The Question of Uncertainties in Nuclear Data Evaluation

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Content

UNCERTAINTY???

What displacement of the person on the left side do you expect?

Nuclear Data Evaluation

Start of Modern Data Evaluation:
recommended values of fundamental physics constants (c, $\hbar$, α_f, ...)
Dunnington (1939); Du Mond and Cohen (1953)

Present Status:
At present Evaluated Nuclear Data Files represent a consistent set of cross sections and associated quantities for all relevant reaction processes. Most data files are limited to the energy region below 20MeV.

There exist several nuclear data libraries with evaluated cross section data, but only few files contain uncertainty information → the reliability Is still an open question.

Required developments

Required developments

- modern transmutation and fusion research require an extension of the energy range up to about 150 MeV → scarcity of data and therefore increased use of models required.
- the inclusion of uncertainty information is a longstandig demand from the user community → cross section covariance matrices

Example: Reliable uncertainty of k_{eff} is required

$$\Delta^2 k_{eff} = \sum_{\rho}\sum_{\eta} \frac{\partial \mathcal{K}}{\partial \sigma_{\rho}} \left\langle \Delta\sigma_{\rho} \Delta\sigma_{\eta} \right\rangle \frac{\partial \mathcal{K}}{\partial \sigma_{\eta}}$$

cross section covariances

Uncertainty information

σ_ρ cross section values given in the file.

ρ characterizes reaction channel ρ and energy E_ρ

$k = \mathcal{K}(\sigma_\rho)$ quantity to be considered, e.g. k_{eff}

$$\Delta^2 k_{eff} = \sum_\rho \sum_\eta \frac{\partial \mathcal{K}}{\partial \sigma_\rho} \left\langle \Delta\sigma_\rho \Delta\sigma_\eta \right\rangle \frac{\partial \mathcal{K}}{\partial \sigma_\eta}$$

Covariance Matrix provides the proper information

The off-diagonal elements $\left\langle \Delta\sigma_\rho \Delta\sigma_\eta \right\rangle$ $\rho \neq \eta$ **describe the correlation of cross sections**

The covariance matrix

The covariance matrix is a typical concept of probability theory

$$\langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle = \cdots \int d\sigma_\rho \int d\sigma_\eta \cdots p(\cdots \sigma_\rho \sigma_\eta \cdots)\left(\sigma_\rho - \langle \sigma_\rho \rangle\right)\left(\sigma_\eta - \langle \sigma_\eta \rangle\right)$$

Expectation value $\langle \sigma_\rho \rangle = \cdots \int d\sigma_\rho \cdots p(\cdots \sigma_\rho \cdots)\sigma_\rho$

In nuclear data evaluation one intends by the inclusion of the covariance matrix to provide the means for inferences based on incomplete and/or unreliable data

What is the probability distribution in the context of Nuclear Data Evaluation?

Covariances for Modelling

Estimate of the uncertainty and the covariance matrices for reaction cross sections calculated within well defined models.

Requests on the procedure:

- use of basic tools
- minimal bias – assumptions
- use of mathematical and physical constraints
- use of available *a-priori* knowledge
- treat all models equally (phenomenological – microscopical)

Sources of uncertainties

The covariance matrix:

$$\langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle = \cdots \int d\sigma_\rho \int d\sigma_\eta \cdots p(\cdots \sigma_\rho \sigma_\eta \cdots)\left(\sigma_\rho - \langle \sigma_\rho \rangle\right)\left(\sigma_\eta - \langle \sigma_\eta \rangle\right)$$

The contributions to the covariance matrix of the model are

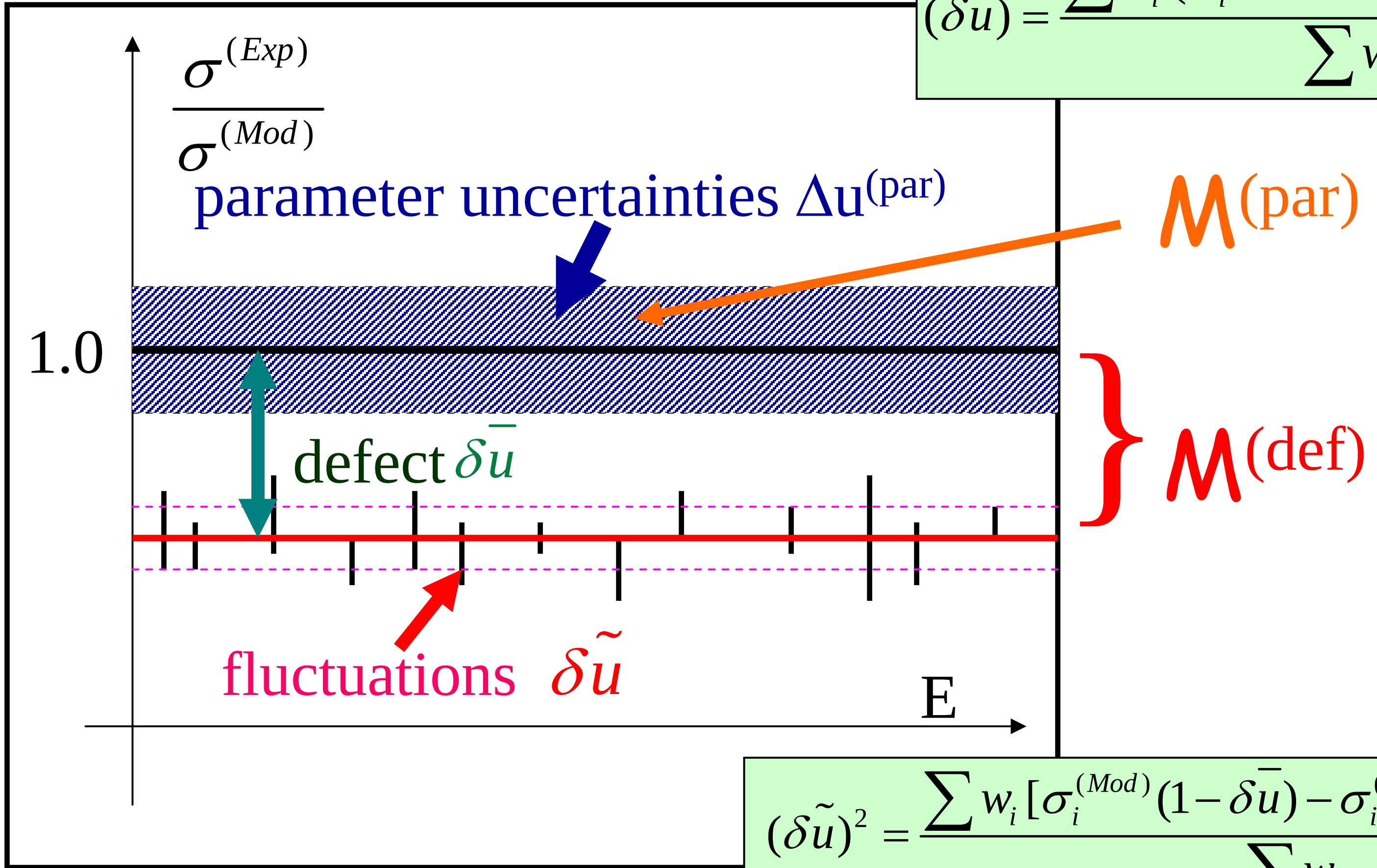
$$M^{(\mathrm{mod})} = M^{(\mathrm{par})} + M^{(\mathrm{num})} + M^{(\mathrm{def})}$$

parameter uncertainties

numerical implementation error

Task 1:
deficiency of the model
non-statistical error

Explanation of terms



$$(\delta\bar{u}) = \frac{\sum w_i (\sigma_i^{(Mod)} - \sigma_i^{(Exp)})/(\sigma_i^{(Mod)})}{\sum w_i}$$

$$(\delta\tilde{u})^2 = \frac{\sum w_i [\sigma_i^{(Mod)}(1-\delta\bar{u}) - \sigma_i^{(Exp)}]^2/(\sigma_i^{(Mod)})^2}{\sum w_i}$$

Methods for covariances

Activities to include covariance information

- covariances from experiment (Vonach, Tagesen)
- Monte Carlo techniques (Smith, Koning),
- KALMAN-filter (Kawano, Herman)
- χ^2 based determination of correlations (Bauge)

All these procedures require experimental data for the determination of the covariance matrices

general problems: (a) uncertainties tend to too small values
(b) correlations either to weak or too strong

Interpretations of probabilities

OBJECTIVE SCHOOL:
Probability of an event is an objective property of the event always accessible by observation of frequency ratios in a random experiment, such as coin tossing

SUBJECTIVE SCHOOL:
Probabilities are expressions of human ignorance; it expresses the expectation based on available information that the event will occur. Detailed verification is not expected.

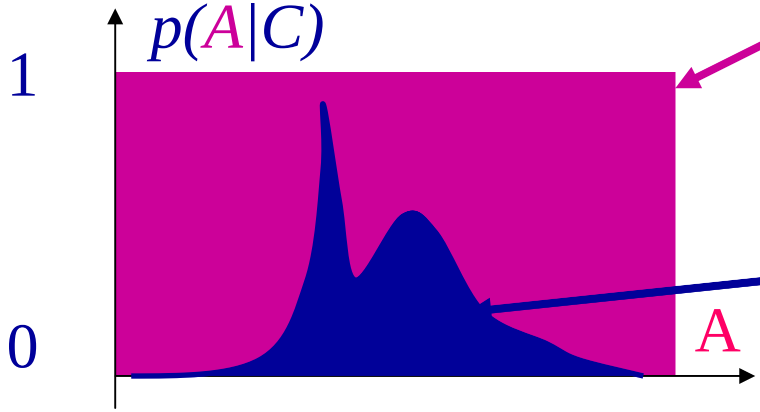
Objective and Subjective schools of thought are mathematically identical, but their concepts cannot be united (Cox, 1946).

- Probabilities are not relative frequencies
- Superior schemes of logical inference (Fuzzy logic, artificial intellegence) are equivalent to probability theory at best.

The subjective point of view is wider and allows to deal with the questions related to nuclear data evaluation.

Formalism

Nuclear data evaluation is essentially a statistical process which implies the subjective point of view in statistics



$p(\bar{A}|C)$ probability that event A does not occur when the condition C is true

$p(A|C)$ probability for the occurence of event A when the condition C is true

Basics of probability theory

- At present significant worldwide effort for the determination of covariance matrices (integral cross sections)

$$M_{ij} = \left\langle \Delta\sigma_i \Delta\sigma_j \right\rangle \qquad \mathrm{i} = \{\mathrm{c_i}, E_i\}$$

- Nuclear data evaluation is essentially a statistical analysis within a subjective point of view. Based essentially on the two fundamental relationships of probability theory

sum rule $\quad p(x \mid M) + p(\overline{x} \mid M) = 1$

product rule $\quad p(x\sigma \mid M) = p(x \mid \sigma M)\, p(\sigma \mid M) = p(\sigma \mid xM)\, p(x \mid M)$

- Bayes theorem:

$$p(x \mid \sigma M) = \frac{p(\sigma \mid xM)\, p(x \mid M)}{p(\sigma \mid M)}$$

Likelihood
Prior

Bayes theorem and nuclear data evaluation

The statistically correct procedure to generate an evaluated nuclear data file is given by the strict application of Bayes theorem.

Bayes Theorem (1763):

P(A|BC) = P(B|AC) P(A|C) / P(B|C)

posterior = likelihood x prior / evidence

A ... model parameter B ... data C ... other information

from experiment (→ likelihood)

Choice of proper prior ? Jaynes (→ prior)

INFORMATION THEORY (Shannon 1949)

Information entropy: $$H(\underline{p}) = -K \sum_{i=1}^{N} p_i \ln p_i$$

The amount of uncertainty is maximal if the entropy is maximal.

The likelihood function

The likelihood $p(\underline{y}\,|\,\underline{x}, M, I)$ gives the probability that the data set $\underline{y}$ is measured for a model *M* with parameters $\underline{x}$ and the additional Information *I*.

$$p(\underline{y}\,|\,\underline{x}, M, I) \propto \exp\left[-\frac{1}{2}(\underline{\sigma}^{\exp} - \underline{\sigma}^{M})^{T}\mathbf{B}^{-1}(\underline{\sigma}^{\exp} - \underline{\sigma}^{M})\right]$$

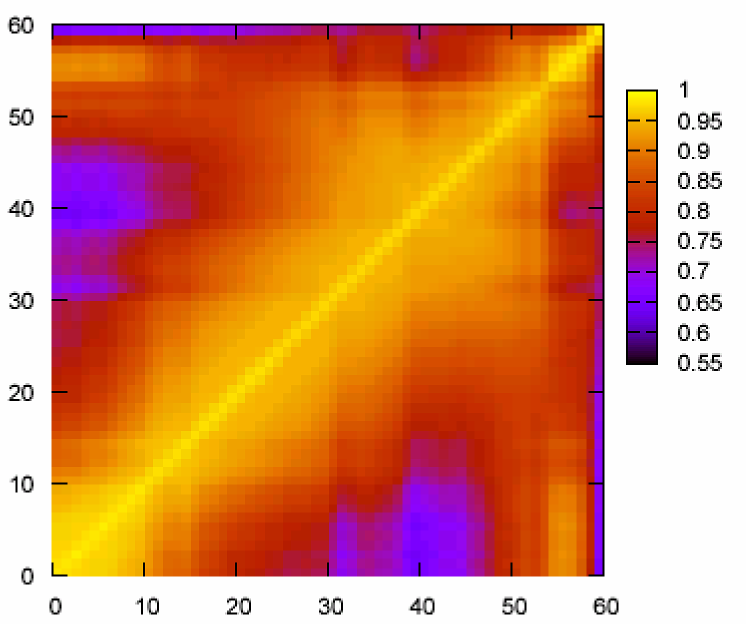
with the experimental covariance matrix **B** with elements

$$B_{\rho\eta} = \left\langle \Delta\sigma_{\rho}^{\exp}\Delta\sigma_{\eta}^{\exp} \right\rangle$$

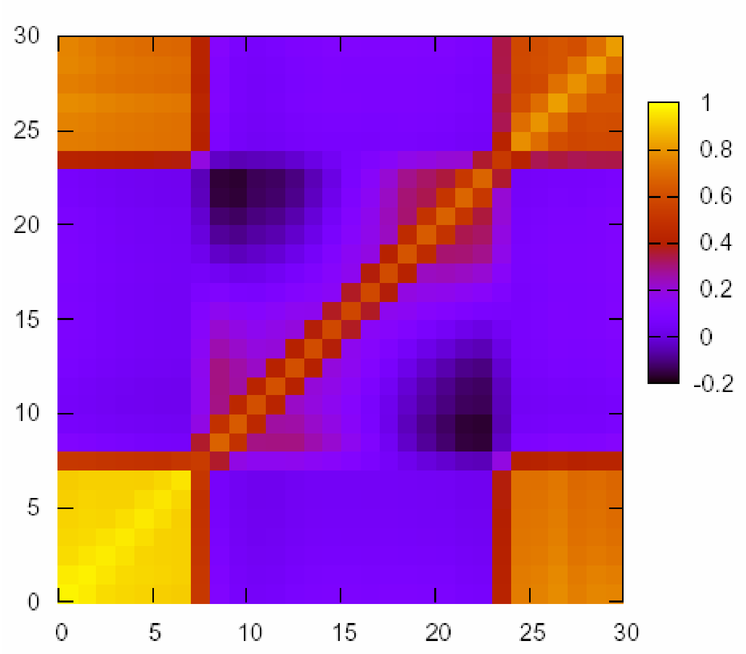
The covariance matrix B should be provided by the experiment. Usually not available neither in the paper nor in the EXFOR file !!!

Covariances of n_TOF experiment

$^{232}Th(n,\gamma)$



$^{151}Sm(n,\gamma)$



normalized covariance matrix **B**

Bayesian statistics

The statistically correct procedure to generate an evaluated nuclear data file is given by the strict application of Bayes theorem.

Bayes Theorem (1763):

p(A|BC) = p(B|AC) p(A|C) / p(B|C)

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A ... model parameter B ... data C ... other information

MC techniques
Kalman filter
χ^2-methods

from experiment

Vonach, Tagesen

Choice of proper prior ?

Determination of prior

The information entropy of a probability distribution is given by

$$H(\underline{p}) = -K \sum_{i=1}^{N} p_i \ln p_i$$

INFORMATION THEORY (Shannon 1949)
Jaynes, Phys. Rev. 106, 620 (1957)

The lack of information on the systems implies that the uncertainty about the actual status is maximal

↓

Information entropy is maximal

Choice of proper prior

For most cases where there is no obvious prior Baye proposed to apply
Laplace principle of insufficient reasoning, i.e. a uniform distribution

Main criticism from objectivist: the choice of prior is arbitrary !!!

INFORMATION THEORY (Shannon 1949)

Information entropy: $$H(\underline{p}) = -K \sum_{i=1}^{N} p_i \ln p_i$$

The amount of uncertainty is maximal if the entropy is maximal.

Assumption: Besides the marginalisation we know an expection value

$$\delta \tilde{H}(\underline{p}, \lambda_0, \lambda_1) = \delta \left[-K \sum_{i=1}^{N} p_i \ln p_i - \lambda_0 K \left(\sum_{i=1}^{N} p_i - 1 \right) - \lambda_1 K \left(\sum_{i=1}^{N} p_i f_i - f \right) \right] = 0$$

Maximum Entropy

Assumption: Besides the marginalisation we know an expection value

$$\delta \tilde{H}(\underline{p},\lambda_0,\lambda_1) = \delta\left[-K\sum_{i=1}^{N} p_i \ln p_i - \lambda_0 K\left(\sum_{i=1}^{N} p_i - 1\right) - \lambda_1 K\left(\sum_{i=1}^{N} p_i f_i - f\right)\right] = 0$$

Lagrange parameter λ_i

Prior:

$$p_i = \frac{1}{Z(\lambda)}\exp(\lambda f_i)$$

Partition function:

$$Z(\lambda) = \sum_{i=1}^{N}\exp(\lambda f_i)$$

Determination of λ:

$$f = \frac{\partial}{\partial\mu}\ln Z(\lambda)$$

Variance of λ:

$$\Delta^2 f = \frac{\partial^2}{\partial\mu^2}\ln Z(\lambda)$$

Problem: continuous parameters

There seems to be a basic arbitrariness about priors in the case of a continuous variable → root of criticisms on Bayesian statistics (A. Wald (1950))

$p(\lambda)\, d\lambda \propto d\lambda$ → for $\tau=1/\lambda$ we obtain $p(1/\tau)d\tau / \tau^2 = p(\tau)\, d\tau \propto d\tau/\tau^2$
$p(\tau)\, d\tau \propto d\tau$ → for $\lambda=1/\tau$ we obtain $p(1/\lambda)d\lambda / \lambda^2 = p(\lambda)\, d\lambda \propto d\lambda/\lambda^2$

In two problems with the same prior information, the same prior probabilities should be assigned. A transformation of coordinates does not change the prior information

Principle required to provide parameter space with a proper rigidity (e.g. concept of invariant line element)

Transformation group

The invariance of the information with respect to trans-formation groups determines the measure unambiguously (E.T. Jaynes, 1968, 1973)

<u>Concept:</u>

Location – the prior must be invariant under a shift c

$$\mathbf{p(\mu)\, d\mu = p(\mu+c)\, d\lambda(\mu+c) \propto d\mu} \qquad \boldsymbol{m(x)=const.}$$

scale – invariance under rescaling

$$\mathbf{p(\mu)\, d\mu = p(c\mu)\, d\lambda(c\mu) \propto d\mu/\mu} \qquad \boldsymbol{m(x)=1/x}$$

Prior for continuous parameters

The concept which provides rigidity is an *invariant measure* function *m(x)*. (Jaynes, 1963)

Information entropy

$$p(x) = \frac{1}{Z(\lambda)}\; m(x)\;\exp\big(\lambda f(x)\big)$$

Partition function:

$$f = \frac{\partial}{\partial\mu} \ln Z(\lambda)$$

Theory for prior determination

Principle of maximal information entropy

$$\delta\left[\int da_1 \cdots \int da_N\, p(\underline{a})\ \log\left(\frac{p(\underline{a})}{m(\underline{a})}\right)\right.$$

Information Entropy

$$\left.-\left[\lambda_0\left(\int da_1 \cdots da_N\, p(\underline{a})-1\right)+\sum_{k=1}^{K}\lambda_k G_k\left(p(\underline{a})\right)\right]\right] = 0$$

Constraints

prior $p(x)=\frac{1}{Z(\lambda)}\ \mathrm{m(x)}\exp\left(\lambda f(x)\right)$ **Determination of Lagrange par. λ**

partition function $Z(\lambda)=\int dx\ m(x)\ \exp\left(\lambda f(x)\right)$ **variance**

Invariant measure to account for continuous parameters:

for scaling parameters:

Data Evaluation: The steps

- What data should be evaluated : observables, energy region
- Available evaluated data files
- The applicable theoretical description → prior
- Experimental data sets and associated covariances → likelihood
- Perform Bayesian Update procedure → posterior
- Construct consistent ENDF-File

The Input for the Prior

Issues to be fixed beforehand:

set of independet cross section,
energy grid (standard)

Basic assumptions: Model

mean values of the parameters a_i,
physical boundaries of the parameters $a_i^<$, $a_i^>$
correlations between parameters
other physical constraints (e.g. sum rules)

Construction principle for prior:

Parameters are introduced as scaling parameters,
i.e. $x_i = a_i\, x_i^0$, x_i^0 is the mean value of x_i

Apart from the known properties and constraints complete ignorance is assumed,

Method of maximum information entropy taking into account the physical properties and constraints

Apriori probability

The apriori probability distribution is constructed by the principle of maximal information entropy under the given constraints

$$\delta\left[\int da_1 \cdots \int da_N \, p(\underline{a}) \, \log\left(\frac{p(\underline{a})}{m(\underline{a})}\right)\right]$$

$$= -\left[\lambda_0\left(\int da_1 \cdots da_N \, p(\underline{a}) - 1\right) + \sum_{k=1}^{K} \lambda_k G_k\left(p(\underline{a})\right)\right] = 0$$

Depending on the available information (constraints G) this can become a quite complicated procedure. Therefore we applied a simplified version which should maintain the basic features.

Prior: uncorrelated parameters

For uncorrelated parameters the probability distribution reduces to a product form

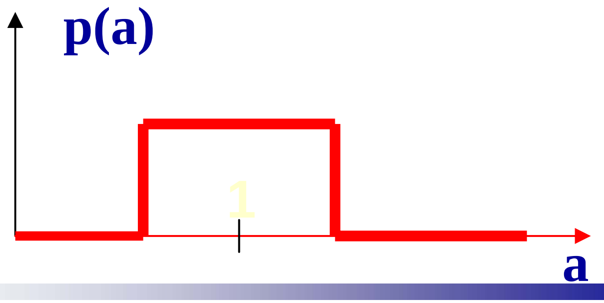
$$p(\underline{a}) = p(a_1)\, p(a_2) \cdots p(a_M)$$

Where the probability distribution for each parameter is given by the condition of complete ignorance

$$p(a_i) = \frac{1}{Z(\lambda_i)} \frac{1}{a_i} \exp(\lambda_i\, a_i) \quad \text{with } Z(\lambda_i) = \int da_i \frac{1}{a_i} \exp(\lambda_i\, a_i)$$

The Lagrange parameter is determined by $1 = \dfrac{\partial}{\partial \lambda} \log Z(\lambda)$

The bounds on the parameter space can be entered via a Bayesian update with a proper likelihood function



Parameter correlation

a) **Uncorrelated parameters** $\langle \Delta a_i \Delta a_j \rangle = \Delta^2 a_i\, \delta_i$

b) **Uncorrelated cross sections – ideal experiment**

$$\left\langle \Delta\sigma_i \Delta\sigma_j \right\rangle = \sum_{l=1}^{M}\sum_{m=1}^{M} \frac{\partial \sigma_i(E_i)}{\partial a_l} \left\langle \Delta a_l \Delta a_m \right\rangle \frac{\partial \sigma_j(E_j)}{\partial a_m} = \delta_{ij} (\sigma_i)^2\, \delta^2 u$$

c) **Inherent correlation related to invariance of the characteristic observable, e.g. σ_{tot} for optical model**

$$\sum_{i=1}^{N} \frac{\partial \sigma_i(E_i)}{\partial a_l} \frac{1}{\Delta^2 \sigma_i} \frac{\partial \sigma_i(E_i)}{\partial a_m} = \left(A^{-1}\right)_{lm} \quad \text{with} \quad A = \left(\left\langle \Delta a_l \Delta a_m \right\rangle\right)$$

For b) and c) the parameter correlation matrix $\langle \Delta a_l\, \Delta a_m \rangle$ can be Determined from a linear equation.

Disentangle correlations

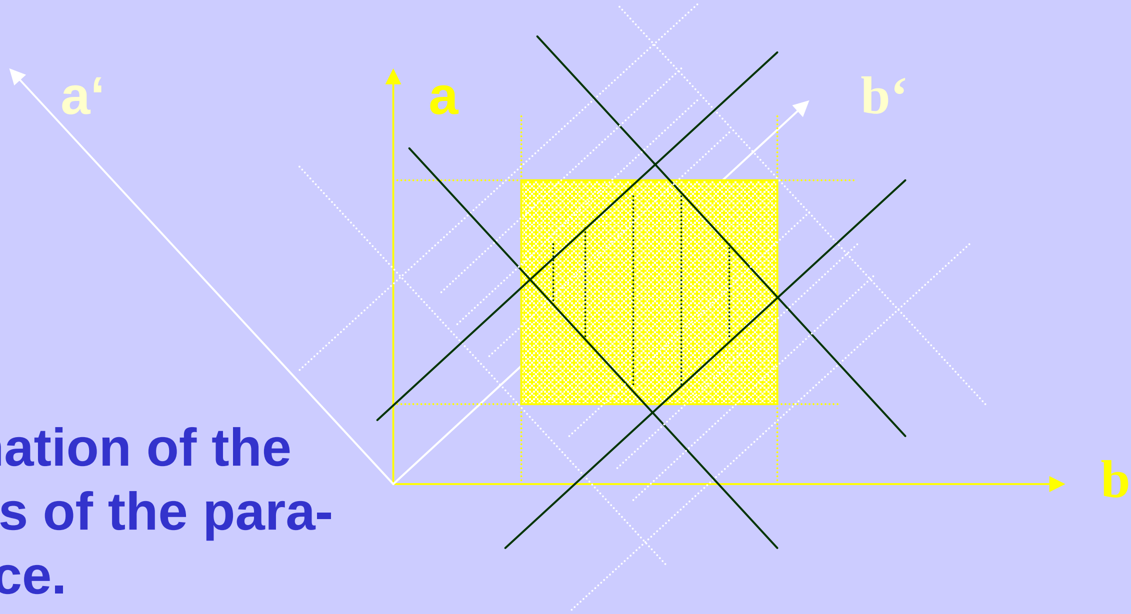
The probability distribution of the correlated parameters is not anymore a product form – Therefore we transform

The parameter vector to the eigenstates of $\mathcal{A}$ =(<$\Delta a_l \Delta a_m$>)

$$A = UDU^T \qquad D \text{ is diagonal}$$

U **contains the structure of the correlations, but not the size of** $\mathscr{E}$***u***

Problem: Transformation of the boundaries of the parameter space.



Covariances from Modelling – Prior

The following sources of uncertainties of model calcualtions can be identified:

- Uncertainties in the model parameters
- Errors in the numerical implementation and calculation
- Conceptual failure of the model

The covariance matrix of the model is composed of the contributions

$$\mathcal{M}^{(mod)} = \mathcal{M}^{(par)} + \mathcal{M}^{(num)} + \mathcal{M}^{(def)}$$

parameter uncertainties

statistically well defined
Procedure discussed before

numerical implementation error

non-statistical error, usually well known, but assumed negligible in our considerations

Deficiency of the model

Non-statistical error, strongly related to the predictive power of the model, problem of quantitative estimate

Model Defects

Normalization <N>=1 with <Δ^2N>

x_ρ...external variables (e.g.E_ρ,θ_ρ)

Nuclear Model: $$\sigma_\rho = \mathbf{N}\, \eta_\rho^{(mod)}\, (x_\rho;\mathbf{a})$$

η_ρ...observables (e.g.σ_{tot},σ_R) **model parameters: a={a_1,a_2,...,a_N}**

ρ denotes type of observable and corresponding external variables

Alternative procedure see previous JEFFDOC-888 on Covariances

Model Error

For a reliable estimate of the model error via $\mathcal{M}^{(def)}$ we evaluate first the mean model error δu as the average quadratic deviation of the model cross sections from experimental values in equivalent systems (neighboring isotopes, proton-nucleus data):

$$(\delta u)^2 = \frac{\sum w_i (\delta u_i)^2}{\sum w_i} \quad \text{with} \quad (\delta u_i)^2 = [\sigma_i^{(exp)} - \sigma_i^{(mod)}]^2 / (\sigma_i^{(mod)})^2, \quad w_i = (\sigma_i^{(mod)})^2 / (\Delta\sigma_i^{(exp)})^2$$

Note: The observable could be a true angle integrated cross section, $\sigma_{tot}, \sigma_R, \ldots$, or a partial integrated one constructed from differential cross sections via

$$\sigma_i = \sum_j \sin\theta_j \; d\sigma_i/d\Omega(E_i,\theta_j) \quad \text{with} \quad \Delta\sigma_i = \sum_j \sin\theta_j \; \Delta(d\sigma_i/d\Omega(E_i,\theta_j))$$

The **variance** of the model is given by

$$M_{i,j}^{(def)} = \langle \Delta\sigma_i^{(mod)}(E_i)\, \Delta\sigma_i^{(mod)}(E_i) \rangle = (\delta u)^2\, \sigma_i^{(mod)}(E_i)\, \sigma_i^{(mod)}(E_i)$$

Covariance of Model Deficiencies

Ansatz:

from JEFFDOC-888

$$M_{i,j}^{(def)} = <\Delta\sigma_i^{(mod)}(E_i)\, \Delta\sigma_j^{(mod)}(E_j)> = (\delta u)^2\, \sigma_i^{(mod)}(E_i)\, \sigma_j^{(mod)}(E_j)\, C_{i,j}$$

The correlation matrix C must satisfy the following conditions:

- $C_{i,i} = 1$ the diagonal of $M^{(def)}$ is given by the variance
- for increasing $\Delta=|E_i-E_j|$ the matrix elements $|C_{i,j}|$ must decrease
- the rate of decrease of $|C_{i,j}|$ must depend on the reproductive power of the model, i.e. for a perfect model $C_{i,j} = 1$

$$C_{i,j} = \exp\left[-\left(\frac{\delta u}{\delta u_0}\right) \ln\frac{E^>}{E^<}\right]$$

for i,j denoting the same type of observable otherwise $C_{i,j} = 0$.

$\delta u_0 = 0.01$ characterize a perfect model; $E^> = \max(E_i,E_j)$, $E^< = \min(E_i,E_j)$

Bayesian update

The statistically correct procedure to generate an evaluated nuclear data file is given by the strict application of Bayes theorem.

Bayes Theorem (1763):

p(A|BC) = p(B|AC) p(A|C) / p(B|C)

posterior = likelihood x prior / evidence

A ... model parameter B ... data C ... other information

from experiment

Choice of proper prior ?

Vonach, Tagesen

Linearized Bayesian update

The specific likelihood function yields the following Linearisation of the Bayesian update procedure (e.g. Fröhner)

$$x' = x + M(1+Q)^{-1}G^T V^{-1}(D - T) \qquad \text{parameter vector}$$

$$= x + (M^{-1} + W)^{-1}G^T V^{-1}(D - T)$$

$$M' = M(1+Q)^{-1} = (M^{-1} + W)^{-1} \qquad \text{covariance matrix}$$

$$\text{with} \quad Q = G^T V^{-1} G M = W M \qquad G \ \text{sensitivity matrix}$$

A least square fit is characterized by the relationship

$$x' = x + W^{-1}G^T V^{-1}(D - T)$$

$$M' = W^{-1} \quad \text{hence } M^{-1} = 0 \text{ no apriori knowledge}$$

Applications

Application to ^{208}Pb, ^{16}O and ^{6}Li with emphasis on the uncertainty related to the optical model (phenomenological and microscopic).

(a) phenomenological optical model of Koning and Delaroche in total 18 potential parameters

(b) nuclear matter approach of Amos et al. (few parameters)

Phenomenological optical model

Use of the optical model of Koning and Delaroche for ^{208}Pb

Volume terms							Der. term	
r_v	a_v	v_1	v_2	v_3	w_1	w_2	r_{vd}	a_{vd}
1.244	0.646	50.6	0.0069	0.000015	15.6	88.0	1.246	0.510

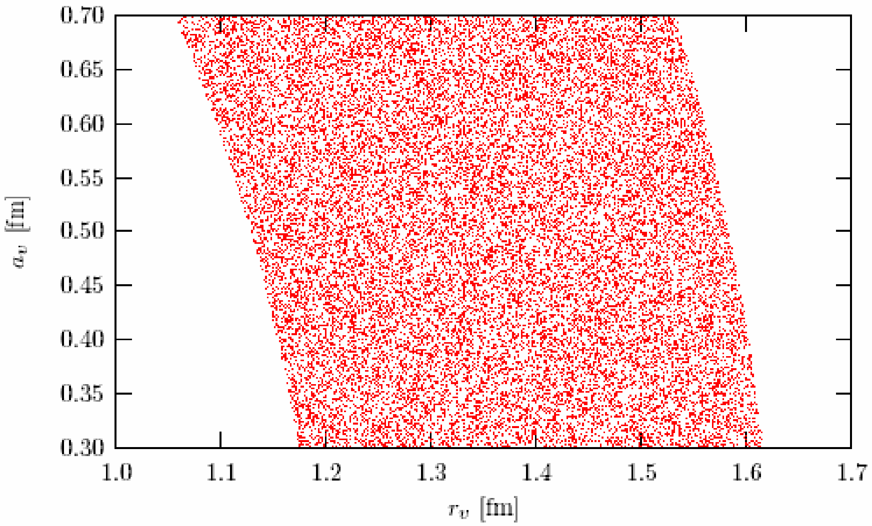
d_1	d_2	d_3	r_{vso}	a_{vso}	v_{so1}	v_{so2}	w_{so1}	w_{so2}
13.8	0.0180	13.80	1.080	0.570	6.6	0.0035	-3.1	160.0
Der. terms			Spin-orbit terms					

<u>Key question</u> – range of physically admissable parameter values

real potential depth – number of nodes
radius – limits from charge radius and nuclear force
difuseness – limits from charge distr. and nuclear range

unitarity, sum rules, ...

admissible range of parameters



dependence on a_v of admissible range in r_v

$$\sqrt{\langle r^2\rangle_{charge}} \le \sqrt{\langle r^2\rangle_{OM}} \le \sqrt{\langle r^2\rangle_{charge}} + \sqrt{\langle r^2\rangle_{force}}$$

$$\langle r^2\rangle = \frac{\int d^3r\, r^2 V(r)}{\int d^3r\, V(r)}$$

		$r^<$ (fm)	$r^>$ (fm)	$r^<$ (%)	$r^>$ (%)
r_v	1.244	1.050	1.550	15.6	24.6
r_{vd}	1.246	1.051	1.552	15.6	24.6
r_{so}	1.080	0.911	1.346	15.6	24.6

admissible range in a_v

$$\rho(|\mathbf{x}|) = \frac{\rho_0}{1+\exp\left[(|\mathbf{x}|-c)/z\right]},$$

z defines lower boundary

$$(\rho * v)_{\mathbf{s}} = (\mathcal{F}^{-1}(F\rho \times Fv)_{\mathbf{k}})_{\mathbf{s}}$$

upper boundary defined by convolution with M3Y

		$a^<$ (fm)	$a^>$ (fm)	$a^<$ (%)	$a^>$ (%)
a_v	0.646	0.549	0.800	15.0	23.8
a_{vd}	0.510	0.487	0.632	15.0	23.8
a_{so}	0.570	0.484	0.706	15.0	23.8

Energy dependence estimated

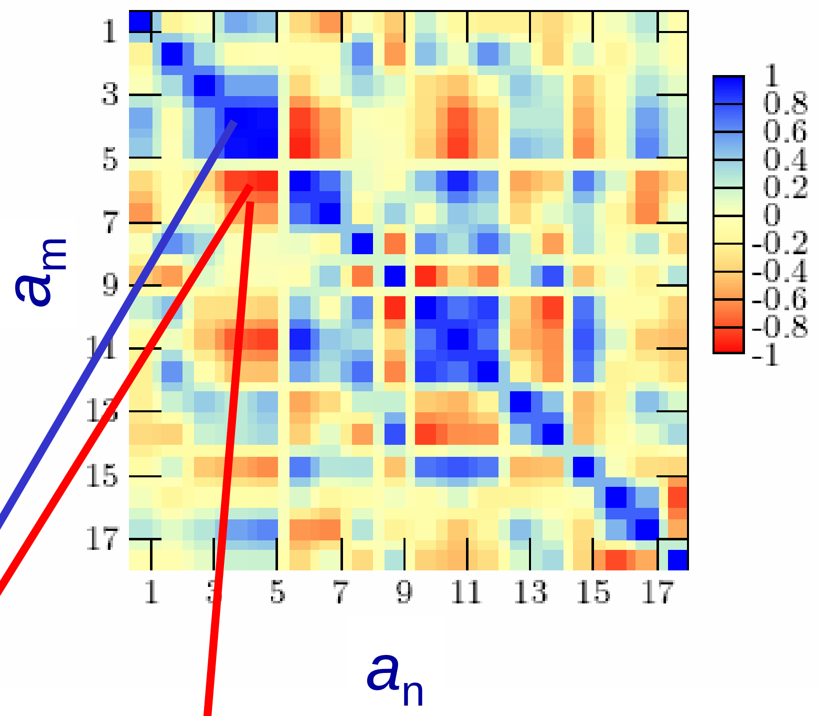
		$v^<$	$v^>$	$v^<$ (%)	$v^>$ (%)
v_1	50.6	46.0	56.0	9.1	9.1
v_2	0.0069	0.0058	0.0079	15.0	15.0
v_3	0.000015	0.000013	0.000017	15.0	15.0
v_{so1}	6.6	5.28	7.92	20.0	20.0
v_{so2}	0.0035	0.0028	0.0042	20.0	20.0

		$w^<$	$w^>$	$w^<$ (%)	$w^>$ (%)
w_1	15.6	12.48	18.72	10.0	10.0
w_2	88.0	70.4	105.6	20.0	20.0
w_{so1}	−3.1	−3.72	−2.48	20.0	20.0
w_{so2}	160.0	128.0	192.0	20.0	20.0

		$d^<$	$d^>$	$d^<$ (%)	$d^>$ (%)
d_1	13.8	11.04	16.56	10.0	10.0
d_2	0.018	0.014	0.022	20.0	20.0
d_3	13.8	11.04	16.56	20.0	20.0

Correlations of parameters

Parameter correlations extracted from the assumption that σ_{tot}, σ_{non}, $\sigma(n,p)$, $\sigma(n,d)$, $\sigma(n,\gamma)$ are reproduced at 200 energies between 4,8 – 100 MeV within a small error band δu=1%

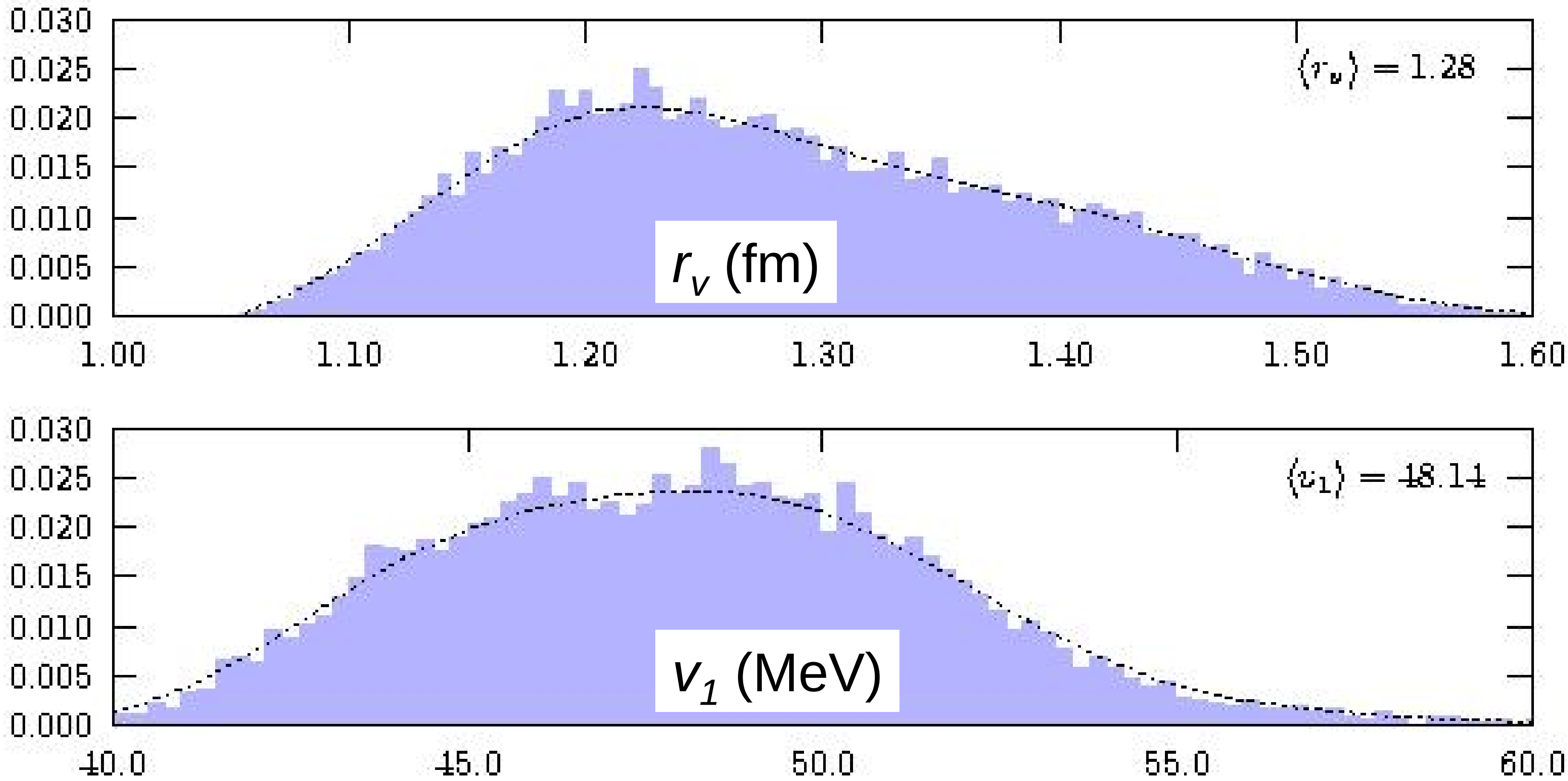


$$C_{m,n} = \frac{\langle \Delta a_m \Delta a_m \rangle}{\sqrt{\langle \Delta^2 a_m \rangle \langle \Delta^2 a_n \rangle}}$$

r_v	a_v	v_1	v_2	v_3	w_1	w_2	r_{vd}	a_{vd}
1.244	0.646	50.6	0.0069	0.000015	15.6	88.0	1.246	0.510
d_1	d_2	d_3	r_{vso}	a_{vso}	v_{so1}	v_{so2}	w_{so1}	w_{so2}
13.8	0.0180	13.80	1.080	0.570	6.6	0.0035	-3.1	160.0

Parameter distributions for ^{208}Pb

potential parameters



Level density parameters

Fermi gas level density

$$\rho_F(E_x, J, \Pi) = \frac{1}{2}\,\frac{2J+1}{2\sqrt{2\pi}\sigma_c^2}\,\frac{\sqrt{\pi}}{12}\,\frac{\exp(2\sqrt{aU})}{a^{1/4}U^{5/4}}\exp\left[\frac{(J+\frac{1}{2})^2}{2\sigma_c^2}\right]$$

$$\sigma_c^2 = c\ A^{2/3}\sqrt{a\ U}$$

$$a(E) = \hat{a}\left[1 + \delta W \frac{1-\exp(-\gamma U)}{U}\right]$$

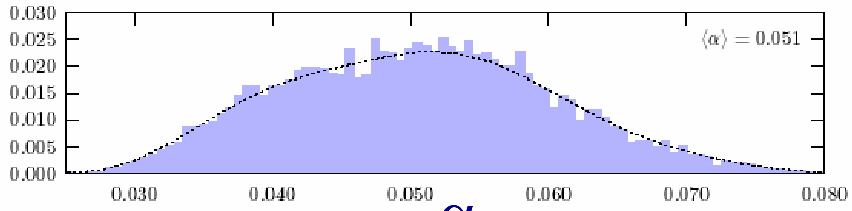
admissible range as given in TALYS

$0{,}04 < \alpha < 0{,}1$

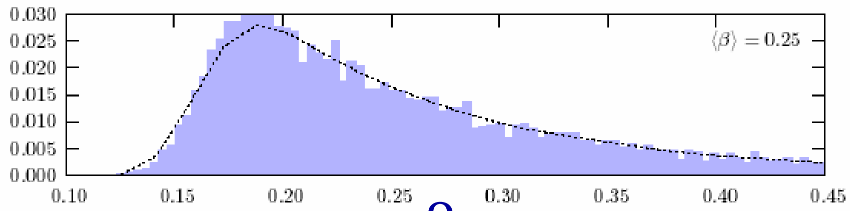
$0{,}06 < \beta < 0{,}5$

level density parameters

$$\hat{a} = \alpha A + \beta A^{2/3}$$

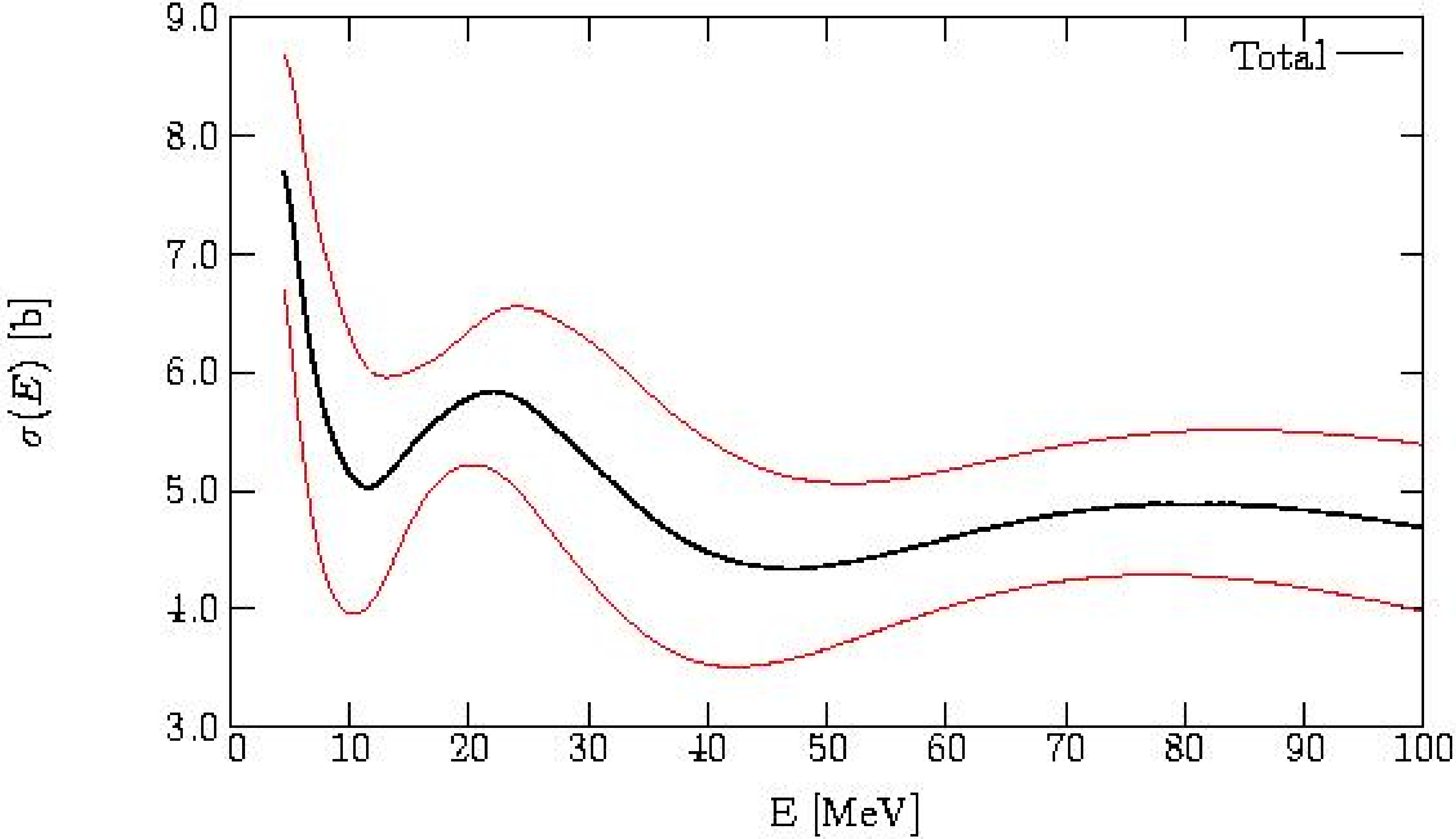


α

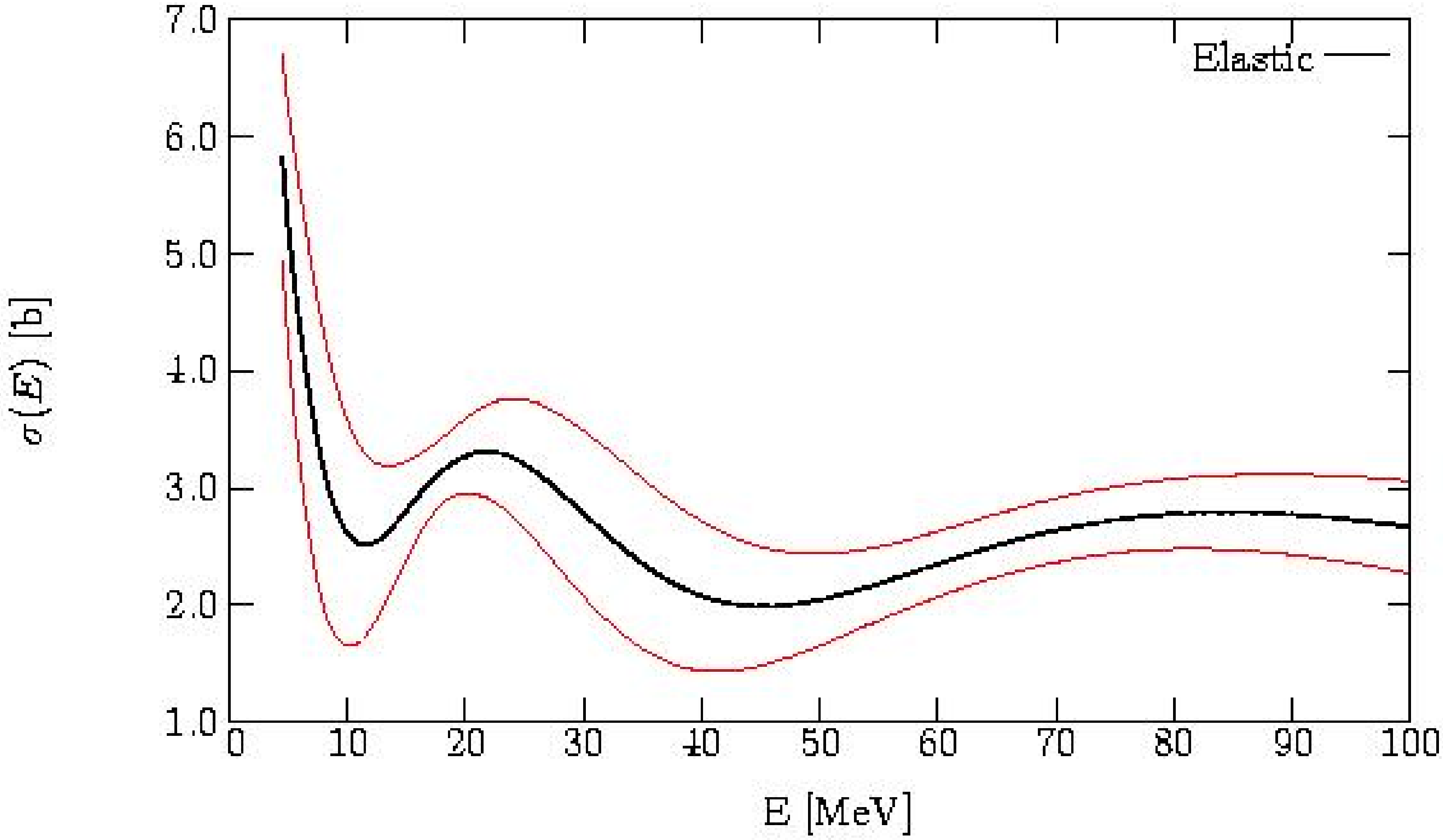


β

Cross section error bands

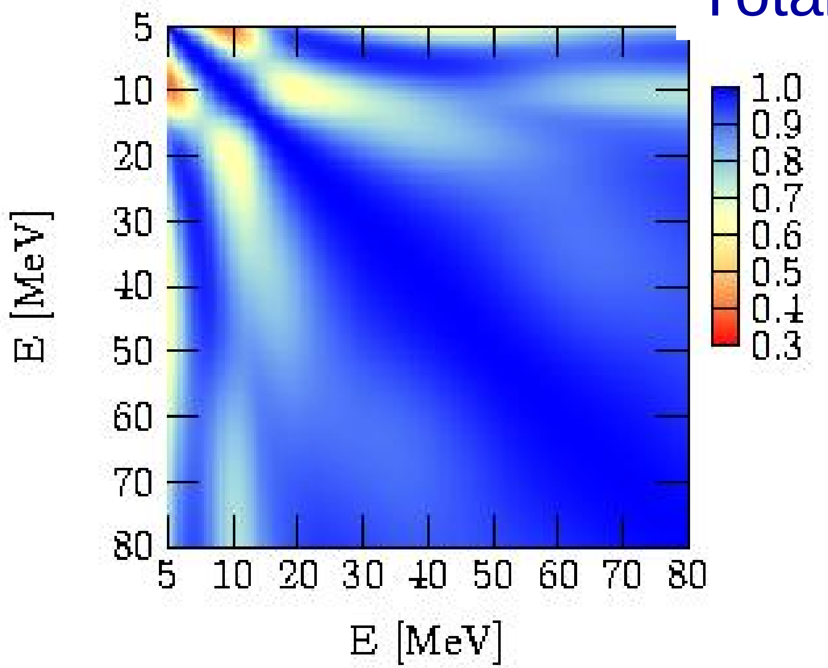


Cross section error bands

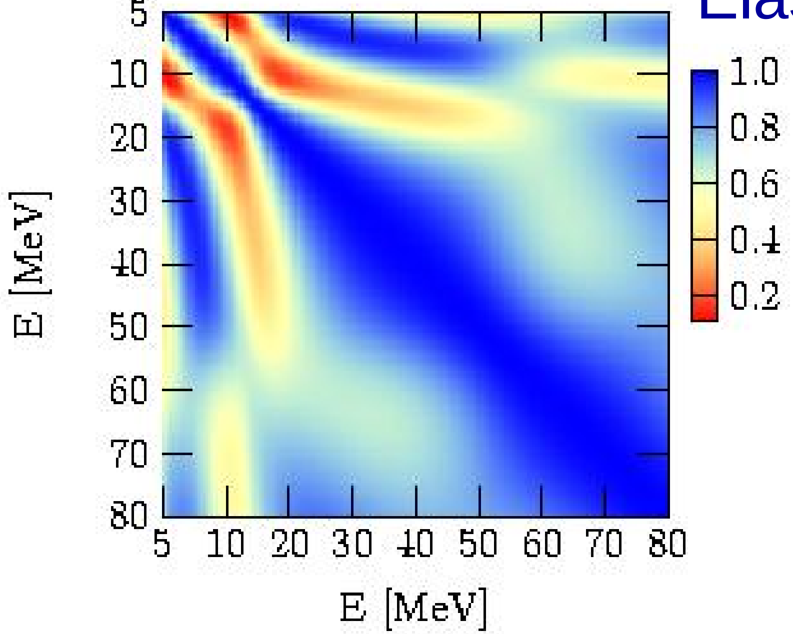


Correlations of cross sections

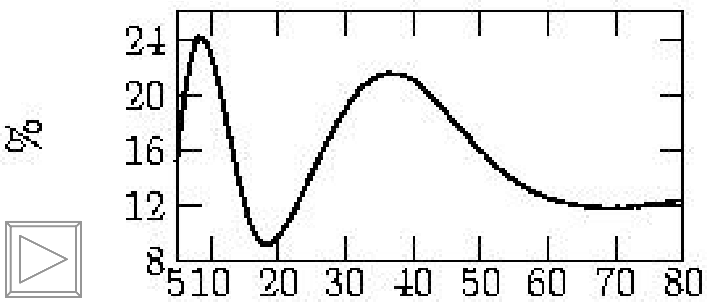
Total



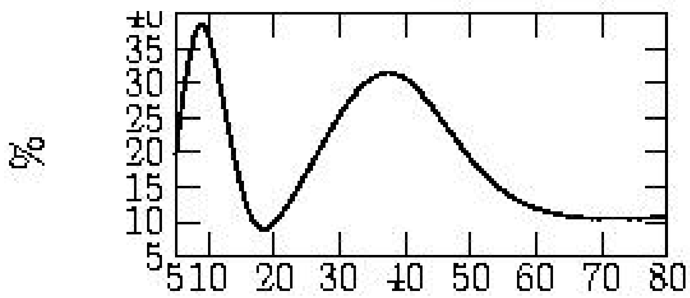
Elastic



Varianz



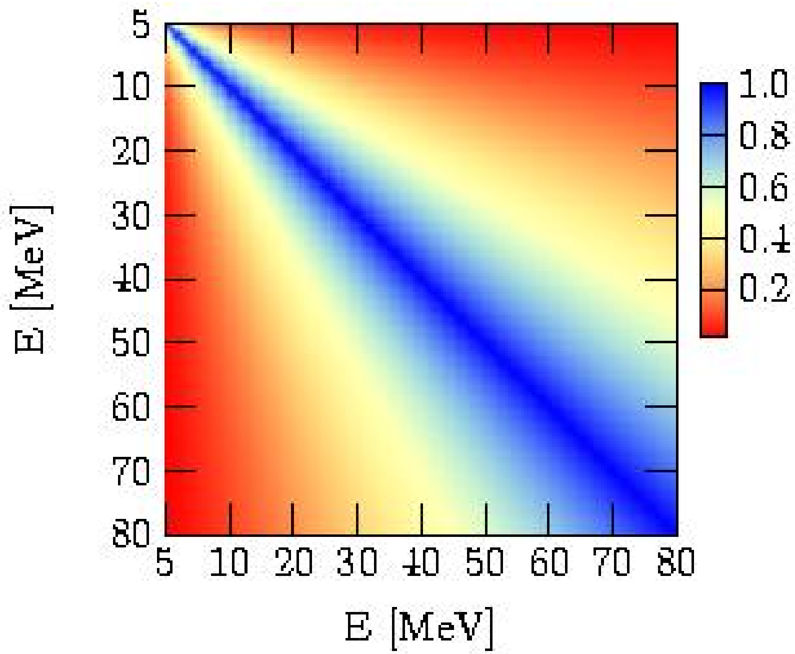
Varianz

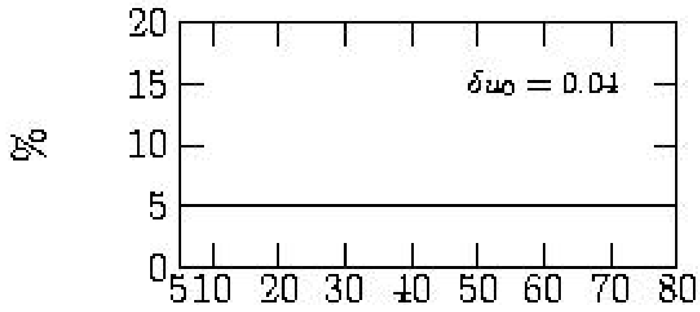


Model defects

In addition one has to include the covariance matrix due to model defects. At present we follow the suggestions made at the nuclear data conference 2004.

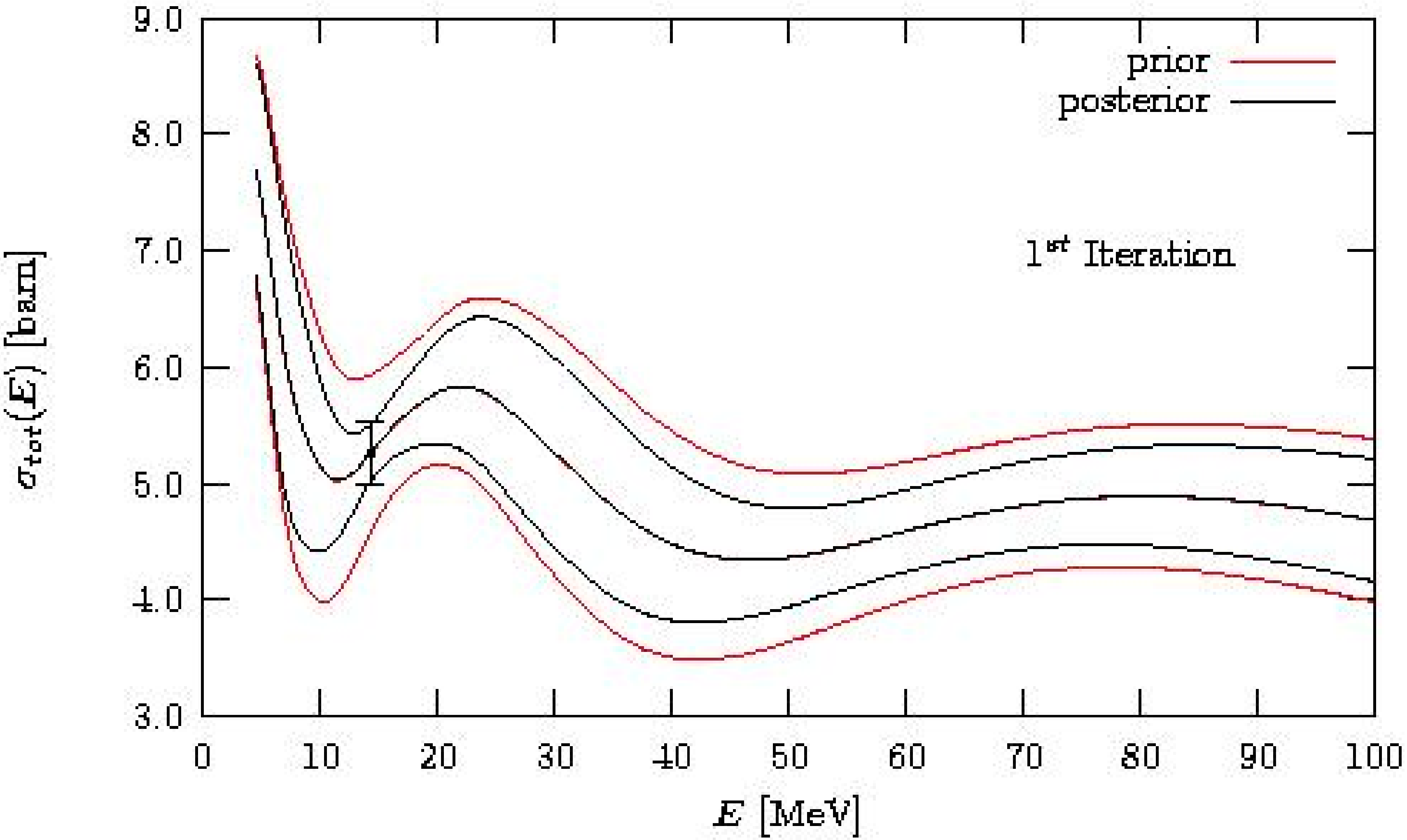
The mean deviation of the optical potential of Koning and Delaroche is about 4% up to 80 MeV





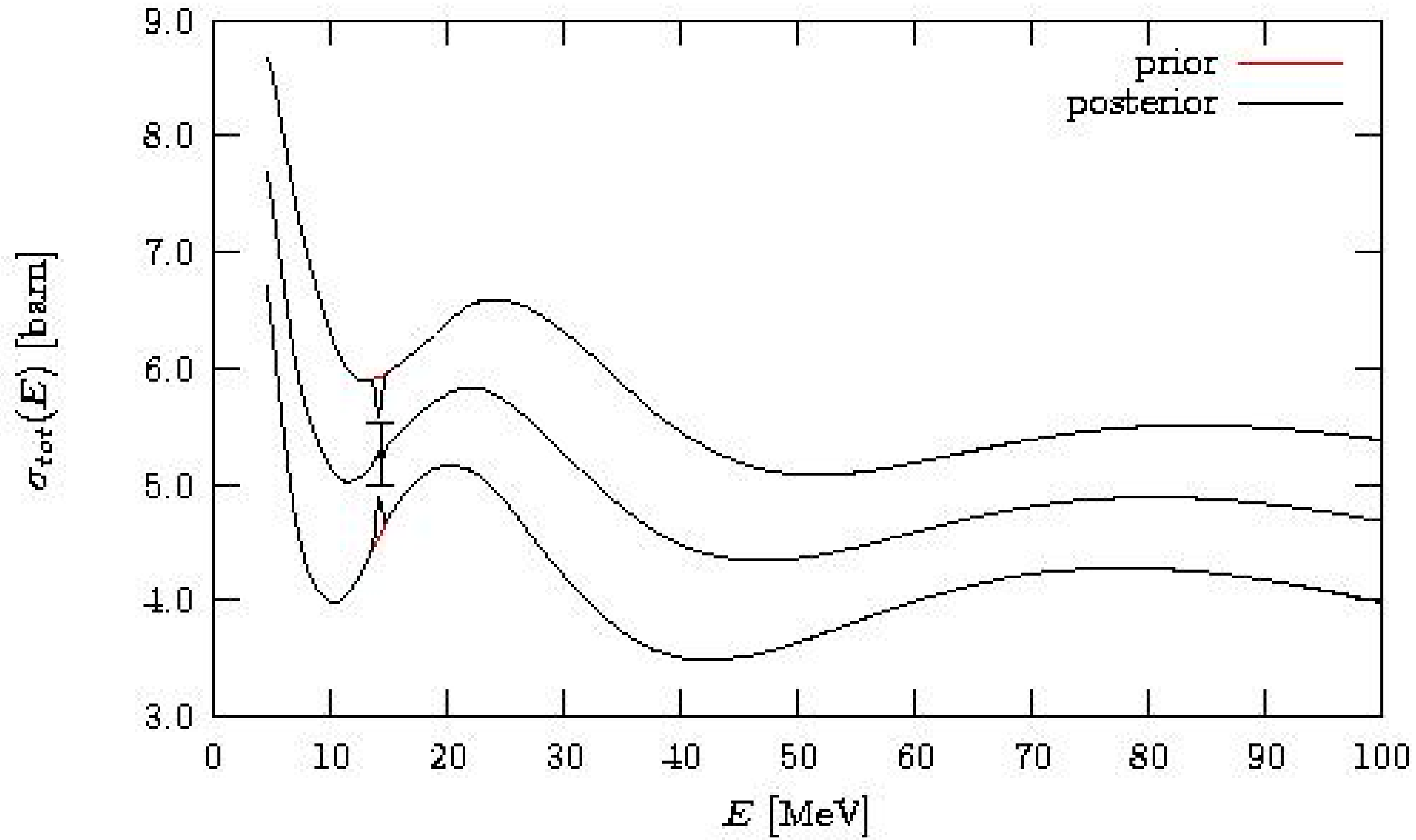
Bayes update procedure

Experimental data are included via Bayes update procedure



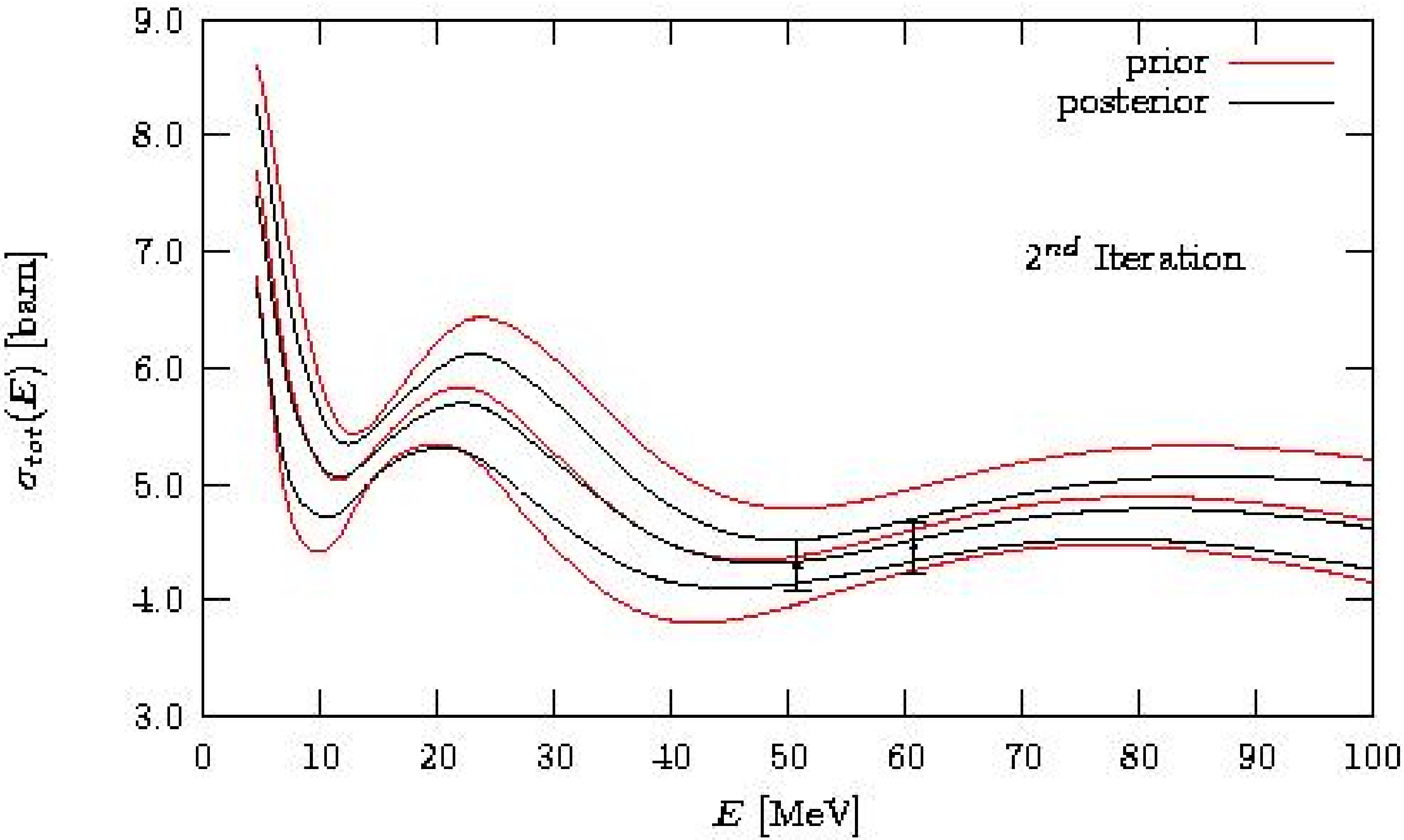
Importance of correlations

Off diagonal elements set to zero → fluctuations

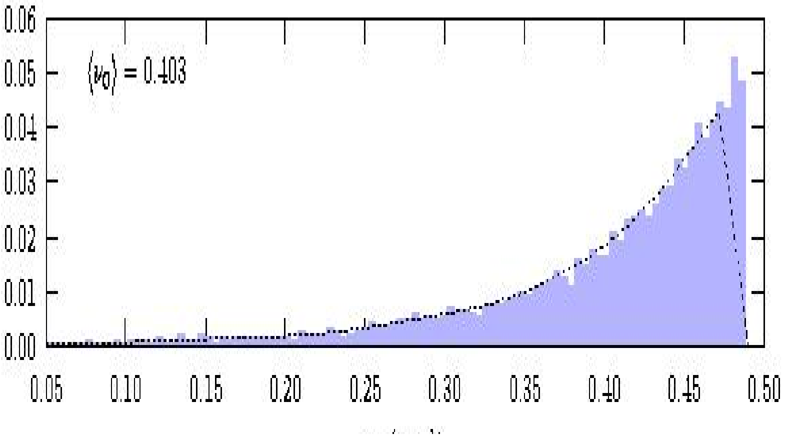


2nd Bayes update

Full convolutions of probabilities performed

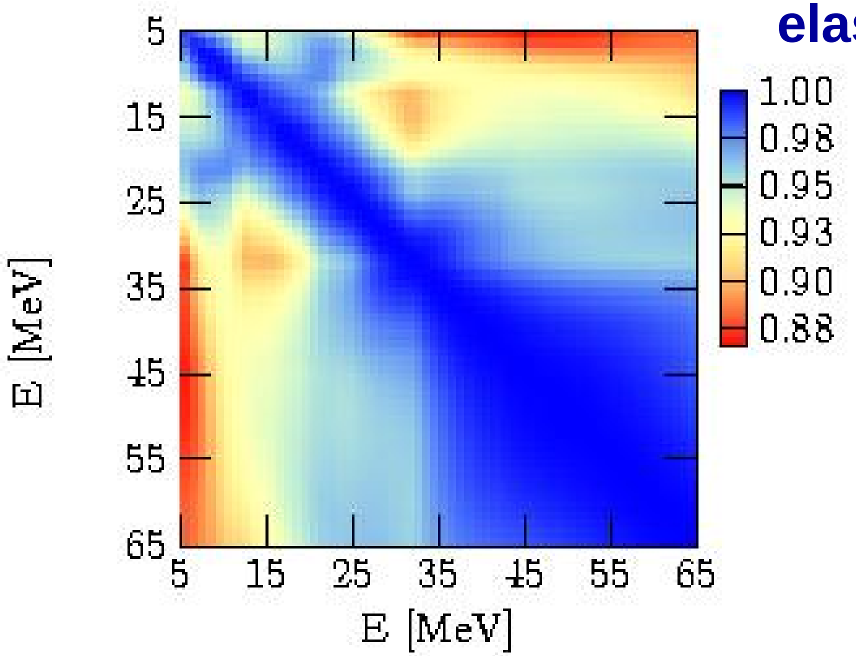


Nuclear matter approach

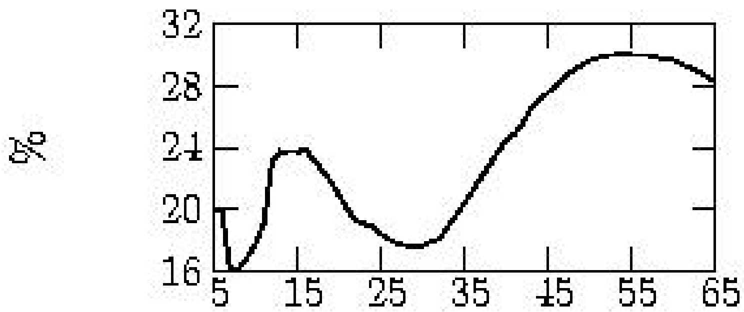


Oscillator frequency

elastic



Varianz



Comparison of methods

At present the following techniques for the determination of covariance matrices for modelling are under investigation:

- Monte Carlo simulations (Smith, Koning, Trkov,...)
- Forward Backward χ^2-fit (Bauge)
- Kalman-filter driven procedure (Kawano, Herman, Talou,...)
- Prior based on maximum entropy and subsequent Bayesian update procedure (Leeb)

What are the characteristics of these methods with regard to fundamental statics?
How are these methods related to each other?

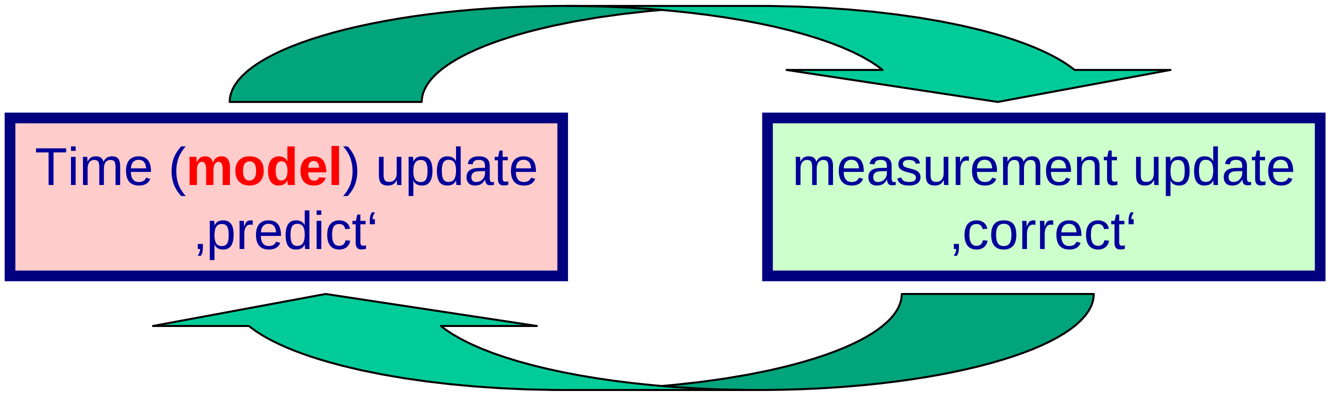
Kalman filter

Kalman filter (1960):

- recursive solution to the discrete-data linear fitting problem
- it is essentially a predictor-corrector type estimator
- optimal with regard to minimize error covariances
- simple and robust algorithm

Major applications: navigation systems, computer graphics

Concept: estimate state of a discrete-time controlled process



Kalman filter – algorithm

Discrete-time process governed by stochastic difference eq.

$x_k = Ax_{k-1} + Bu_k + \omega_k$ learning process

$\sigma_k = Gx_k + \nu_k$ measurement

ω, ν are random variables, covariance Q

Formulation of measurement process

$$\Delta\sigma_k^- = x_k - \langle x_k^- \rangle \quad \text{and} \quad \Delta\sigma_k = x_k - \langle x_k \rangle$$

$$M_k^- = \left\langle \Delta\sigma_k^- \left(\Delta\sigma_k^-\right)^T \right\rangle \quad \text{and} \quad M_k = \left\langle \Delta\sigma_k \left(\Delta\sigma_k\right)^T \right\rangle$$

$$\langle x_k \rangle = \langle x_k^- \rangle + K\left(\sigma_k - G\langle x_k^- \rangle\right)$$

Kalman filter – algorithm

$$\Delta\sigma_k^- = x_k - \langle x_k^- \rangle \quad \text{and} \quad \Delta\sigma_k = x_k - \langle x_k \rangle$$

$$M_k^- = \left\langle \Delta\sigma_k^- \left(\Delta\sigma_k^-\right)^T \right\rangle \quad \text{and} \quad M_k = \left\langle \Delta\sigma_k \left(\Delta\sigma_k\right)^T \right\rangle$$

$$\langle x_k \rangle = \langle x_k^- \rangle + K\left(\sigma_k - G\langle x_k^- \rangle\right)$$

Evaluation of *M* and minimizing the trace of the covariance Matrix by adjustment of *K* leads to

$$K_k = M_k^- G^T \left(G M_k^- G^T + V\right)^{-1}$$

Kalman filter – algorithm

Learning update equations

$$\langle x_k^- \rangle = A\langle x_k \rangle + Bu_k$$

$$M_k^- = AM_{k-1}A^T + Q$$

The prior correlations depend on the optimization algorithm

Measurement update equations

$$K_k = M_k^- G^T \left(GM_k^- G^T + V\right)^{-1}$$

$$\langle x_k \rangle = \langle x_k^- \rangle + K_k\left(\sigma_k - G\langle x_k^- \rangle\right)$$

$$M_k = \left(1 - K_k G\right)M_k^-$$

The **same relationships** for **expectation values** and **covariance matrices**, but normal distributions for linear problems are assumed, otherwise inverse distribution with respect to the model function.

Relationship of methods

The comparison of available techniques shows the following relationship to basic statistics:

a) MC simulations assume adhoc parameter distributions, ignore parameter correlations and contain no linearisation, but uncontrollable a-priori assumptions.

b) Forward backward χ^2-fits are consistent least square fits, which contain correlations, but there is no controlled a-priori knowledge included in the process (except x-boundaries).

c) The Kalman filter technique is essentially an approximate Bayesian update procedure, which provides the same expectation values and covariances using normal (linear process) or model defined parameter distributions. Prior?

d) a basic prior determination allows a full Bayesian update procedure similar to the analysis of experimental data.

Conclusions

- well defined procedure for prior associated with parameter uncertainties developed
  start: complete ignorance → apriori information
- physical boundaries for some parameters established
- method successfully applied to ^{208}Pb, ^{16}O, ^{6}Li
- importance of correlations

Open Problems

There are still several open problems in the determination of reliable covariance matrices

Required Developments

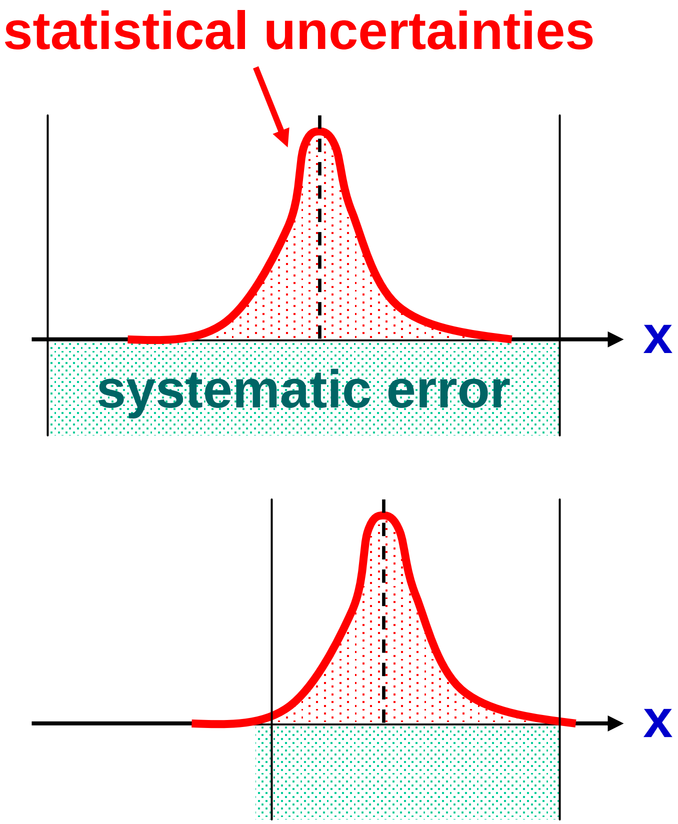
- **consistent method for model defects**
- **systematic errors and Bayesian update procedure**
- **relationship of different methods of covariance determination**
- **benchmark tests with well defined integral experiments**

Technical Requirement

- **Numerical implementation into an automatic code**

Systematic errors and Bayesian update procedure

At present the consistent treatment of systematic errors in a Bayesian update procedure is an open problem.



Fact: If data from experiments of the same type are used in Bayesian update procedure the systematic error is reduced According to statistics – However, the same systematic error should also apply after the update

Consequence: find a mean to formulate the complementarity of different experiments

THANK YOU FOR YOUR ATTENTION