Integral equation for the reading z_{0i} of the detector i:

$$z_{0i} = \int \mathrm{d}E \; R_i(E) \; \Phi_E(E) \qquad i = 1,\ldots,M$$

more exactly: $z_{0i}' = z_{0i} + \varepsilon_i$ (statistically fluctuating ε_i)

$R_i(E)$: response function

(no unique solution of the equation above)

approximation by discretisation (group structure):

$$z_{0i} = \sum_{\nu=1}^{N} R_{i\nu} \, \Phi_\nu \qquad i = 1,\ldots,M$$

$\mathbf{z}_0 = \mathbf{R} \cdot \mathbf{\Phi}$ with $\Phi^{\mathrm{T}} = (\Phi_1,\ldots,\Phi_\nu,\ldots\Phi_N)$ (group fluence)

M < N $\rightarrow\rightarrow$ no unique solution

M > N $\rightarrow\rightarrow$ least-squares

Minimum χ^2 by least-squares methods:

$$\chi^2 = (\mathbf{z}_0 - \mathbf{R} \cdot \mathbf{\Phi})^T \cdot \mathbf{S}_{z0}^{-1} \cdot (\mathbf{z}_0 - \mathbf{R} \cdot \mathbf{\Phi}) \rightarrow \text{Min}$$

solution from the “normal equations”:

$$\mathbf{R}^T \cdot \mathbf{S}_{z0}^{-1} \cdot \mathbf{z}_0 = (\mathbf{R}^T \cdot \mathbf{S}_{z0}^{-1} \cdot \mathbf{R}) \cdot \mathbf{\Phi} = \mathbf{B} \cdot \mathbf{\Phi}$$

N x N “**Structure**” matrix:

$$\mathbf{B} = \mathbf{R}^T \cdot \mathbf{S}_{z0}^{-1} \cdot \mathbf{R}$$

has to be inverted

Matrix **B**
sometimes ill-conditioned (ill-posed problem), even for N < M

Minimum of χ^2 numerically not well-defined,

There might be a multitude of existing solutions

Conclusion:
For ill-conditioned **B**, additional information on the spectrum must be included, for instance:

- ⇒ spectrum is non-negative
- ⇒ spectrum is smooth
- ⇒ spectrum can be developed into a set of standard spectra (thermal, 1/E, fission)
- ⇒ spectrum is known a priori from a MCNP calculation

Linear least-squares **adjustment,** STAY'SL, LEPRICON, DIFBAS, MSITER(MINCHI), LSL, German (European) Standard DIN 1319……….

$$\chi^2 = (\mathbf{z}_0-\mathbf{z})^T \cdot \mathbf{S}_{z0}^{-1} \cdot (\mathbf{z}_0-\mathbf{z})$$ measured information

$$+(\mathbf{R}_0-\mathbf{R})^T \cdot \mathbf{S}_{R0}^{-1} \cdot (\mathbf{R}_0-\mathbf{R})$$ *a priori* information

$$+(\mathbf{\Phi}_0-\mathbf{\Phi})^T \cdot \mathbf{S}_{\Phi 0}^{-1} \cdot (\mathbf{\Phi}_0-\mathbf{\Phi})$$ *a priori* information

χ^2 to be minimised under constraint $\mathbf{z} = \mathbf{R}\,\mathbf{\Phi}$

Solution:

$$\mathbf{\Phi} = \mathbf{\Phi}_0 + \mathbf{S}_{\Phi 0} \cdot \mathbf{R}_0 \cdot \mathbf{W}^{-1} \cdot (\mathbf{z}_0 - \mathbf{R}_0 \cdot \mathbf{\Phi}_0)$$

Uncertainty matrix:

$$\mathbf{S}_{\Phi} = \mathbf{S}_{\Phi 0} - \mathbf{S}_{\Phi 0} \cdot \mathbf{R}_0 \cdot \mathbf{W}^{-1} \cdot \mathbf{R}_0 \cdot \mathbf{S}_{\Phi 0}$$

(due to minus sign reduction of uncertainty)

With weighting matrix

$$\mathbf{W} = \mathbf{S}_{z0} + \mathbf{\Phi}_0 \cdot \mathbf{S}_{R0} \cdot \mathbf{\Phi}_0 + \mathbf{R}_0 \cdot \mathbf{S}_{\Phi 0} \cdot \mathbf{R}_0$$

- ⇒ consistent a priori information needed, no guess
- ⇒ correct uncertainty analysis (reactor dosimetry !)
- ⇒ but: negative fluence values are possible

Codes, using a priori information on fluence

STAY'SL
LEPRICON
LSL
MSITER(MINCHI)
DIFBAS
BUNKI
MAXED……….

a priori information on fluence and response functions added to χ^2

ADJUSTMENT

Consequent uncertainty analysis possible

Codes, using constraint of non-negative fluence:

Non-linear least squares, solution depends on start spectrum, no exact uncertainty analysis.

SAND-II	Unfolded for $\mathrm{Log}(\Phi_v)$
GRAVEL	" " "
LSL-M2	" " "
LOUHI	Unfolded for Φ_v^2

Other codes which must be mentioned:

Neural networks (BUGS)	uncertainty propagation now possible, Bayesian methods)
Genetic algorithms(BONDI-97)	(survival of the fittest)
Singular value decomposition	(infinity equals zero ?)
Codes with smoothing routines	e. g. FERDOR (FORIST)
Maximum Entropy (MIEKE, UNFANA, MAXED)	(uncertainty propagation !!)

Each code or algorithm is based on an individual model, independent from each other, therefore: quantitative comparison of quality (judging) is difficult

Monte Carlo Unfolding (MIEKE, Maximum Entropy)

$$\chi^2 = (\mathbf{z}_0 - \mathbf{R}\cdot\boldsymbol{\Phi})^{\mathrm{T}} \cdot \mathbf{S}_{z0}^{-1} \cdot (\mathbf{z}_0 - \mathbf{R}\cdot\boldsymbol{\Phi}) \;\rightarrow\; \mathrm{Min}$$

minimum χ^2

⇑ ⇑

equivalent

⇓ ⇓

maximum likelihood:

$$P(\boldsymbol{\Phi}) = \mathrm{const}\cdot\exp(-\frac{\beta}{2}\chi^2(\boldsymbol{\Phi}))$$

Most probable fluence values might not exist,
but it is possible to calculate expectation values:

$$\langle \Phi_\nu \rangle = \frac{\int \mathrm{d}\Phi_1 \ldots \mathrm{d}\Phi_M \; \Phi_\nu \; \exp(-\frac{\beta}{2}\chi^2(\boldsymbol{\Phi}))}{\int \mathrm{d}\Phi_1 \ldots \mathrm{d}\Phi_M \; \exp(-\frac{\beta}{2}\chi^2(\boldsymbol{\Phi}))}$$

covariance matrix:

$$S_{\Phi,\nu\mu} = \langle \Phi_\nu \, \Phi_\mu \rangle - \langle \Phi_\nu \rangle \langle \Phi_\mu \rangle$$

>Integrals by importance sampling (Metropolis)
>β from the constraint $<\chi^2> = M$

Consistent uncertainty propagation possible,
2 components of uncertainty:
(from ambiguity and from propagation of uncertainties)

Maximum Entropy:

$$S = -\int \mathrm{d}^M x \;\; P(\mathbf{x}) \log(P(\mathbf{x}))$$

MIEKE:

$$P(\mathbf{\Phi}) = \; C_1 \cdot \exp(-\frac{\beta}{2} \cdot \chi^2(\mathbf{\Phi})) \;\; \text{for all} \;\; \Phi_\nu \geq 0$$

UNFANA:

$$P(\mathbf{\Phi}) = \; C_1 \cdot \exp(-\mathbf{b}^{\mathrm{T}} \cdot \mathbf{R} \cdot \mathbf{\Phi})$$

MAXED:

$$P(E) = \frac{\Phi_E(E)}{\Phi}$$

used as probability density

MIEKE: Fluctuation of fluence can be represented as a fluctuation coming from the uncertainties of the measured values and a fluctuation coming from ambiguity:

$$\delta\mathbf{\Phi} = < \frac{\partial \mathbf{\Phi}}{\partial z_0} > \delta z_0 + \delta\mathbf{\Phi}_1$$

The resulting covariance matrix is thus the sum of two parts:

$$\frac{\partial < \mathbf{\Phi} >}{\partial \mathbf{z}_0} \mathbf{S}_{z0} \frac{\partial < \mathbf{\Phi} >}{\partial \mathbf{z}_0} + \mathbf{S}_{\Phi 1} = \mathbf{S}_{\Phi} = < \mathbf{\Phi} \cdot \mathbf{\Phi} > - < \mathbf{\Phi} > \cdot < \mathbf{\Phi} >$$

It can be shown:

$$\frac{\partial < \mathbf{\Phi} >}{\partial \mathbf{z}_0} = -\beta \, \mathbf{S}_{\Phi} \cdot \mathbf{R} \cdot \mathbf{S}_{z0}^{-1}$$

(part coming from uncertainty propagation)

Therefore, the "ambiguity" part of the uncertainty matrix can be defined as:

$$\mathbf{S}_{\Phi 1} = \mathbf{S}_{\Phi} - \beta^2 \mathbf{S}_{\Phi} \cdot \mathbf{B} \cdot \mathbf{S}_{\Phi}$$

In linear least-squares methods there is for a

non-singular matrix **B**: $\beta^2 \mathbf{S}_{\Phi} = \mathbf{B}^{-1}$,

i. e. for non-singular **B** there is no "ambiguity"

Uncertainty propagation due to response matrix uncertainties can be included in most of the programs. In MAXED the corresponding formulas are easy to obtain.

Uncertainty description for response functions should follow the ENDF format.

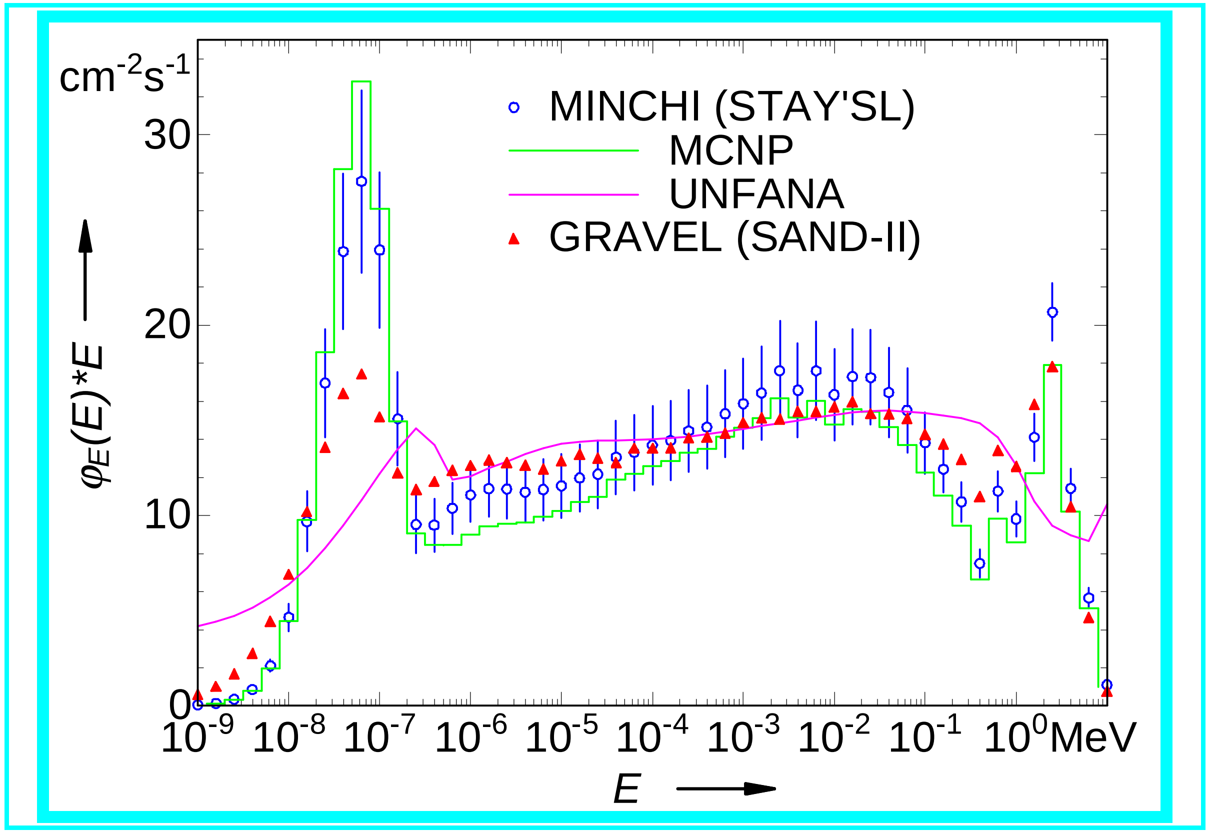
MIEKE: It is possible to include those uncertainties too. The corresponding contribution to the uncertainty matrix is:

$$\frac{\partial < \Phi >}{\partial \mathbf{R}} = \beta \left\{ \mathbf{S}_{\Phi} \cdot \mathbf{S}_{z0}^{-1} \cdot \mathbf{z}_0 - \left(< \Phi\Phi\Phi > - < \Phi >< \Phi\Phi > \right) \cdot \mathbf{R} \cdot \mathbf{S}_{z0}^{-1} \right\}$$

Triplet correlation function can be approximated by:

$$< (\Phi_{\nu} - < \Phi_{\nu} >) (\Phi_{\mu} - < \Phi_{\mu} >) (\Phi_{\lambda} - < \Phi_{\lambda} >)> = 0$$

for all ν, μ, λ.



MINCHI : *A priori* information from the MCNP run was used with reasonable estimated uncertainties

GRAVEL-SAND-II:
Educated guess using the MCNP *a priori* information as start spectrum.

UNFANA: unfolded without any *a priori* information, the solution spectrum looks unphysically.

Uncertainty of fluence 5%-8%,

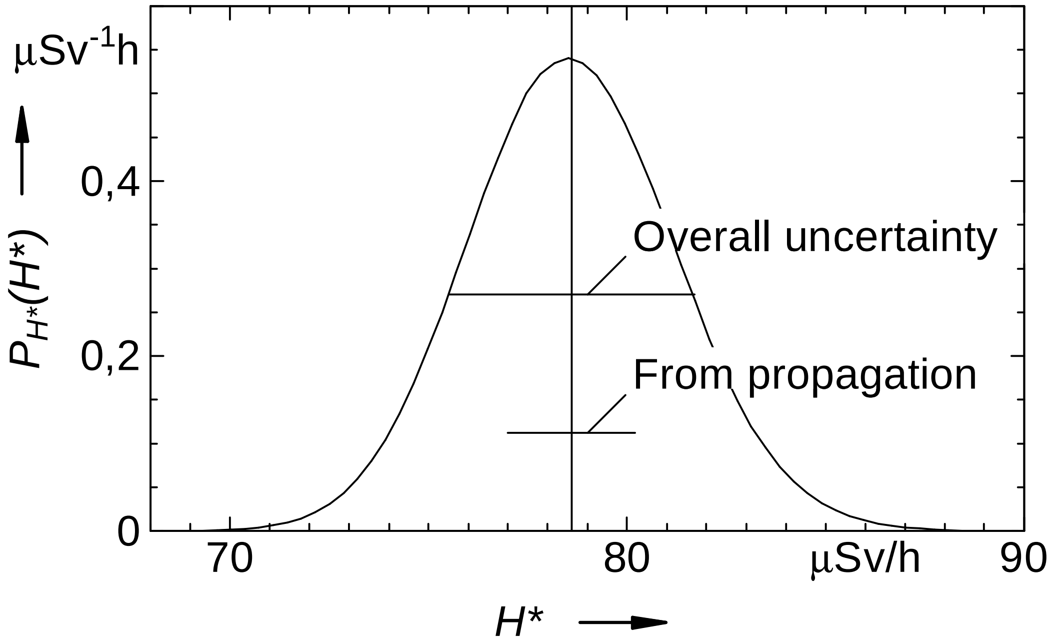
Uncertainty of dose equivalent: 8%-14%

$$P(H^*) = \left\langle \, \delta(H^* - \mathbf{h}^*_{\Phi} \cdot \mathbf{\Phi}) \, \right\rangle$$ and $$H^* = < \mathbf{h}_{\Phi}{}^* \cdot \mathbf{\Phi} >$$

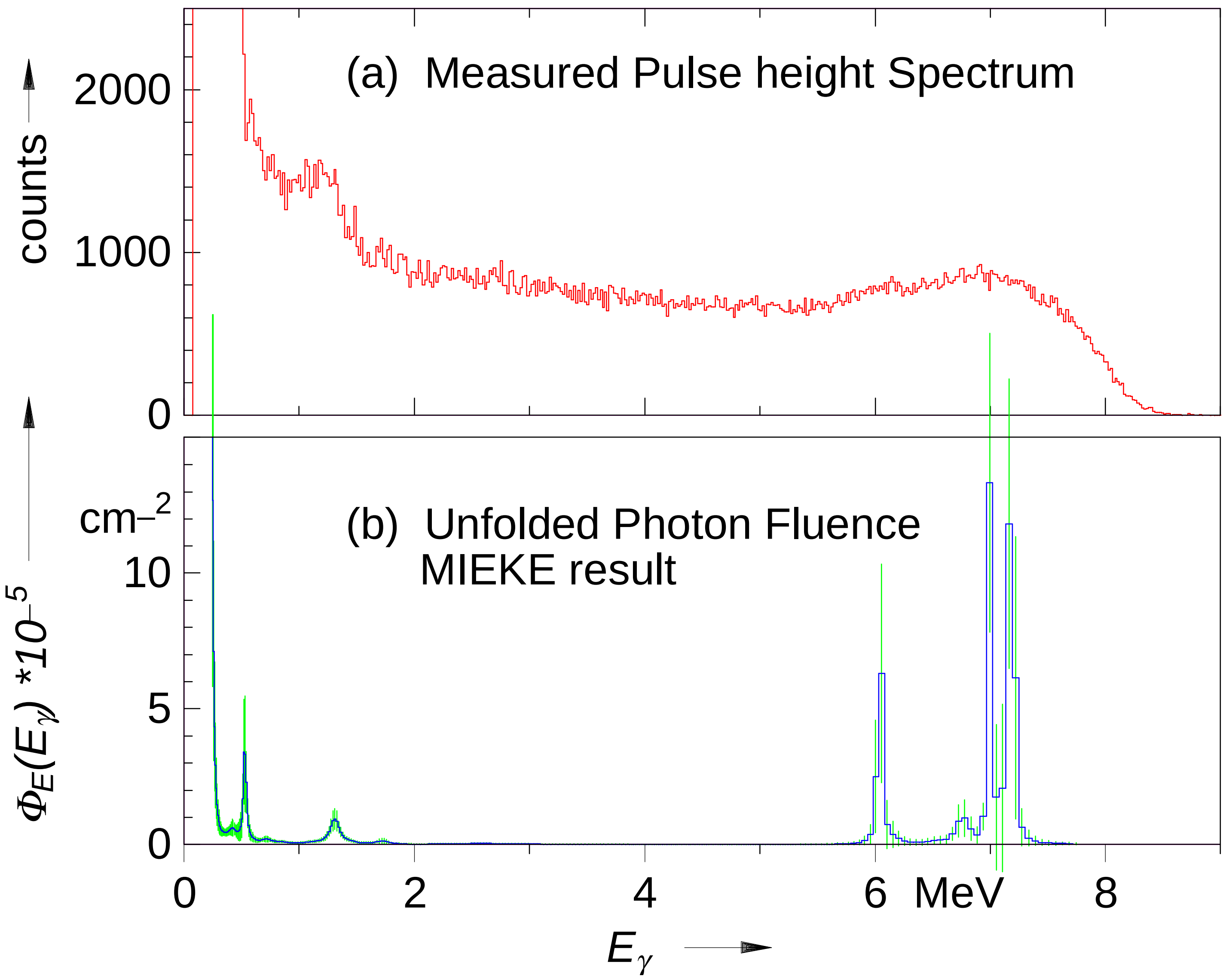
There are 2 contributions to uncertainty:

1. from the usual uncertainty propagation

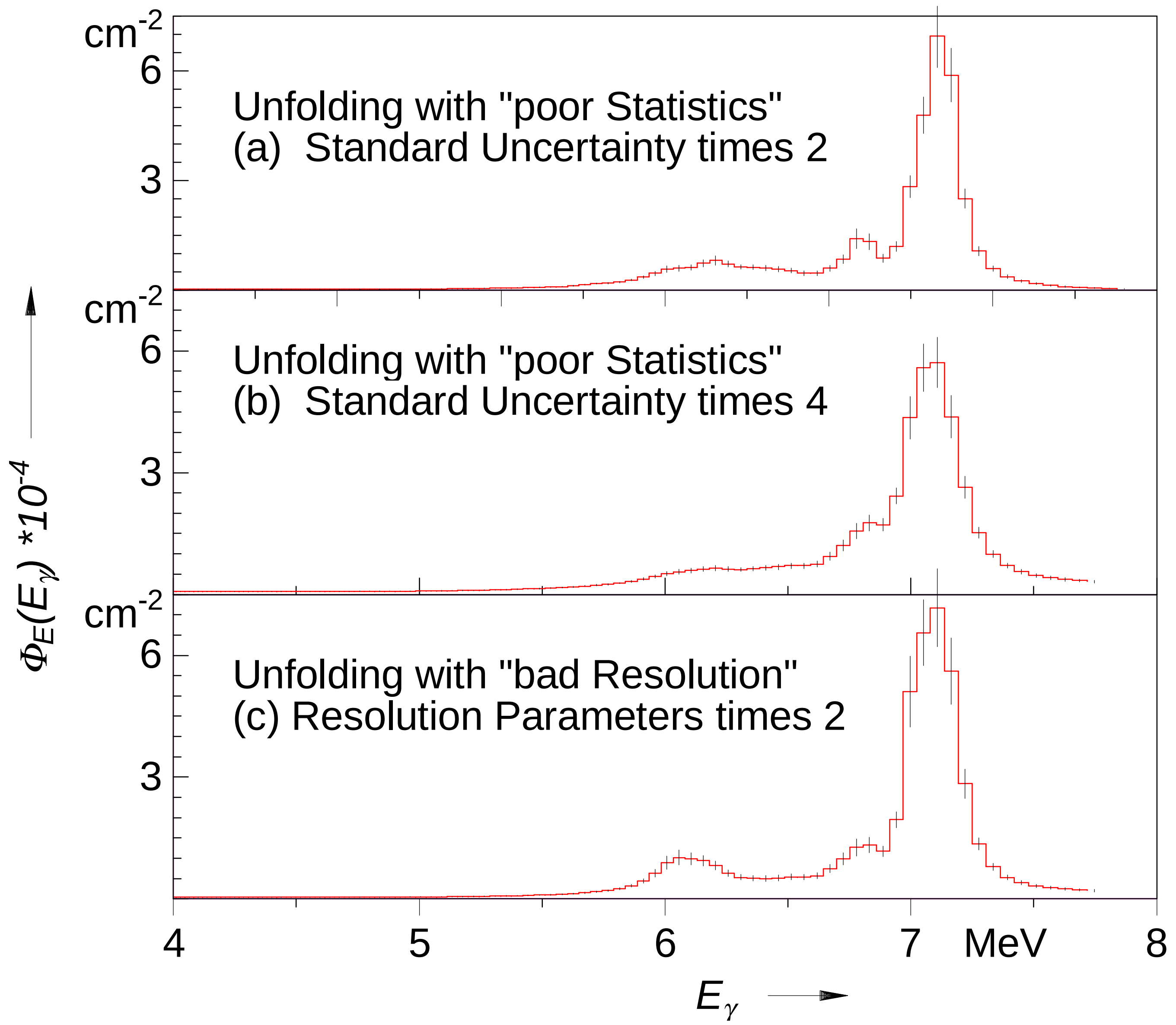
2. from ambiguity



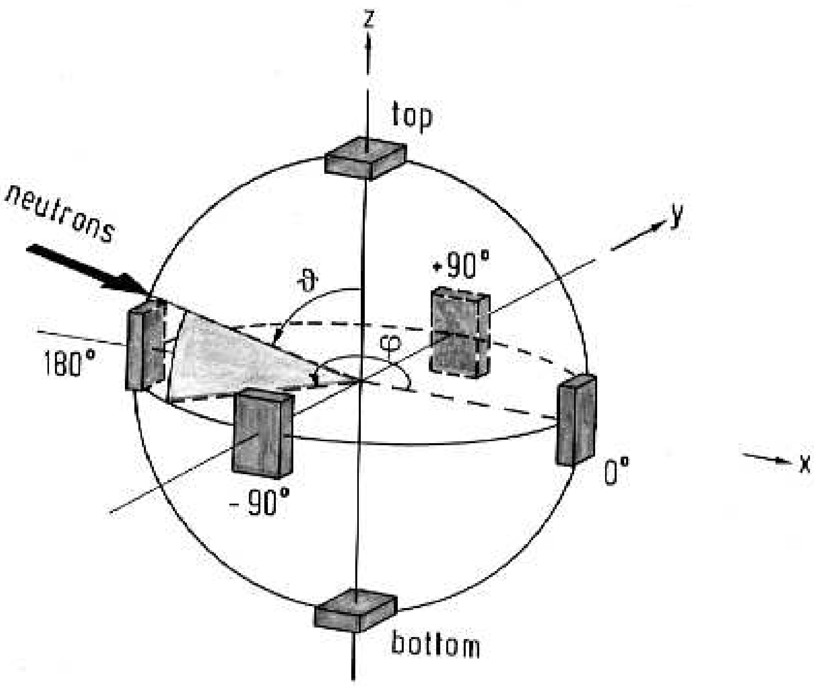
Probability distribution of dose equivalent:



(a) Measured Pulse height Spectrum
counts
2000
1000
0
(b) Unfolded Photon Fluence
MIEKE result
cm–2
10
5
0
Φ_E(E_γ) *10^–5
0
2
4
6 MeV
8
E_γ



cm-2
6
3
Unfolding with "poor Statistics"
(a) Standard Uncertainty times 2
Unfolding with "poor Statistics"
(b) Standard Uncertainty times 4
Unfolding with "bad Resolution"
(c) Resolution Parameters times 2
Φ_E(E_γ) *10^-4
4
5
6
7
MeV
8
E_γ



Luszik-Bhadra et al.

Orientation of a detector characterised by:

$$\mathbf{u}_i = (x_i, y_i, z_i) = (\cos\varphi_i \sin\vartheta_i,\ \sin\varphi_i \sin\vartheta_i,\ \cos\vartheta_i)$$

Cylindrical symmetry is assumed, i.e. response to incident neutrons of the direction $\mathbf{\Omega}$ depends only on $\mathbf{u}_i \cdot \mathbf{\Omega} = \cos\Theta_i$

Group representation in angular and energy groups. for the directional spectral fluence: $\Phi_{\mathbf{\Omega},E}(\mathbf{\Omega}, E)$

Expectation values $<\Phi_{\Omega,E}(\mathbf{\Omega}_l, E_u)>$ and weighted integrals:

$$\int dE\, d^2\Omega\ \ W(\mathbf{\Omega}, E)\ <\Phi_{\mathbf{\Omega},E}(\mathbf{\Omega}, E)>$$

are calculated.

Example for $W(\mathbf{\Omega}, E)$:

directional dose equivalent $h'_{\Phi}(\mathbf{u}_p \cdot \mathbf{\Omega}, E)$, where $\mathbf{u}_p$ characterises the direction investigated ($\cos\alpha = \mathbf{u}_p \cdot \mathbf{\Omega}$)

Summary:

----- Matrix **B** might be ill-conditioned even for M > N

----- STAYS'L, LEPRICON, DIFBAS, MSITER…..
need consistent a priori information, no guess !!
unique solution but negative fluence values possible

----- SAND-II, GRAVEL, LOUHI
always convergence, always positive solution.
For ill-conditioned **B**, multitude of solutions possible.
no uncertainty analysis, only to be used by experts !

----- NEURAL NETWORKS and EVOLUTION strategies.
Interesting alternative, uncertainty handling must be included.

----- Maximum entropy, MIEKE, UNFANA, MAXED
Solution non-negative, consistent uncertainty propagation,
Two components of uncertainty: ambiguity and usual propagation

Unfolding codes should not be used as black boxes, some experience is required,
e.g. GRAVEL, MIEKE, UNFANA, MAXED should be used consecutively.
Each single code is based on an own single model