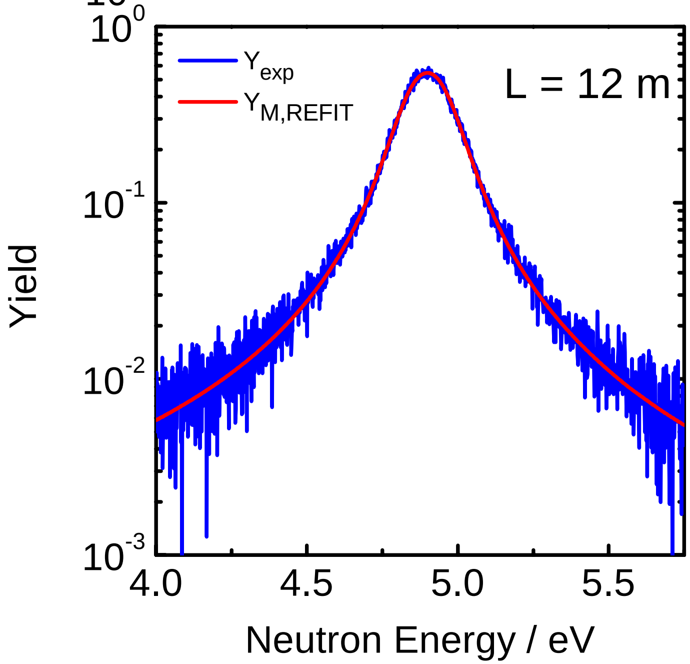
Γ_γ = (124.8 ± 3.7) meV

$\rho(\Gamma_n, \Gamma_\gamma)$ = - 0.96

RSA by REFIT

C_θ : 4.9 eV resonance for ^{197}Au+n (2/3)





$C_{Y,exp}$: only uncorrelated uncertainties due to counting statistics

$\Rightarrow$

$$\Gamma_n = (15.31 \pm 0.12)\ \text{meV}$$
$$\Gamma_\gamma = (118.0 \pm 1.4)\ \text{meV}$$
$$\rho(\Gamma_n, \Gamma_\gamma) = -0.50$$

$\Rightarrow$

$$\Gamma_n = (15.26 \pm 0.15)\ \text{meV}$$
$$\Gamma_\gamma = (118.9 \pm 1.2)\ \text{meV}$$
$$\rho(\Gamma_n, \Gamma_\gamma) = -0.63$$

RSA by REFIT

C_θ : 4.9 eV resonance for $^{197}Au+n$ (3/3)

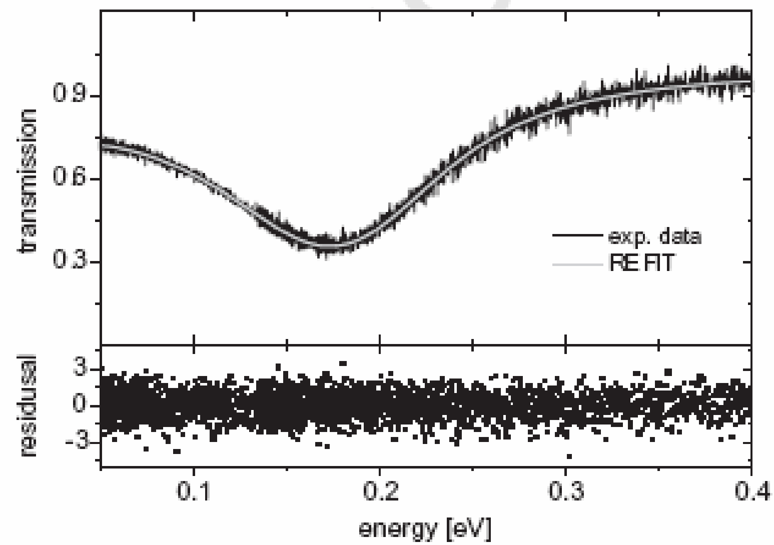
$C_{Z,exp}$: only uncorrelated uncertainties due to counting statistics

Measurements	Γ_n / meV	Γ_γ / meV	$\rho(\Gamma_n, \Gamma_\gamma)$
T1	15.06 ± 0.08	121.7 ± 1.3	0.55
T2	14.66 ± 0.30	124.8 ± 3.7	- 0.96
C1	15.31 ± 0.12	118.0 ± 1.4	- 0.50
C2	15.26 ± 0.15	118.9 ± 1.2	- 0.63
T1 + C1	15.14 ± 0.07	120.0 ± 1.0	0.06
T1 + C2	15.10 ± 0.07	120.2 ± 0.9	- 0.29
T1 + T2 + C1 + C2	15.14 ± 0.06	119.8 ± 0.7	- 0.47

Id-number	Measurement	Distance	Angle (flight path – moderator)	Target thickness
T1	Transmission	50 m	9^o	10 µm
T2	Transmission	50 m	9^o	50 µm
C1	Capture	30 m	0^o	5 µm
C2	Capture	12 m	18^o	5 µm

Cd Resonance Parameters

thickness (at/b)	sample type	flight path length
1.40 10^{-4}	solution	25 m
1.36 10^{-4}	foil	25m
2.24 10^{-4}	foil	25 m



Only uncorrelated uncertainties

Parameter	p / meV			$\rho(p_i,p_j)$		
E_R	178.7	±	0.1	1.00	0.43	0.79
Γ_n	0.640	±	0.001		1.00	0.43
Γ_γ	113.5	±	0.2			1.00

Full Covariance Matrix

Parameter	p / meV			$\rho(p_i,p_j)$		
E_R	178.7	±	0.1	1.00	0.53	0.28
Γ_n	0.640	±	0.004		1.00	0.25
Γ_γ	113.5	±	0.2			1.00

Kopecky et al., NIMB accepted

Data Reduction: Covariance (AGS)

$$\mathbf{Z_1} = F(\mathbf{a_1}, \mathbf{Y_1})$$

Z_1, Y_1 : dimension n
a_1 : dimension k_1

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

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

$\mathbf{V_{a_1}} = \mathbf{L_{a_1}} \mathbf{L_{a_1}}^{\mathbf{T}}$ (Cholesky decomposition)

$$S_{a1} = \left(\frac{\partial Z_1}{\partial a_1}\right) L_{a_1}$$

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

$\left(\frac{\partial \mathbf{Z_1}}{\partial \mathbf{Y_1}}\right)$ only diagonal terms

$$D_{Z1} = \left(\frac{\partial Z_1}{\partial Y_1}\right) D_{Y_1} \left(\frac{\partial Z_1}{\partial Y_1}\right)^T$$

D_{Y_1} → $\mathbf{s^2_{Y1u}}$

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

S_{a_1}: dimension: n x k_1

D_{Z_1}: n values (diagonal)

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

Z, Z_1, Z_2 : dimension n

b : dimension k_b

$$V_b = L_b L_b^T \qquad S_b = \left(\frac{\partial Z}{\partial b}\right) L_b$$

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

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

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

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

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

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

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

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

$$\boxed{V_Z = S_Z S_Z^T + D_Z}$$

dimension: n x k

$k = k_b + k_1 + k_2$

n values (diagonal)

Conditions :

(1) Data reduction starts from spectra subject only to uncorrelated uncertainties

(2) Additional computations using parameters with well defined covariance matrix

(3) Channel – channel operations (+, - , x , ÷) and log, exp, …

Uncertainty propagation results in:

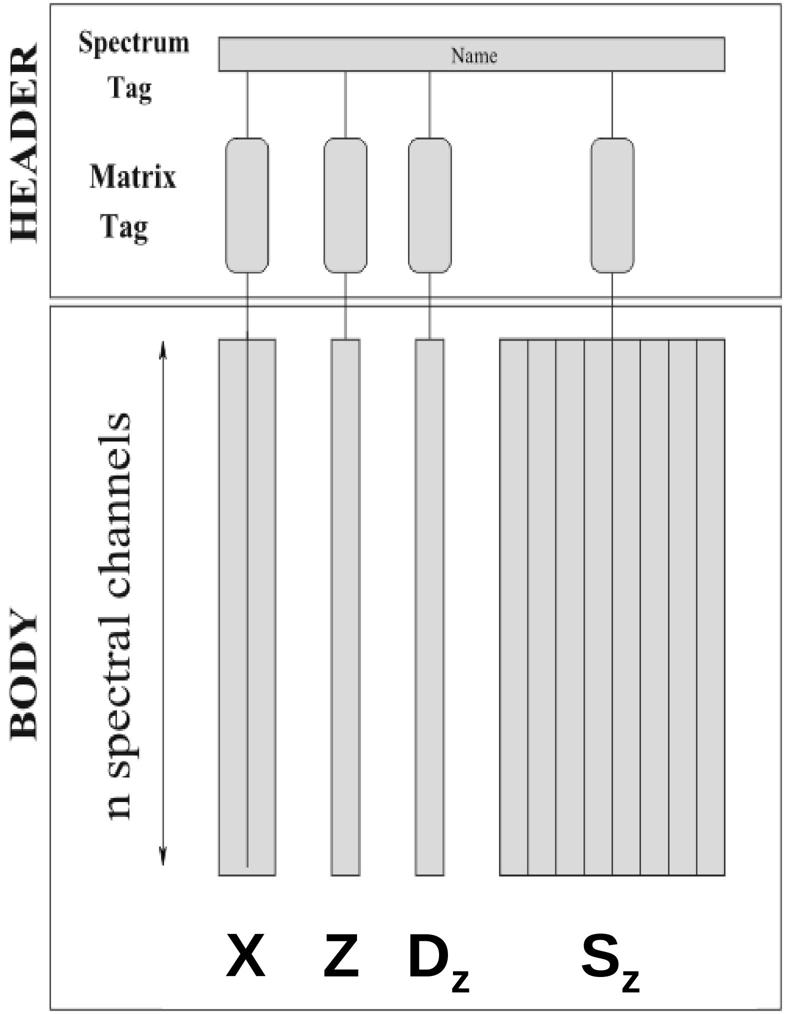
$$\boxed{V_Z = S_Z S_Z^T + D_Z}$$

correlated part
dimension: n x k

uncorrelated part
diagonal : n values

n : length of vector **Z**
k : number of common sources of uncertainties

AGS, File format



Storage

Covariance matrix

n^2 elements (e.g. 32k x 8 bytes → 8 Gb !)

AGS representation

n (k+1) elements (32k, 20 corr. → 5 Mb)

Conclusion

- **Covariance Matrix are required evaluated data files**
  - Try to produce them from experimental data
- **Requires:**
  - Covariance Matrix from exp. Data
  - Good description of experimental data
- **To reduce storage space**
  - Cholesky decomposition and uncorrelated uncertainties