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Consistent procedure for nuclear data evaluation based on modelling

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Content

- Motivation and objectives
- Bayesian statistics

    basics - linearized update - correlated Bayesian update approach (CBUA)
- Prior determination

    concept of maximum entropy – parameter uncertainties – model defects
- Summary and conclusions

The reliability of forecast

1. Motivation

Present status

- essentially a consistent set of cross sections (most files up to 20 MeV)
- reflects our best knowledge of these observables
- covariance information is limited (few files – reliability ?)

New challenges

- novel technologies (ADS, transmutation, …) require data in an extended energy range up to 150 MeV
- optimized design of new facilities require knowledge of the reliability of the evaluated data – (safety margins – costs)

Example: Reliable uncertainty of quantity A_{eff} is required

$$\Delta^2 A_{eff} = \sum_{\rho} \sum_{\eta} \frac{\partial A}{\partial \sigma_\rho} \left\langle \Delta\sigma_\rho \Delta\sigma_\eta \right\rangle \frac{\partial A}{\partial \sigma_\eta}$$

cross section covariances

Objectives

Consequences

- scarcity of experimental data beyond 20 MeV implies evaluations which rely strongly on nuclear model calculations
- uncertainty information associated with nuclear models are required

Objectives

- development of a consistent procedure to estimate the uncertainties associated with the use of nuclear models
  → choice of proper prior

- proper inclusion of experimental data into evaluated data file
  → correlated Bayesian update approach (CBUA)

2. Concept of evaluation

Nuclear data evaluation is essentially a procedure following the rules of Bayesian statistics within a *subjective* interpretation

the probability reflects our expectation
→ no experimental verification

Evaluation is given in terms of
- expectation values of observables

$$\langle \underline{\sigma} \rangle \text{ cross sections,} \qquad \langle \underline{x} \rangle \text{ parameters of nuclear model}$$

- covariance matrices of observables (cross sections)

$$\langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle \qquad \rho, \eta \ldots \text{channel, energy}$$

→ **BAYESIAN STATISTICS**

2.1 Basics of statistics

BAYESIAN STATISTICS

Based on the two fundamental relationships of probability theory

sum rule $p(\underline{x} \mid M) + p(\underline{\bar{x}} \mid M) = 1$

product rule $p(\underline{x} \mid \underline{\sigma} M)\, p(\underline{\sigma} \mid M) = p(\underline{\sigma} \mid \underline{x} M)\, p(\underline{x} \mid M)$

Expectation value:

$$\langle \sigma_\rho \rangle^{\text{apriori}} = \int d^n x \; p(\underline{x} \mid M)\, \sigma_\rho^{\text{model}}(\underline{x}, M)$$

Covariance matrix element:

$$\langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle^{\text{apriori}} = \int d^n x \; p(\underline{x} \mid M)\, \sigma_\rho^{\text{model}}(\underline{x}, M)\, \sigma_\eta^{\text{model}}(\underline{x}, M)$$

Bayes theorem

Bayes Theorem (1763):

$$p(\underline{x}|\underline{\sigma}\,M) \;=\; p(\underline{\sigma}\,|\underline{x}M) \quad p(\underline{x}|M) \;/\; p(\underline{\sigma}\,|M)$$

posterior = likelihood x prior / evidence

$\underline{x}$ ... model parameter $\underline{\sigma}$ ... data M ... other information

from experiment (→ likelihood)

Choice of proper prior ? (→ prior)

Prior and likelihood

- Problem: Prior is dominant in evaluations based on a scarce set of experimental data (extension to 200MeV!).

- Prior: probability for a set of parameters $\underline{x}$ within a well defined model *M*; it contains the full a-priori knowledge

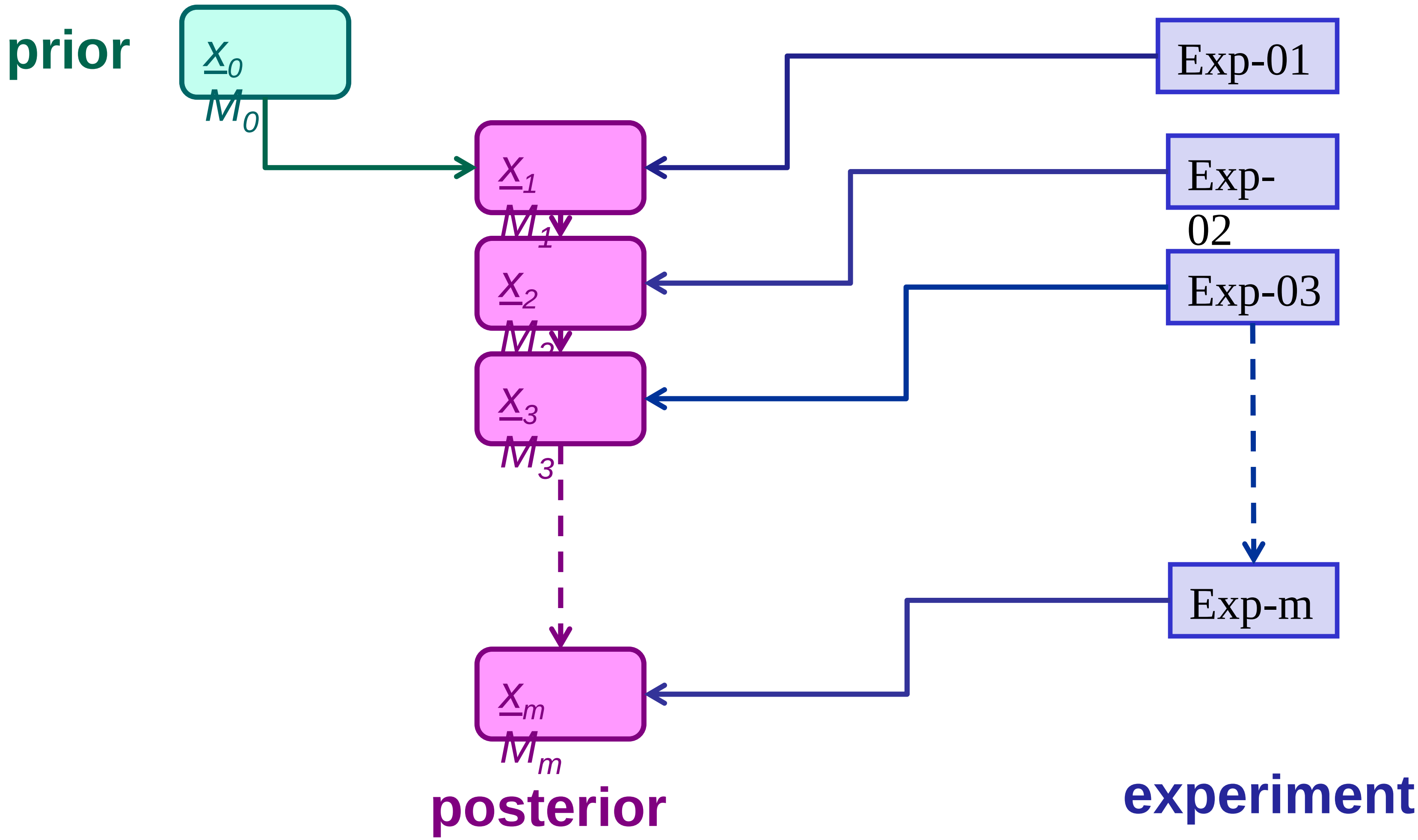
- Likelihood: probability for mesured cross sections $\underline{\sigma}$ at a given set of parameters $\underline{x}$ within a well defined model *M*:

$$p(\underline{\sigma} \mid \underline{x}M) = \frac{1}{\sqrt{(2\pi)^d \det V}} \exp\left[\left(\underline{\sigma} - \underline{S}_M(\underline{x})\right)^T V^{-1} \left(\underline{\sigma} - \underline{S}_M(\underline{x})\right)\right]$$

V experimental covariance matrix

$\sigma_{Model} = S_M(x)$ model value

Bayesian update procedure



Probability update

The Bayesian update procedure in terms of the probability distribution:

$$p\left(\underline{x} \mid \underline{\sigma}_1 \ldots \underline{\sigma}_m M\right) = p\left(\underline{\sigma}_m \mid \underline{x}\underline{\sigma}_1 \ldots \underline{\sigma}_{m-1} M\right) \times \cdots$$

$$\cdots \times p\left(\underline{\sigma}_2 \mid \underline{x}\underline{\sigma}_1 M\right) p\left(\underline{\sigma}_1 \mid \underline{x} M\right) p\left(\underline{x} \mid M\right)$$

2.2 Linearized Bayesian theorem

Assuming normal distributions linearized expression for Bayes theorem can be obtained

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

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

parameter vector

$$M' = M(1+Q)^{-1} = (M^{-1} + W)^{-1}$$

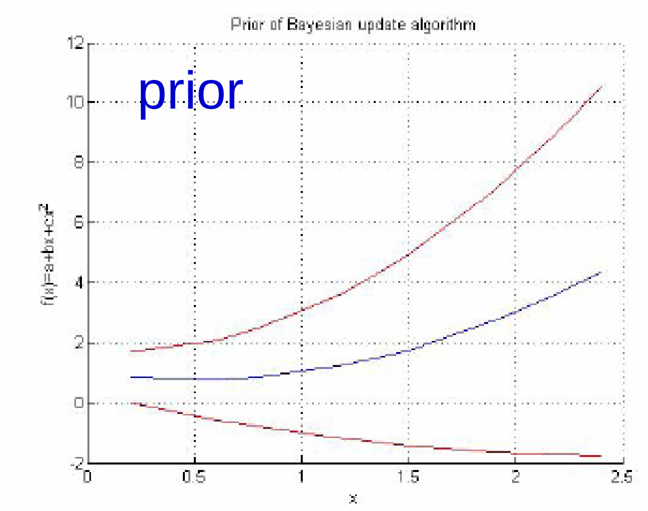
covariance matrix

with $Q = G^T V^{-1} G M = W M$

G sensitivity matrix

V contains all available experimental data of the system
→ used as an update procedure including set per set

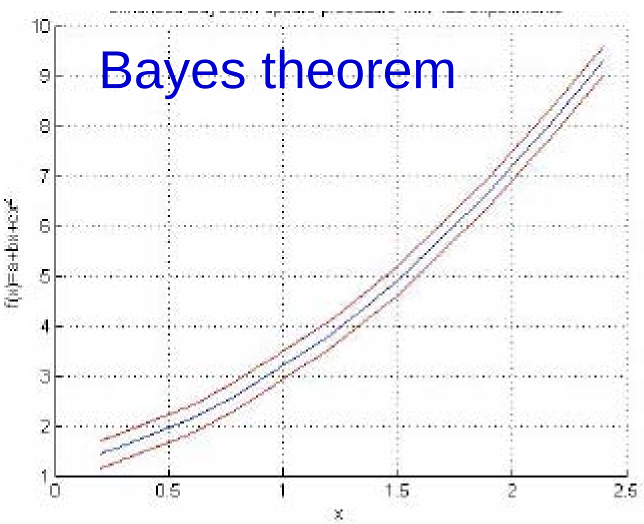
Bayesian update procedure - problem

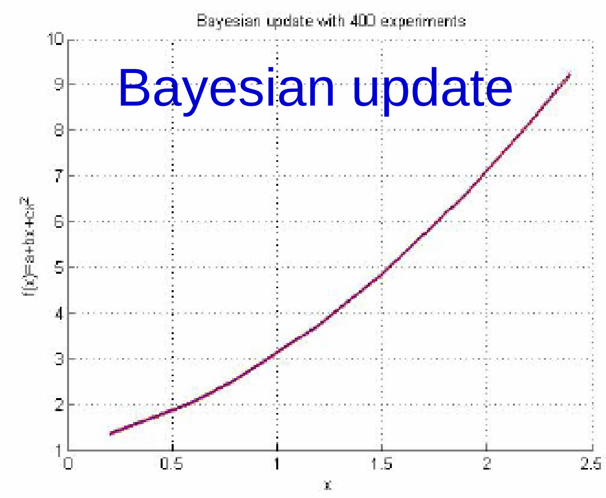


$$f(x)=\left(a+bx+cx^{2}\right)\left[1+d\left(2r-1\right)\right]+e$$

statistical error

systematic error





Mathematical consideration

The aposteriori probability distribution is given by

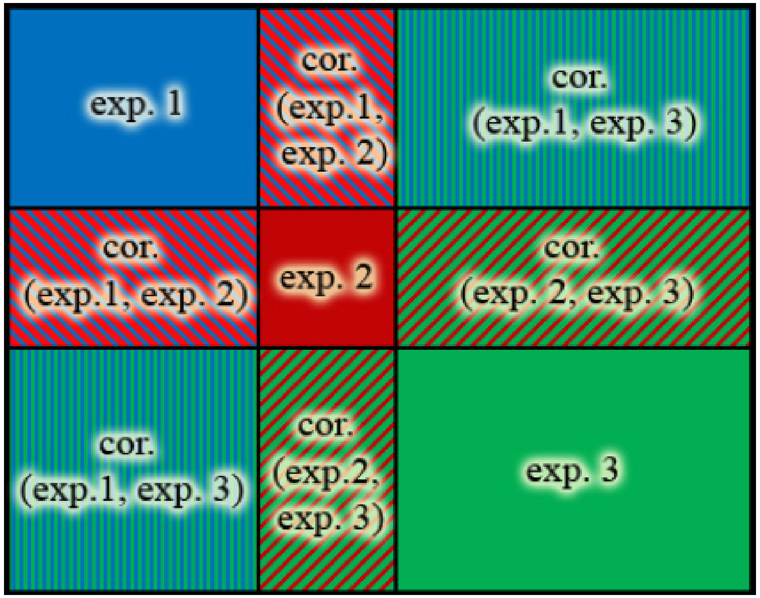
$$p\left(\underline{x}\,|\,\underline{\sigma}_1\ldots\underline{\sigma}_m M\right)=\exp\left(-\left[\underline{\sigma}_m-\underline{S}\left(\underline{x}_{m-1}\right)\right]^T \mathbf{V}_m^{-1}\left[\underline{\sigma}_m-\underline{S}\left(\underline{x}_{m-1}\right)\right]\right)\times\cdots$$

$$\cdots\times\exp\left(-\left[\underline{\sigma}_1-\underline{S}\left(\underline{x}_0\right)\right]^T \mathbf{V}_1^{-1}\left[\underline{\sigma}_1-\underline{S}\left(\underline{x}_0\right)\right]\right)p\left(\underline{x}\,|\,M\right)$$

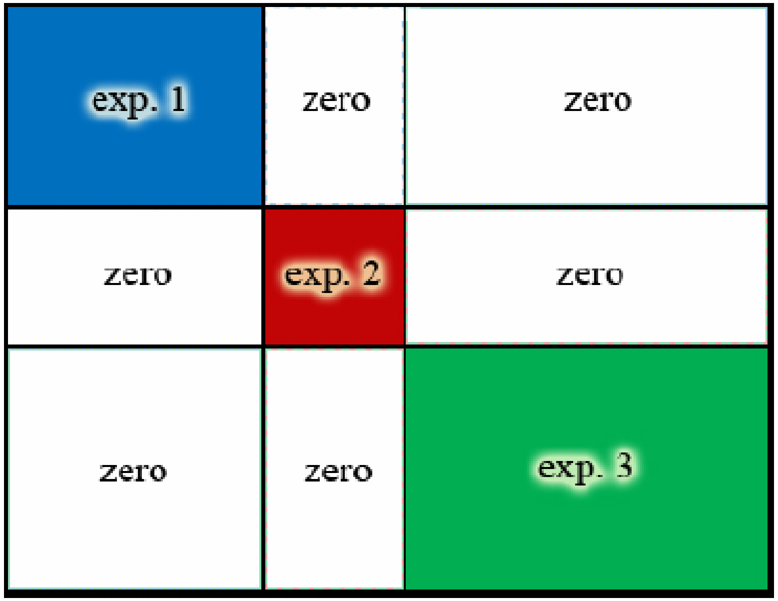
Assume that you made different experiments at different facilitities by the same method, but all with a systematic error of the same order

→ Systematic errors are treated like a statistical uncertainty i.e. $\left\langle \Delta\sigma_\rho \Delta\sigma_\eta \right\rangle \propto 1/m$

Origin of the difference



The ‚experiments' covariance matrix *V* contains all experiments and all correlations



Standard Bayesian update procedure – no correlations between experiments

Where occurs the problem

This effect is a general problem related to all evaluation methods based on a Bayesian update procedure

- Bayes update via Monte Carlo sampling
- Bayes update via linearized version
- Kalman filter techniques
- Generlized least square method

The problem was recognized:
It results in unphysically small uncertainties of observables when many connected data sets are taken into account

→ low fidelity cross section (BNL, Hermann,Pigni)

How to treat systematic errors?

Recent approach: low fidelity covariance matrices

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

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

$$M' = M\cancel{(1+Q)^{-1}} = (M^{-1} \cancel{+W})^{-1}$$

with $Q = G^T V^{-1} G M = WM$

Full linearized version of the Bayesian update procedure

Low fidelity approach assumes

$$M' = M$$

Final covariance matrix is the covariance matrix of the prior M_0

2.3 Correlated Bayesian update approach (CBUA)

Correlations between different experiments are usually not obvious – but may occur even if different setups are used:

- use of same standards
- use of equivalent method

Major Problem

correlations between experiments are almost not quantifiable

global scaling parameter q

Concept of CBUA

The Correlated Bayesian Update Approach (CBUA) should have essentially a similar form to the standard Bayesian update procedure

Keep the simplicity of Bayesian update

- only data of the update step are required
- no history of update procedure
- include correlations between experiments

Basic assumption

Scope of the development:

- keep the simple update strategy
- include correlation terms approximately

exp 1 V_1	corr 12 C
corr 12 C	exp 2 V_2

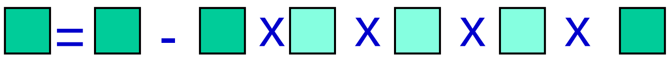
Idea:
Extract analytically the effect of correlations in a calculation via Bayes theorem and perform few, but appropriate approximations

V covariance matrix including 2 experiments

Implementation of CBUA

Standard Bayesian update:

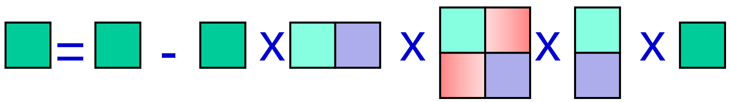
$$\tilde{M}_1 = M_0 - M_0 G_1^T \left(Q_0 + V_1\right)^{-1} G_1 M_0$$



$$\tilde{M}_2 = \tilde{M}_1 - \tilde{M}_1 G_2^T \left(\tilde{Q}_1 + V_2\right)^{-1} G_2 \tilde{M}_1$$

One step Bayesian update:

$$M_2 = M_0 - M_0 \left(G_1^T \quad G_2^T\right) G_2^T \underbrace{\begin{pmatrix} E & H^T \\ H & F \end{pmatrix}}_{(Q+V)^{-1}} \begin{pmatrix} G_1 \\ G_2 \end{pmatrix} M_0$$



<u>Correlated Bayesian Update Approach</u>

$$M_2^{CBUA} = \tilde{M}_2 - M_0 \underbrace{\begin{pmatrix} \text{correlation} \\ \text{dependent terms} \end{pmatrix}}_{\text{additional term dependent on } H} M_0$$

Correlated Bayesian update approach

$$M^{(i)} = \underbrace{M^{(i-1)} - M^{(i-1)}G^T\left(GM^{(i-1)}G^T + V^{(i)}\right)^{-1}GM^{(i-1)}}_{\text{Standard Bayesian update fomula}}$$

$$+ \underbrace{M^{(0)}G^T\left(E_{corr} + F_{corr} + H_{corr} + H^T_{corr}\right)GM^{(0)}}_{\text{additional correlation term}}$$

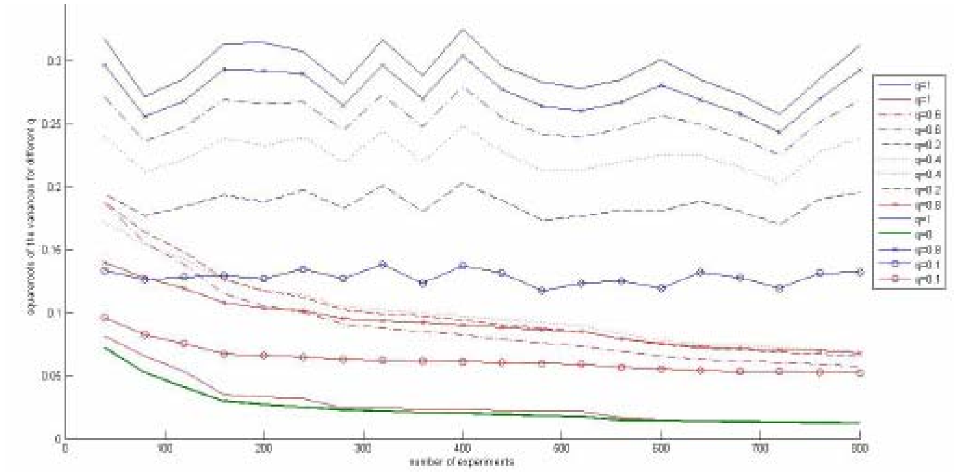
the correlation term vanishes for C=0

The terms E_{corr}, F_{corr} and H_{corr} are expressions in terms of $V^{(i)}$, G, $M^{(0)}$

$$E_{corr} = \left[\left(Q+\tilde{B}\right) - \left(Q+C^T\right)\left(Q+V^{(i)}\right)^{-1}\left(Q+C\right)\right]^{-1}$$
$$-\left[\left(Q+\tilde{B}\right) - Q\left(Q+V^{(i)}\right)^{-1}Q\right]^{-1}$$

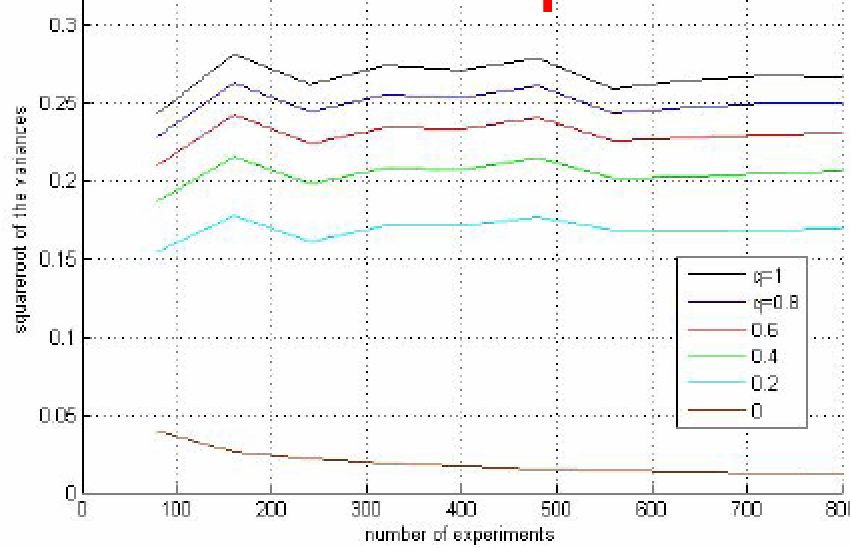
Dependence on correlations

systematic error after a sequence of updating



correlated experiments

anticorrelated experiments



variation of *q*

3. Choice of proper prior

GOAL
It is the primary goal of this work to provide quantitative estimates of the reliability of nuclear model based evaluations

Minimal use of experimental data

There has been considerable effort to define an almost unbiased prior

- concept of maximum entropy including apriori knowledge
- including mathematics and physics constraints as apriori knowledge
- transformation group invariance for continuous parameters

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

contribution determined
In previous projects

numerical
implementation
error

Task 1:
deficiency
of the model
non-statistical error

3.1 Theoretical basis

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:

Determination of λ:

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

Variance of λ:

3.2 parameter uncertainties

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

Information Entropy

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

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: m(x)=1/x

Phenomenological optical potential

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

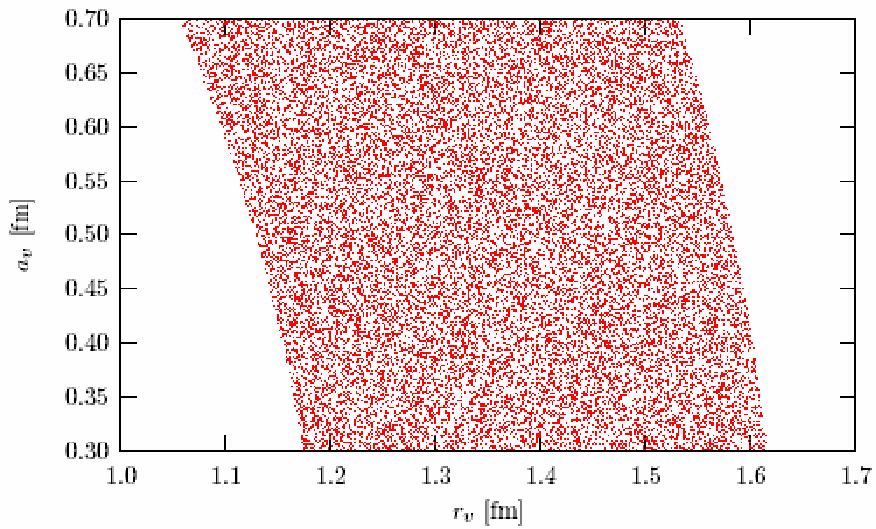
Der. terms			Spin-orbit terms					
d_1	d_2	d_3	r_{vso}	a_{vso}	v_{so1}	v_{so2}	w_{so1}	w_{so2}
13.8	0.0180	13.80	1.080	0.570	6.6	0.0035	-3.1	160.0

Key question – 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

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

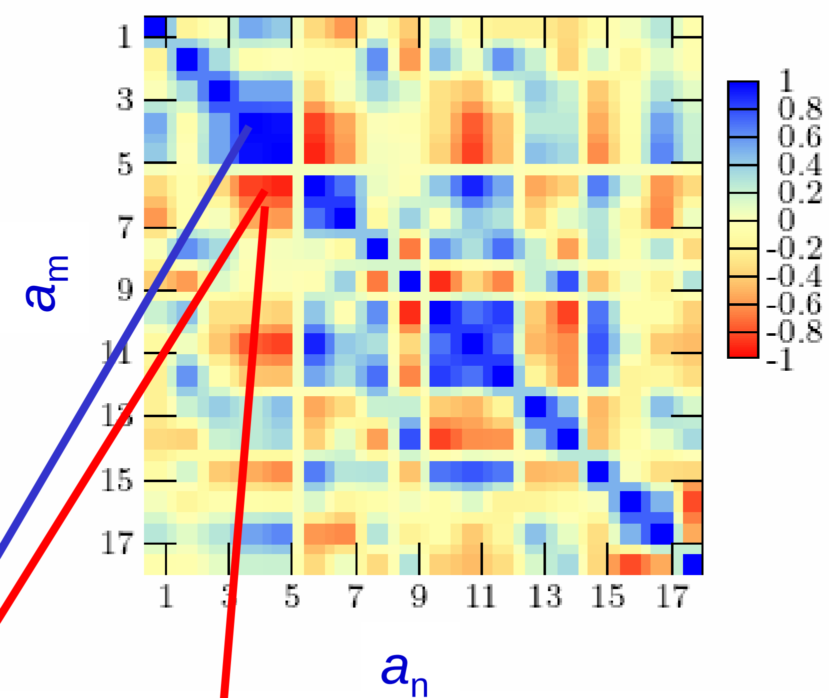
z defines lower boundary

$$(\rho * v)_s = (\mathcal{F}^{-1}(F\rho \times Fv)_k)_s$$

		$a^<$ (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

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%

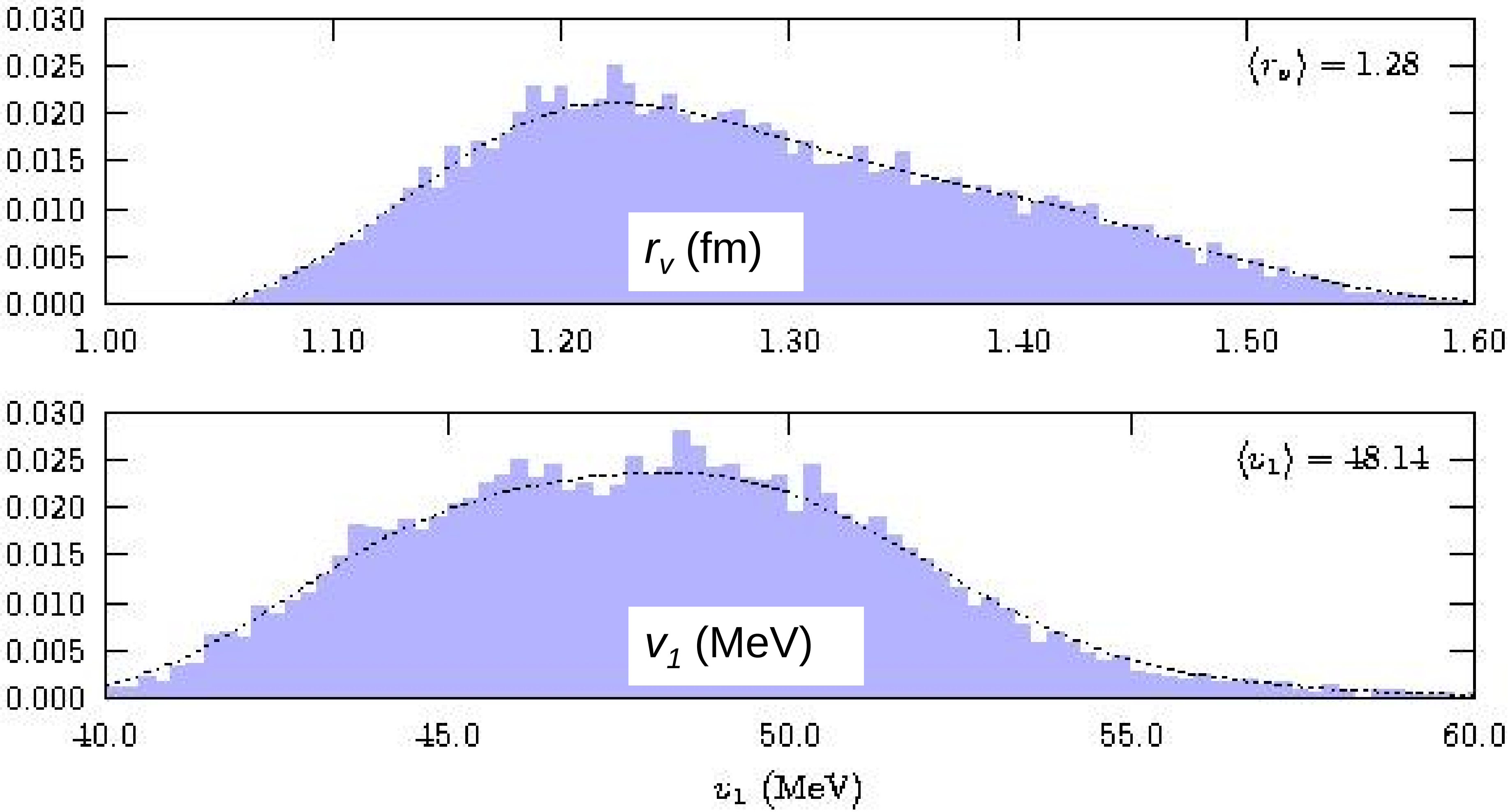


$$C_{m,n} = \frac{\langle \Delta a_m \Delta a_m \rangle}{\sqrt{\langle \Delta^2 a_m \rangle \langle \Delta^2 a_n \rangle}}$$

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 distribution for ^{208}Pb

potential parameters



Level densities for ^{208}Pb

Fermi gas level density

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

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

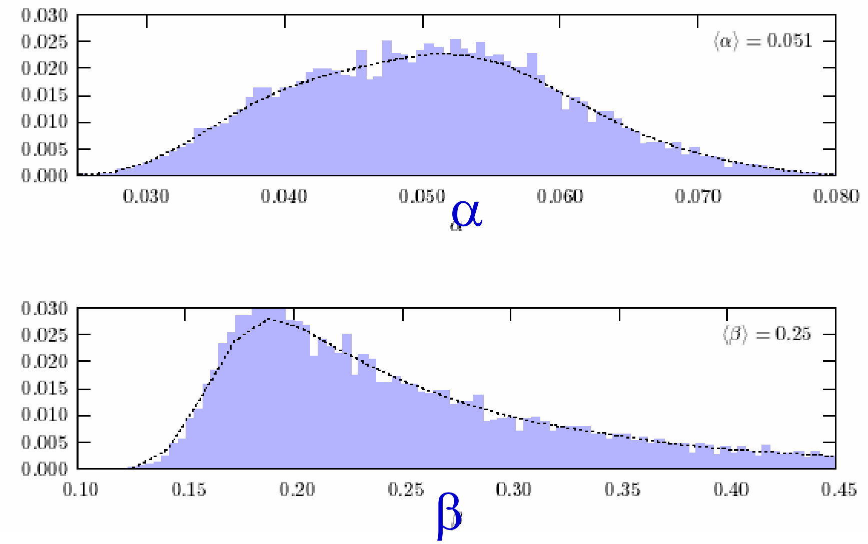
$$a(E) = \hat{a}\left[1 + \delta W \frac{1-\exp(-\gamma U)}{U}\right]$$

admissible range as given in TALYS

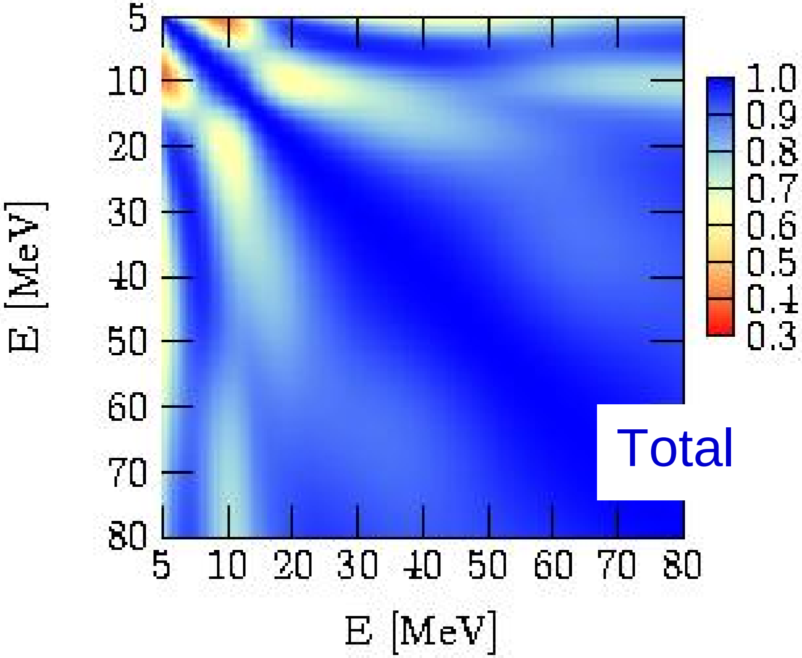
0,04 < a < 0,1
0,06 < b < 0,5

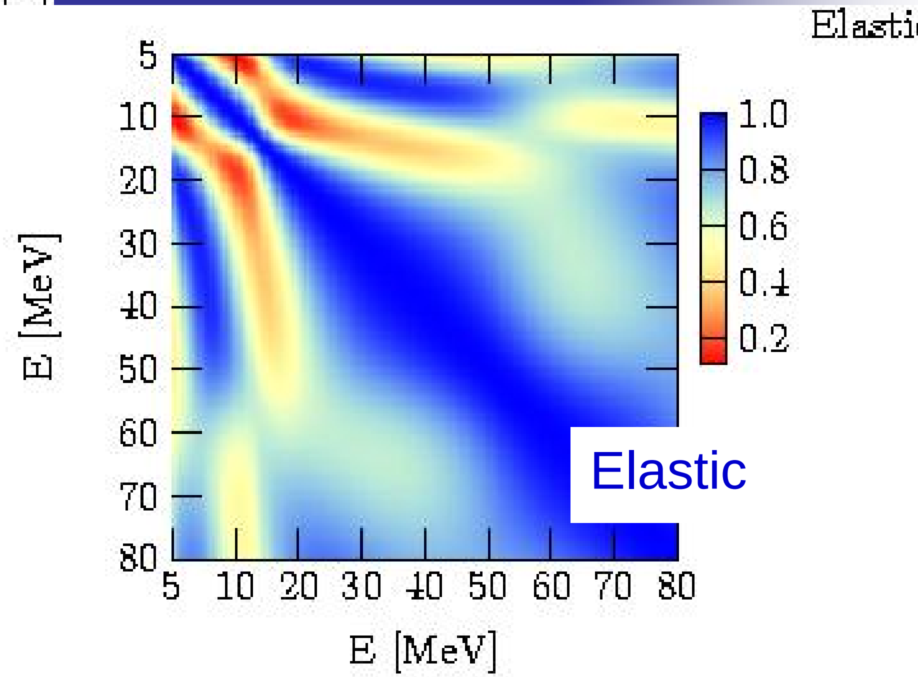
level density parameters

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

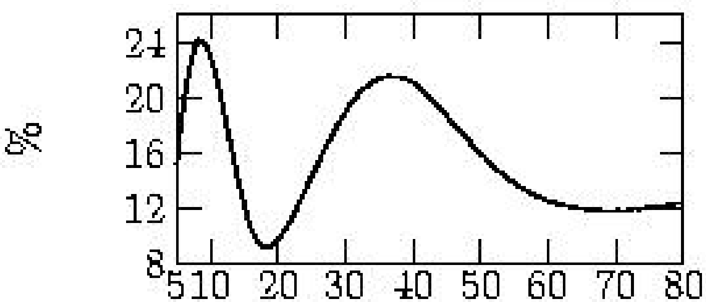


Correlations of cross section

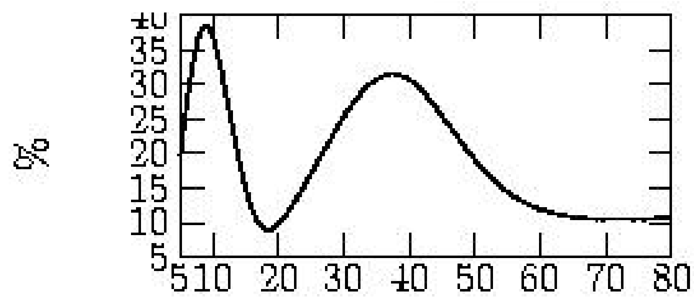




Varianz

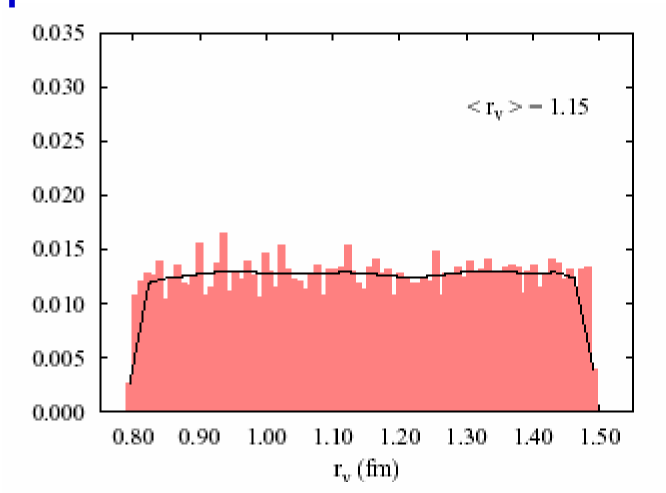


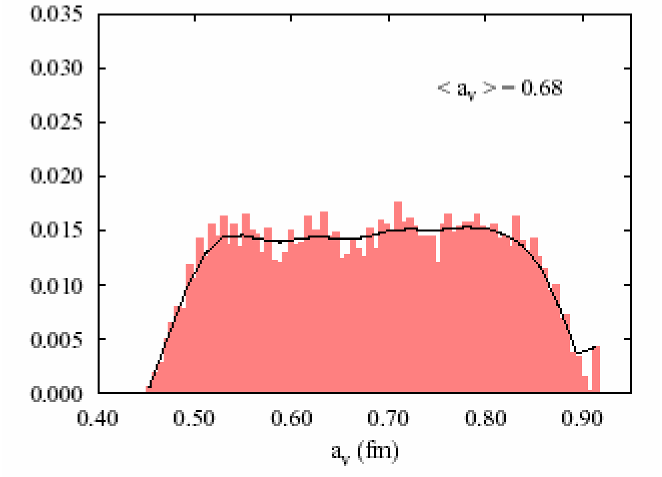
Varianz



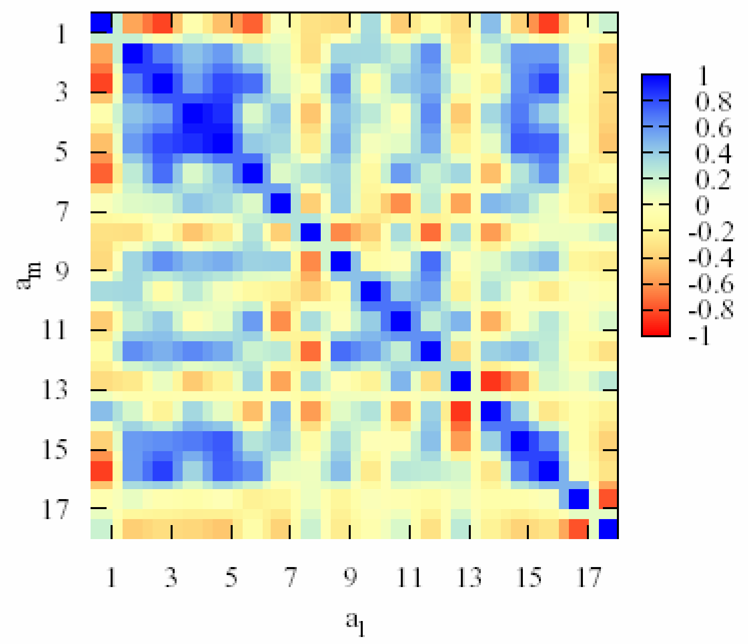
Parameter distributions and correlations

parameter distributions

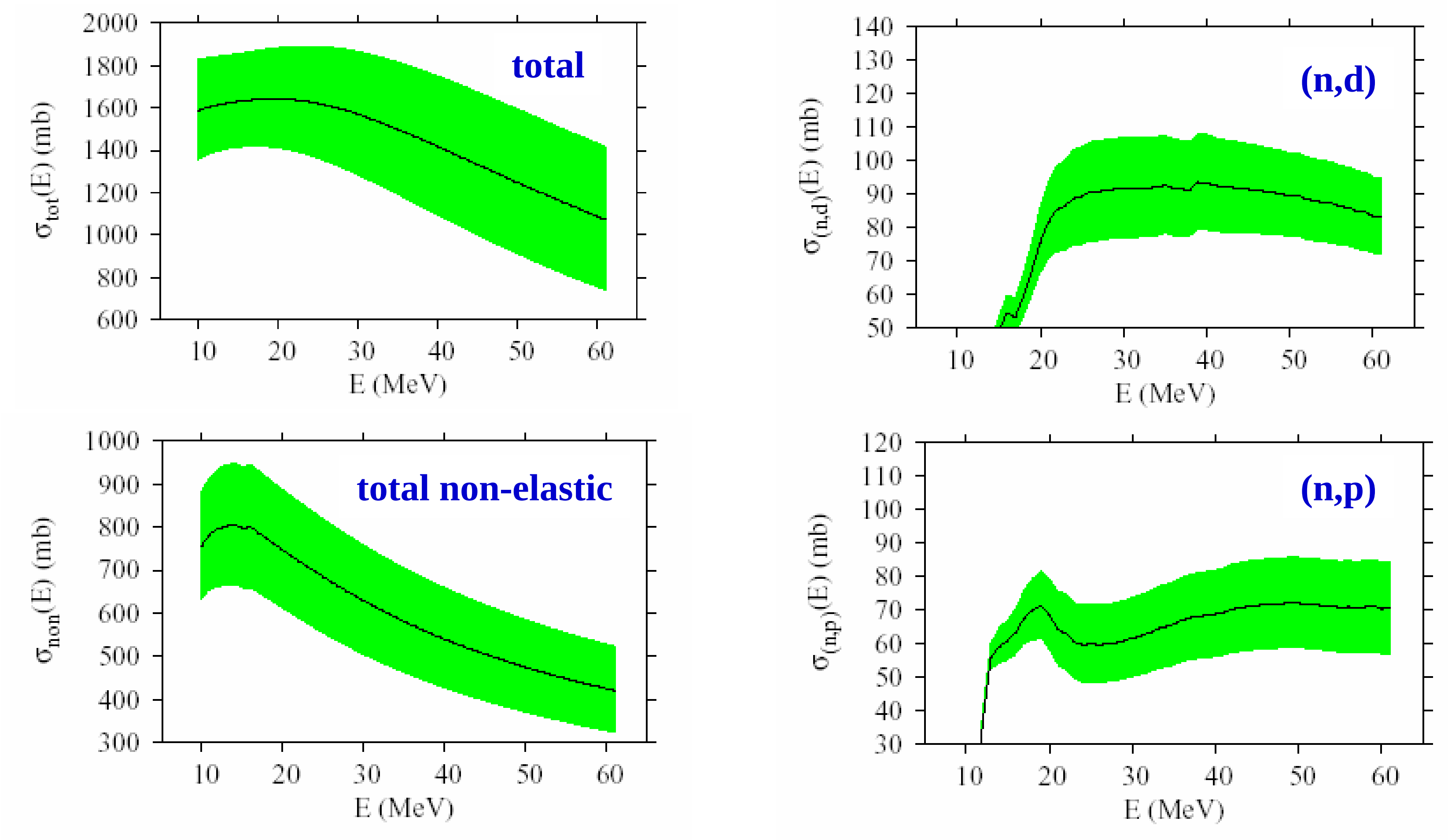




parameter correlations



Error bands of cross sections

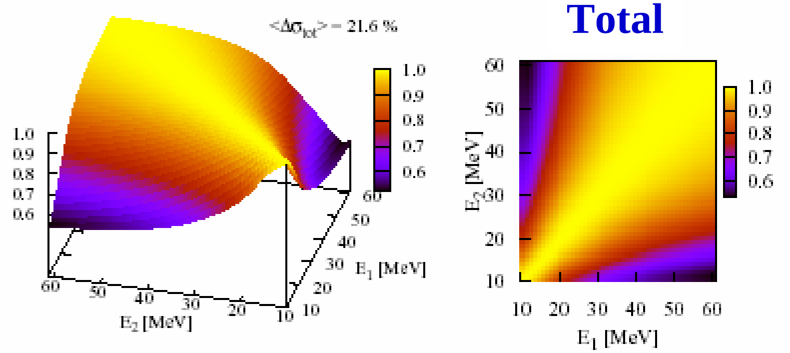


Cross sections

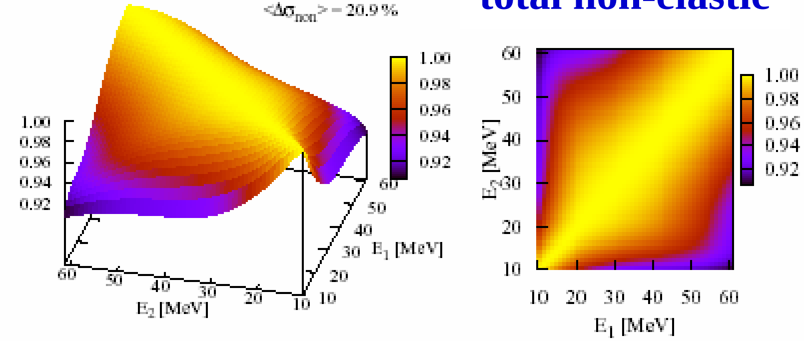
cross section correlation matrix

$$\langle \Delta\sigma(E_1)\Delta\sigma(E_2) \rangle$$

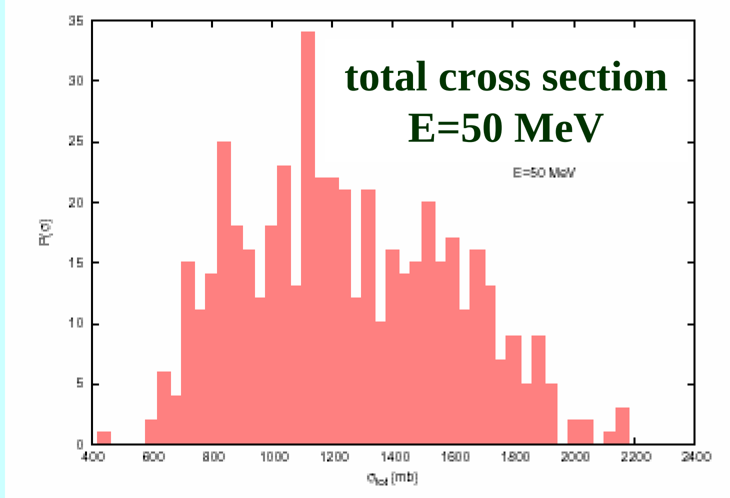
Total



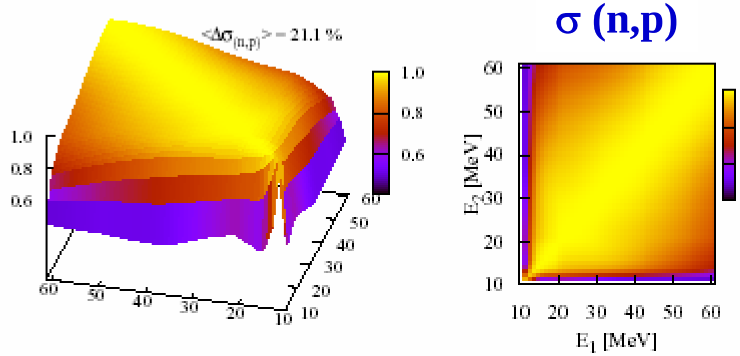
total non-elastic



cross section distribution



σ (n,p)

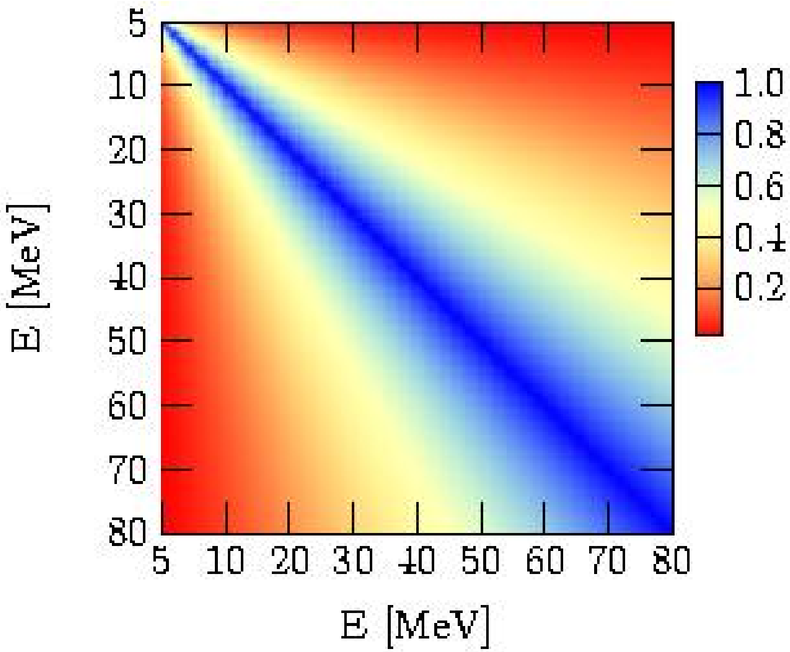


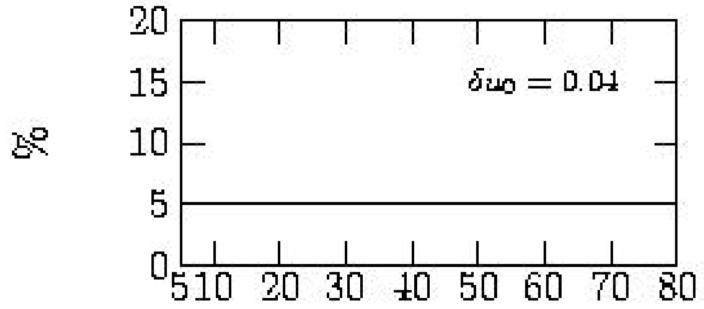
3.3 Model defects

Following the suggestions made at the nuclear data conference 2004 the covariance matrix of the model defects is generated via an empirical ansatz

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

Present subtask aims at a more sophisticated approach based on experimental data similar to SACS of Forrest and Kopecky,
Fusion Engineering and Design 82 (2007) 93





Phenomenological ansatz

A possible 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 $\boldsymbol{M}^{(def)}$ 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; $E^{>} = \max(E_i,E_j)$, $E^{<} = \min(E_i,E_j)$

Consistent methods for model defects

Problem: non statistical nature
no unique definition

Method A:

channel dependent, but energy independent scaling of model
Scaling factor is constant and covariance matrix in energy
both determined from neighboring nuclei
→ Correlations, not completely statistically defined

Method B:

Scaling factors are channel and energy dependent
redefinition of model
No correlations – covariance matrix is only diagonal
statistically defined

Model A - scaling

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Global scaling factor for one reaction channel

$$\overline{N} = \frac{\sum_{all\ r} \sigma_{\exp}(E_r)}{\sum_{all\ r} \sigma_{the}(E_r)} = \sum_{all\ r} \overbrace{\frac{\sigma_{the}(E_r)}{\sum_{all\ r} \sigma_{the}(E_r)}}^{\text{weight}} \overbrace{\frac{\sigma_{\exp}(E_r)}{\sigma_{the}(E_r)}}^{\text{local scale } N(E_r)}$$

$$\overline{N}_E = \frac{\sum_{r \in E-bin} \sigma_{\exp}(E_r)}{\sum_{r \in E-bin} \sigma_{the}(E_r)} \qquad \text{mean scale for each energy bin}$$

$$\left\langle \Delta\sigma(E)\Delta\sigma(E')\right\rangle_{def} = \sigma_{the}(E)\sigma_{the}(E')(\overline{N}_E - \overline{N})(\overline{N}_{E'} - \overline{N})$$

This coarse approximation provides a covariance matrix

PROBLEM: not statistically defined; correlations are 1 or -1

Model B - remodelling

Define scaling factor for each reaction and energy bin

$$N(E_r) = \frac{\sigma_{\exp}(E_r)}{\sigma_{the}(E_r)} \qquad \sigma_{\exp}(E_r) \text{ from neighbouring nuclei}$$

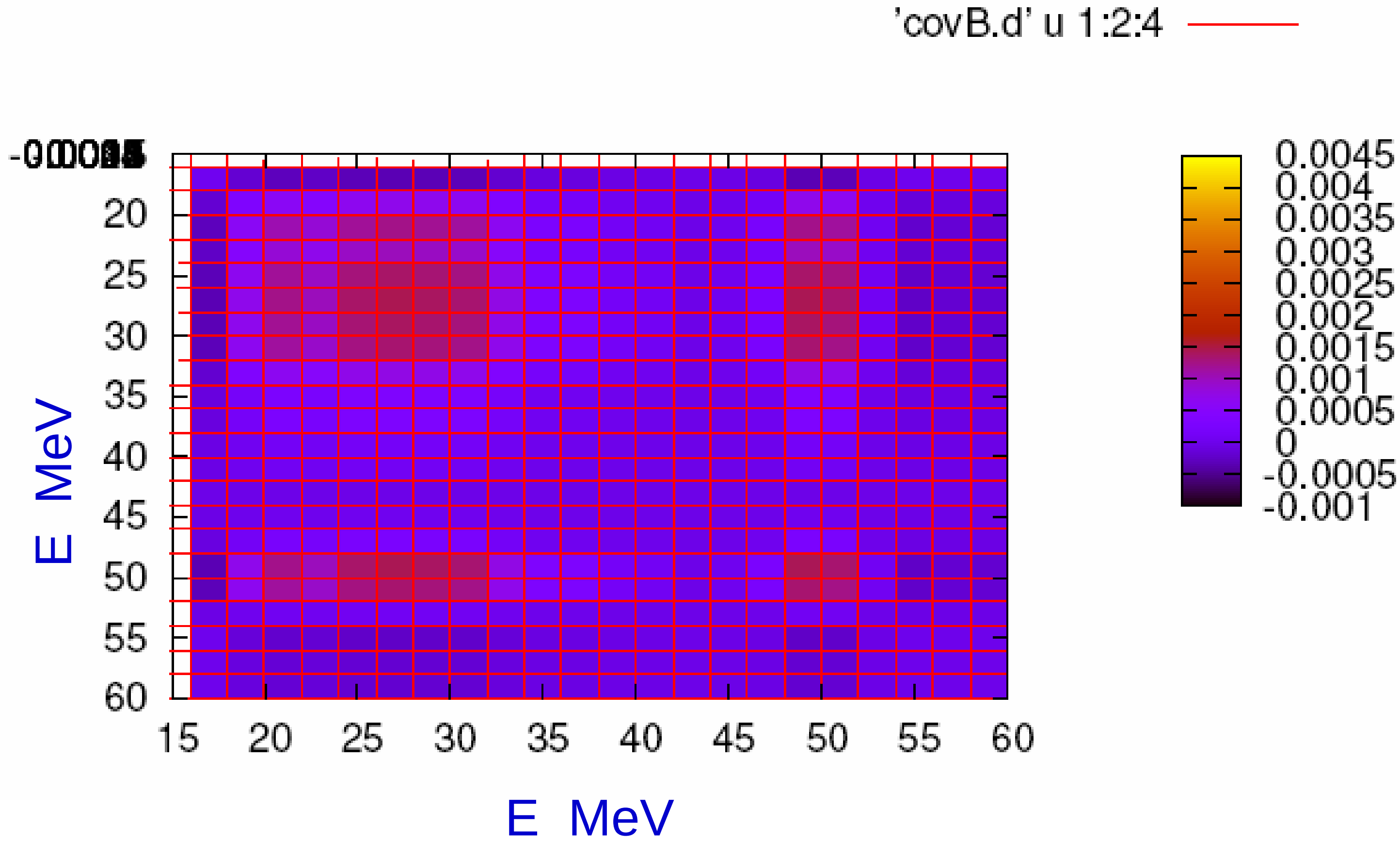
$$N_E = \frac{1}{R} \sum_{r \in E-bin} N(E_r) \qquad \Delta^2 N_E = \frac{1}{R} \sum_{r \in E-bin} \left(N(E_r) - N_E\right)^2$$

$$\langle \Delta\sigma(E) \Delta\sigma(E') \rangle_{def} = \sigma_{the}(E) \sigma_{the}(E) \Delta^2 N_E \delta_{EE'}$$

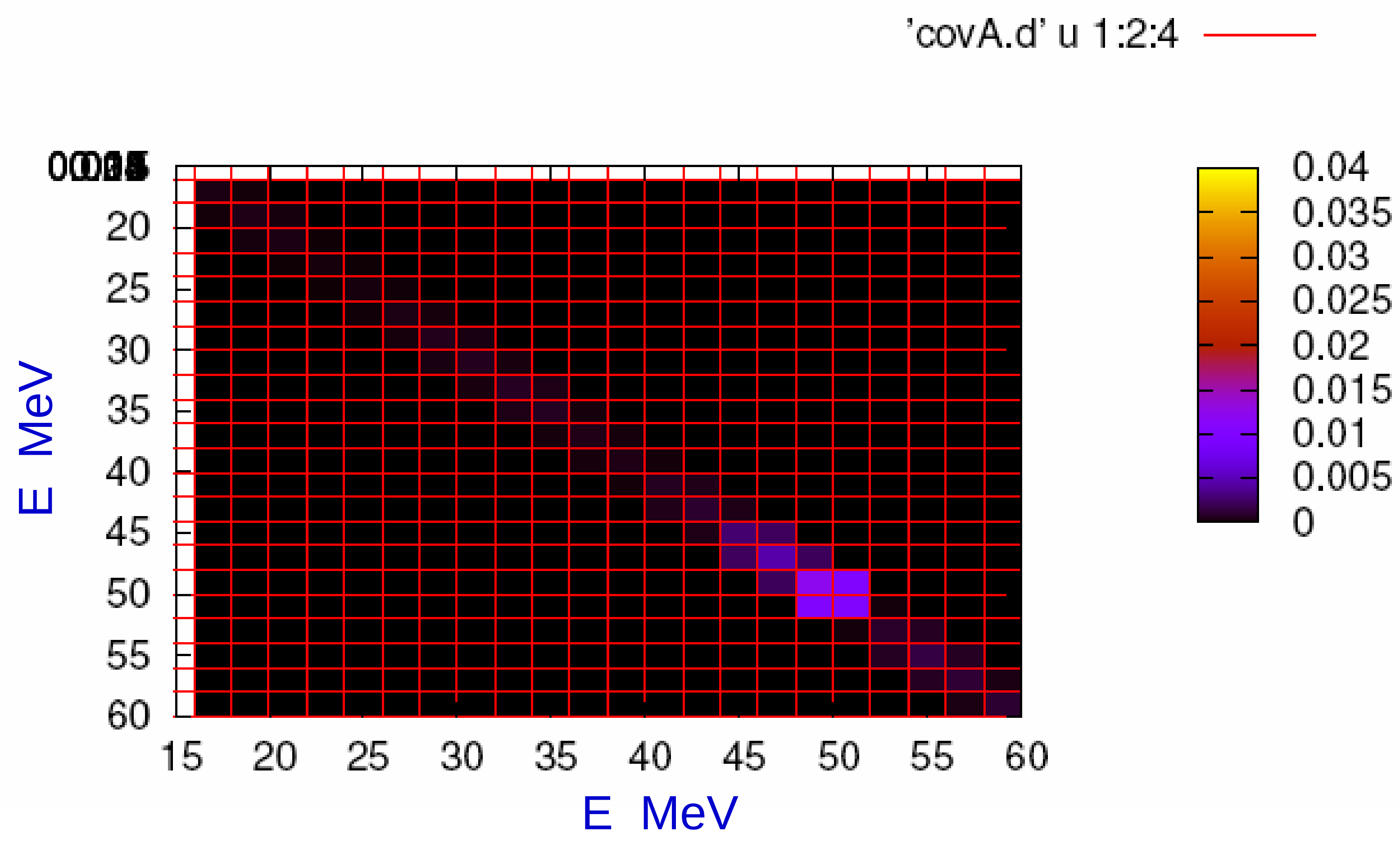
This method represents a redefinition of the model
→only diagonal elements of the covariance matrix, no correlations

PROBLEM:
Requires good experimental data from neighboring nuclei for reliable estimates

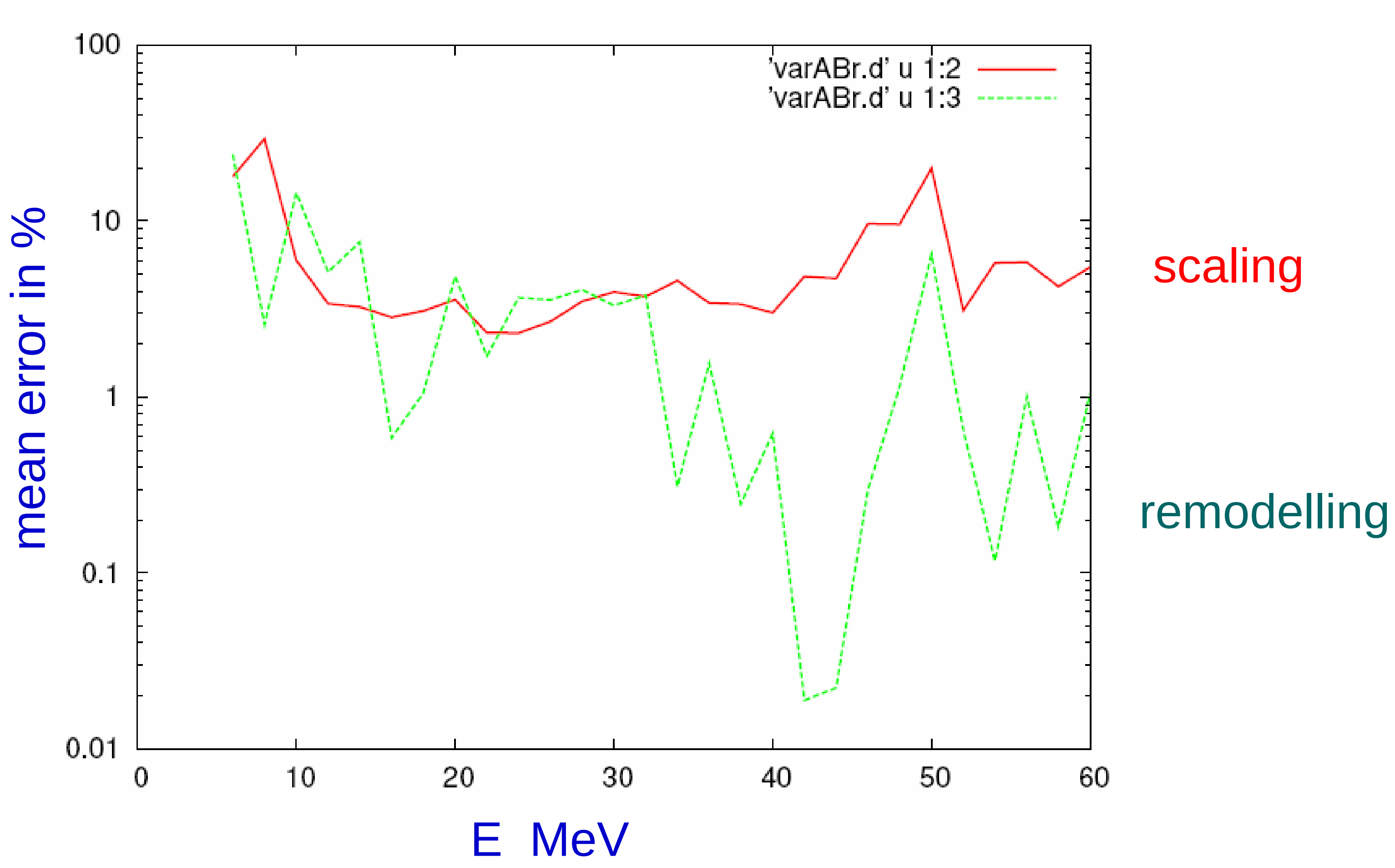
Model defects - scaling



Model defects - remodelling



Model defects – mean error



Open Problems - Summary

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**

THANK YOU FOR YOUR ATTENTION