Cross Section Measurements and Uncertainties of Cross Section Data

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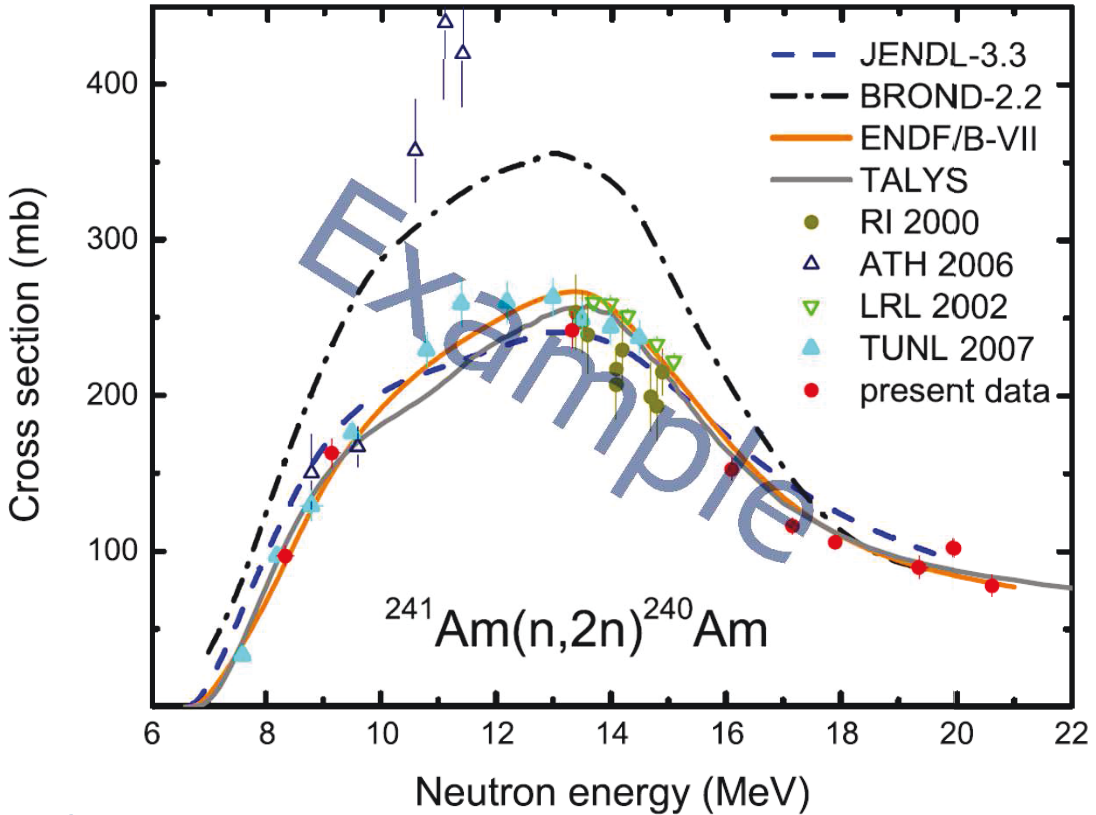
Uncertainties of measurements



Methodology

“Evaluation of measurement data - Guide to the expression of uncertainty in measurement”

Joint Committee for Guides in Metrology, *JCGM 100:2008, www.bipm.org (2008)*

General

Systematic

Standardized

Developed by experts for measurements relied upon in application

Concepts and terminology

Summary of the procedure

Illustration

European
Commission

Concepts

Quantity, measurand

True value

indeterminate, unknowable

Measured value or measurement result

corrected for systematic error

(qualify what you report!)

Error

measured minus true value

indeterminate, unknowable

Uncertainty

parameter associated with the measurement result characterizing the distribution in values that could reasonably be attributed to the measured quantity

… for a given quantity and measurement result there is an infinite number of values dispersed around it, consistent with the data and one’s knowledge, that can be attributed to the measurand with varying degree of credibility.

Uncertainties

Error

Every measurement is in error

All measurements are imperfect

- imperfect realization of quantity
- random variations
- inadequate corrections
- incomplete knowledge
  - *number of nuclei*
  - *detection efficiency*
  - *fluence measurement*
  - *multiple scattering*
  - *standard cross section*
  - *calibration sources*
  - *statistics*

Error *is unknowable, however sources of error may be recognized and should be corrected for:*

Measurement result

=

corrected result

Systematic error

Mean error that would result from infinitely many measurements under repeatability conditions

Correction (factor)

Value added (multiplied) to compensate for systematic error

Random error

Error minus systematic error

Uncertainties

Uncertainty

Several ways to express

one standard deviation

a multiple thereof

fwhm, half width…

Many contributing components

standardized approach

estimate one total std. deviation

uncertainty propagation

uncertainty budget

Method of evaluation

Assess distribution, mean and standard deviation of measurement outcome.

Mean ⇨ measurement result

Std.dev. ⇨ measurement uncertainty

Type A method of determination:

repetition of the experiment to obtain, mean and expt. standard deviation

Type B method of determination:

scientific judgment: *previous measurements, experience/knowledge, specification manufacturer, (calibration) certificates,reference data (handbooks)*

Procedure

1. Set up mathematical relation measured quantity (Y) and input quantities (X)
2. Estimate the inputs (x)
3. Estimate the standard uncertainties for the inputs: u(x)
4. Estimate covariances of input uncertainties: $u(x_i, x_j)$
5. Find the measured quantity (y) from the inputs
6. Estimate the combined standard uncertainties and covariances $u_c(y_k)$ and $u_c(y_k, y_l)$
7. Report result with standard uncertainties and covariances and uncertainty budget.

$$Y_k = f_k(X_1, X_2, \ldots X_N)$$

$$X_i \rightarrow x_i$$

$$\rightarrow u(x_i)$$

$$\rightarrow u(x_i, x_j) = C(x_i, x_j)u(x_i)u(x_j)$$

$$y_k = f_k(x_1, x_2, \ldots x_N)$$

$$u_c^2(y_k) = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial f_k}{\partial x_i} \frac{\partial f_k}{\partial x_j} u(x_i, x_j)$$

$$u_c(y_k, y_l) = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial f_k}{\partial x_i} \frac{\partial f_l}{\partial x_j} u(x_i, x_j)$$

$$u_c(y_k, y_l) = \sum_{i=1}^{N} \sum_{j=1}^{N} S_{ki} S_{lj} C(x_i, x_j) r(x_i) r(x_j)$$

Reporting

1. Be clear about definition of the uncertainty (combined standard uncertainty, state coverage factor if any, fwhm, …)

2. For nuclear data work the combined standard uncertainty is to be preferred. Harmonization

3. Notation
   - **$\sigma = 30.5$ b with $u_c = 0.3$ b**
   - **$\sigma = 30.5(3)$ b**
   - **$\sigma = 30.5(0.3)$ b**
   - **$\sigma = (30.5 \pm 0.3)$ b**

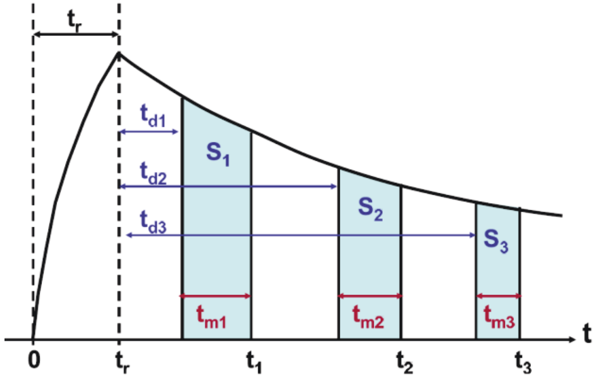
A. Measurement expression

B. Input quantities, values, uncertainties, correlations

C. Final results, combined standard uncertainties, correlations

Activation data evaluation

$$\sigma_{\rm Am} = \sigma_{\rm Al}\frac{S_{\rm Am}}{S_{\rm Al}}\frac{\left[I\epsilon f_{\Sigma} f_r n\Phi_0\right]_{\rm Al}}{\left[I\epsilon f_{\Sigma} f_r n\Phi_0\right]_{\rm Am}}\cdot\prod_k\frac{C_{\rm k,Am}}{C_{\rm k,Al}}$$



σ_{Al}	Reference cross section
S	Counts for gamma
I	gamma-ray intensity
ε	absolute detection efficiency
f_Σ	cooling time factor
f_r	irradiation time factor
n	number of nuclides
Φ_0	mean neutron flux
C_k	correction factors for
	* low energy neutrons
	* intensity fluctuations

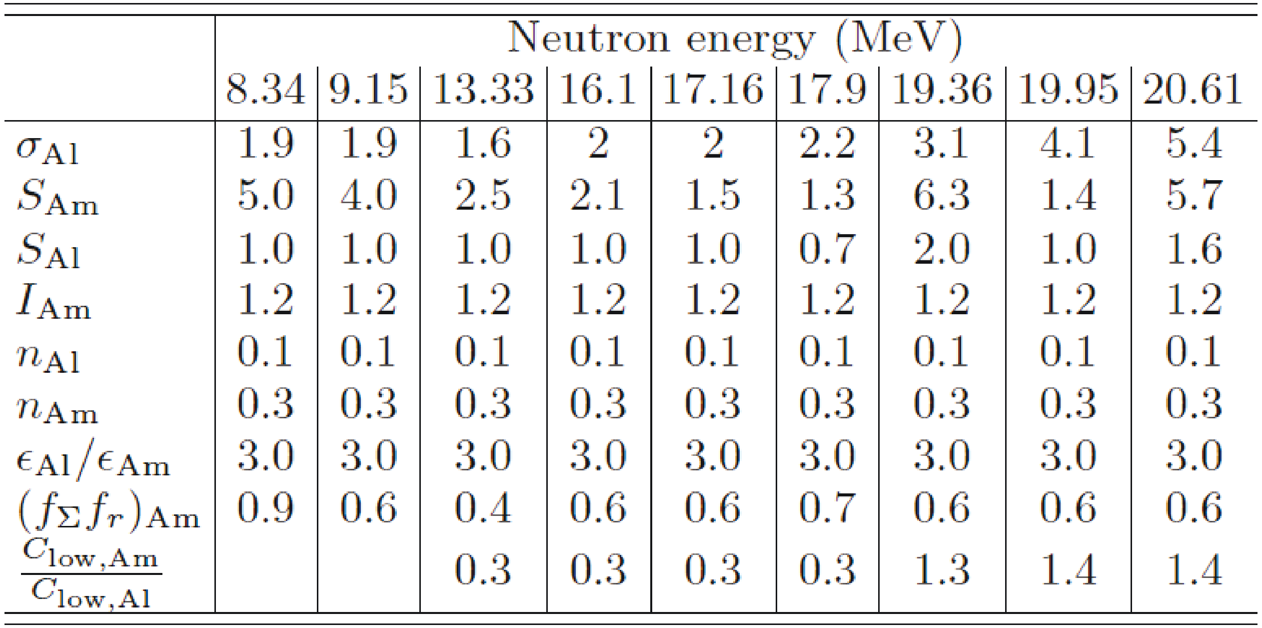
$$f_{\Sigma} = \frac{1}{\lambda}\sum e^{-\lambda t_{d_i}}(1-e^{-\lambda t_{m_i}})$$

$$f_r = 1 - e^{-\lambda t_r}$$

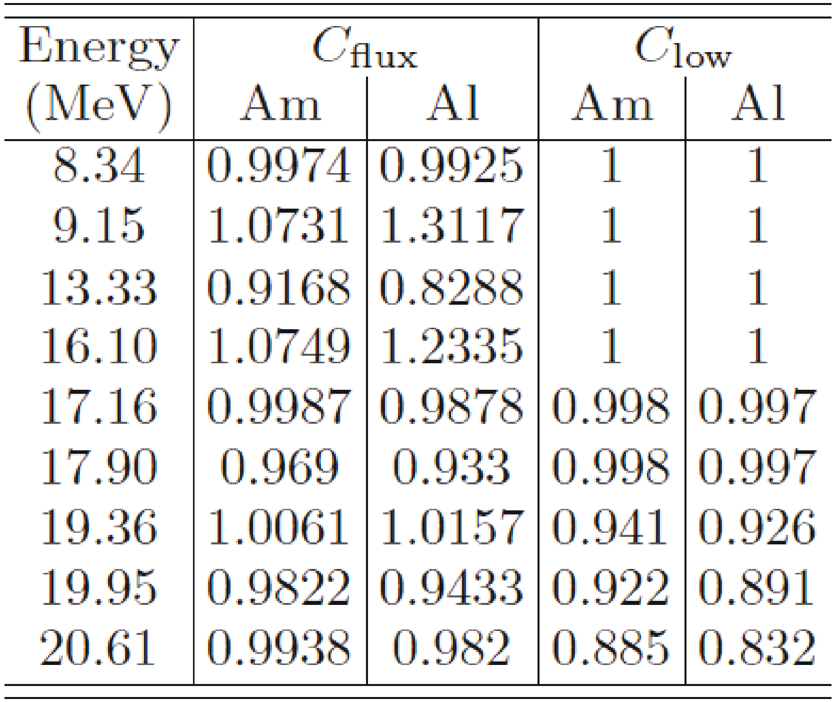
$$C_{\rm flux} = \frac{\bar{\Phi}(1-e^{-\lambda t_r})}{\sum_{i=1}^{m}\Phi_i(1-e^{-\lambda\Delta t})e^{-\lambda(m-i)\Delta t}}$$

$$C_{\rm low} = 1 - \frac{\int_0^{E_c}\Phi(E)\sigma(E)dE}{\int_0^{\infty}\Phi(E)\sigma(E)dE}.$$

Activation data reporting



	Neutron energy (MeV)								
	8.34	9.15	13.33	16.1	17.16	17.9	19.36	19.95	20.61
σ_{Al}	1.9	1.9	1.6	2	2	2.2	3.1	4.1	5.4
S_{Am}	5.0	4.0	2.5	2.1	1.5	1.3	6.3	1.4	5.7
S_{Al}	1.0	1.0	1.0	1.0	1.0	0.7	2.0	1.0	1.6
I_{Am}	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
n_{Al}	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
n_{Am}	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
$\epsilon_{\mathrm{Al}}/\epsilon_{\mathrm{Am}}$	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0
$(f_{\Sigma} f_r)_{\mathrm{Am}}$	0.9	0.6	0.4	0.6	0.6	0.7	0.6	0.6	0.6
$\frac{C_{\mathrm{low,Am}}}{C_{\mathrm{low,Al}}}$			0.3	0.3	0.3	0.3	1.3	1.4	1.4



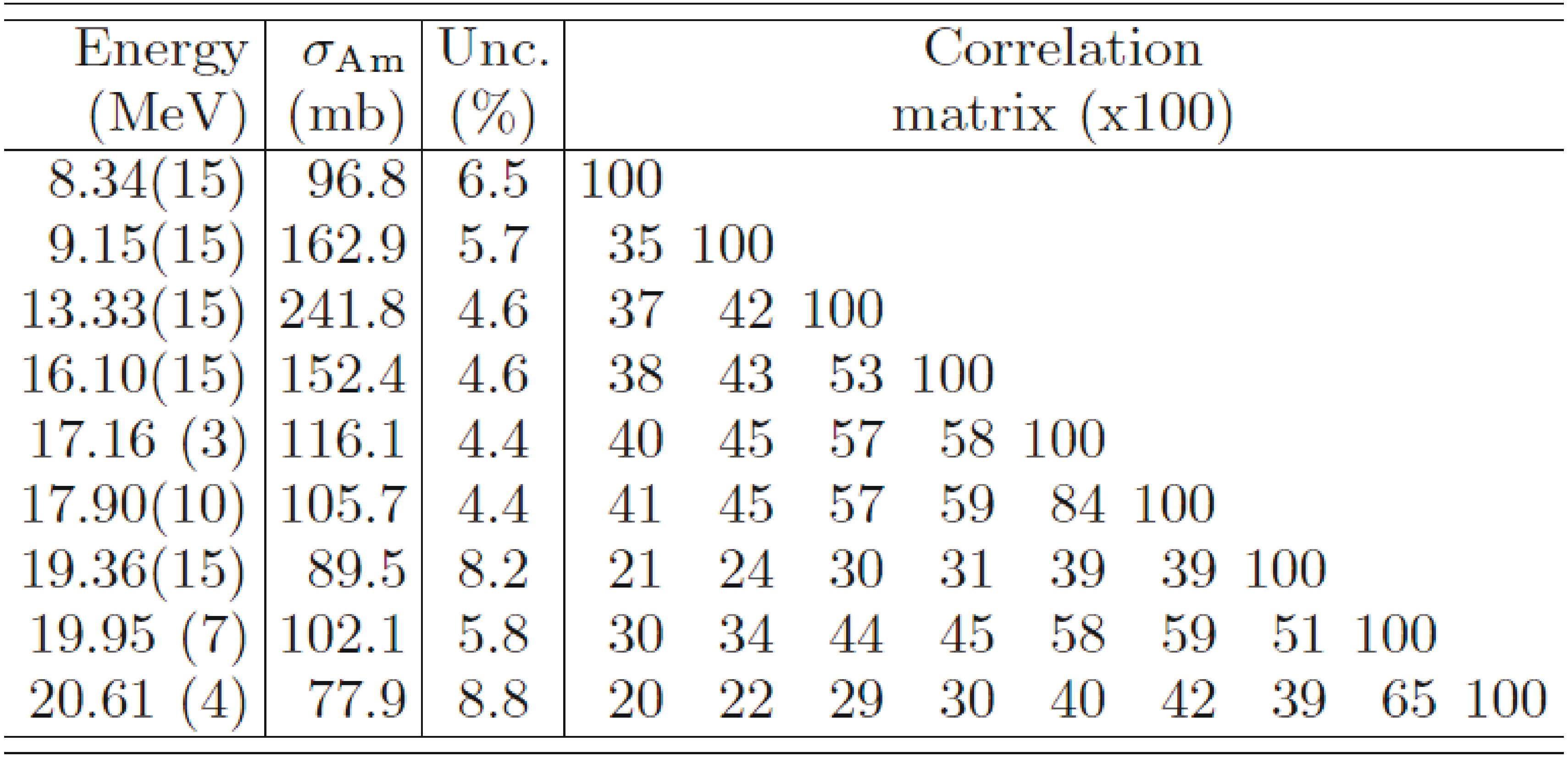
Energy (MeV)	C_{flux}		C_{low}	
	Am	Al	Am	Al
8.34	0.9974	0.9925	1	1
9.15	1.0731	1.3117	1	1
13.33	0.9168	0.8288	1	1
16.10	1.0749	1.2335	1	1
17.16	0.9987	0.9878	0.998	0.997
17.90	0.969	0.933	0.998	0.997
19.36	1.0061	1.0157	0.941	0.926
19.95	0.9822	0.9433	0.922	0.891
20.61	0.9938	0.982	0.885	0.832

% uncertainties for components in the activation formula

σ_{Al} uncertainty correlations taken from the evaluation

$\varepsilon_{\mathrm{Al}}/\varepsilon_{\mathrm{Am}}$ uncertainty fully correlated w. neutron energy

Activation reporting



Energy (MeV)	σ_{Am} (mb)	Unc. (%)	Correlation matrix (x100)								
8.34(15)	96.8	6.5	100								
9.15(15)	162.9	5.7	35	100							
13.33(15)	241.8	4.6	37	42	100						
16.10(15)	152.4	4.6	38	43	53	100					
17.16 (3)	116.1	4.4	40	45	57	58	100				
17.90(10)	105.7	4.4	41	45	57	59	84	100			
19.36(15)	89.5	8.2	21	24	30	31	39	39	100		
19.95 (7)	102.1	5.8	30	34	44	45	58	59	51	100	
20.61 (4)	77.9	8.8	20	22	29	30	40	42	39	65	100

Monte Carlo evaluation

A. Negret et al., GAINS data for inelastic scattering by (n,n'g).

Randomization of the input quantities

Case-by-case propagation of inputs to measured quantities

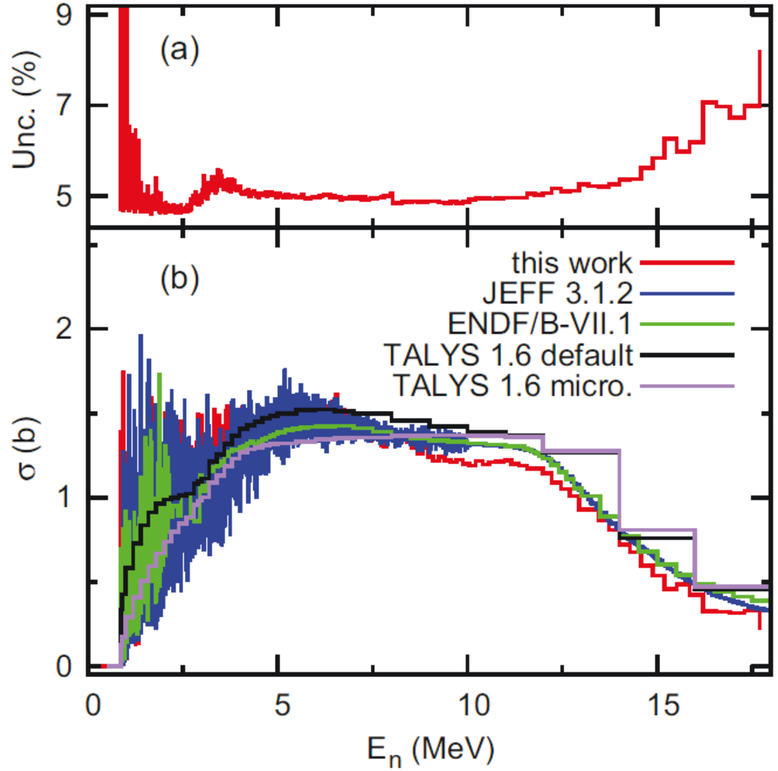
Statistical generation of covariance matrices and cross-covariance matrices

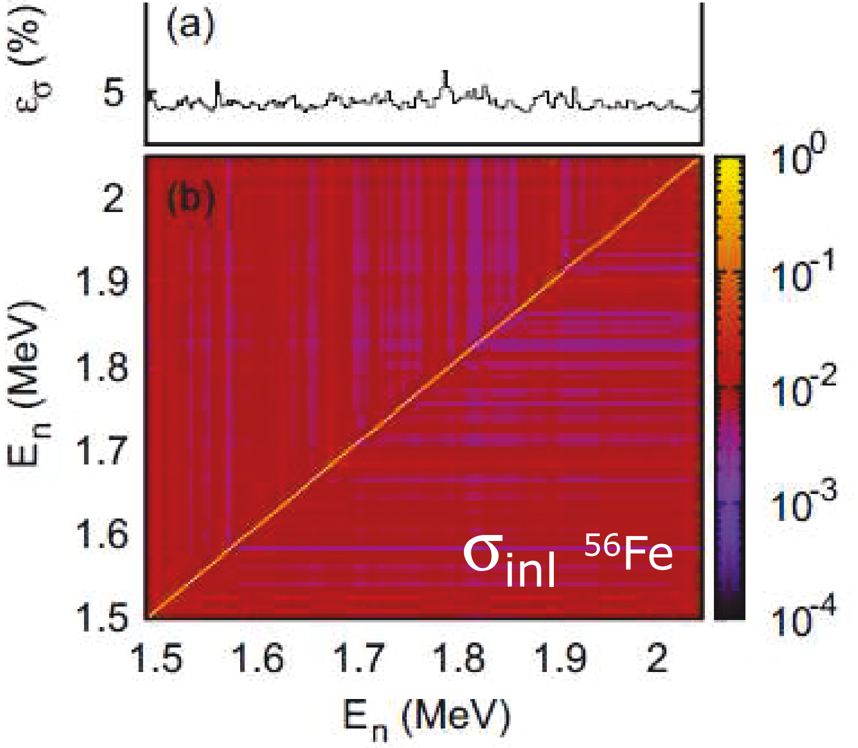
$$\mathrm{cov}(x,y) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

Examples ^{28}Si and ^{56}Fe:

A. Negret et al. NDS119(2014)179

A. Negret et al. PRC90(2014)034602





AGS method

Bastian and Schillebeeckx

Analytic propagation of uncertainties for (TOF) Spectra

Compact covariance matrix representation

Compact EXFOR standard

Automated in code package AGS (Analysis of Geel Spectra)

See NRAS 2014 Neutron resonance analysis school 2014, Geel … December 2014

B. Becker et al. J.Instr.07(2012)P11002

B. Becker et al. NDS118(2014)381

‘Bastian’ representation of covariance matrix:

$$\mathbf{V}_{\vec{Z}} = \mathbf{U}_{\vec{Z}} + \mathbf{S}_{\vec{Z}}\mathbf{S}_{\vec{Z}}^{T}$$

U: Uncorrelated/diagonal component

S S^T is the correlated component

S: n x k matrix

k is the number of operations (a small number)

k+1 columns of n rows to store

Much less than n x n !

Additional reading

N. Otuka and D.L. Smith, NDS120 (2014) 281 (Uncertainties in EXFOR)

D.L. Smith and N. Otuka NDS113 (2012) 3006 (Uncertainties in meas.)

D.L. Smith NDS 112 (2011) 3037 (Uncertainties ENDF/B-VII.1)

Uncertainties in measurement

Summary

There is an excellent guide on what to do

Its use should be promoted

Reporting should be as complete as possible

Correlations make this a challenge in data storage for large data sets, but there are solutions (AGS)

Cautions

A small uncertainty does not guarantee a small error: incomplete knowledge ⇨ incomplete corrections

Do not over- or underestimate uncertainties! Use all your current knowledge as best as possible.

1. overestimation leads to needless caution of users, attempts to remeasure, disregard for your hard work, difficulty identifying incomplete knowledge
2. underestimation leads to misplaced trust, undue weight of the result in evaluations, biased predictions