WHAT IS THE PROPER EVALUATION METHOD: some basic considerations

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Nuclear Data Evaluation

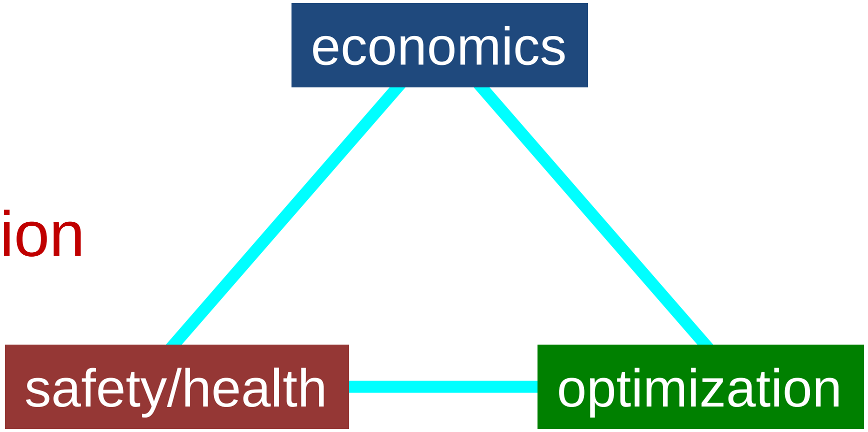
Scope: provides best knowledge of observables

- consistent set of cross sections, spectra …
- basic principles satisfied (unitarity, sum rules, …)
- compatible with a-priori knowledge

Interest: motivated by application

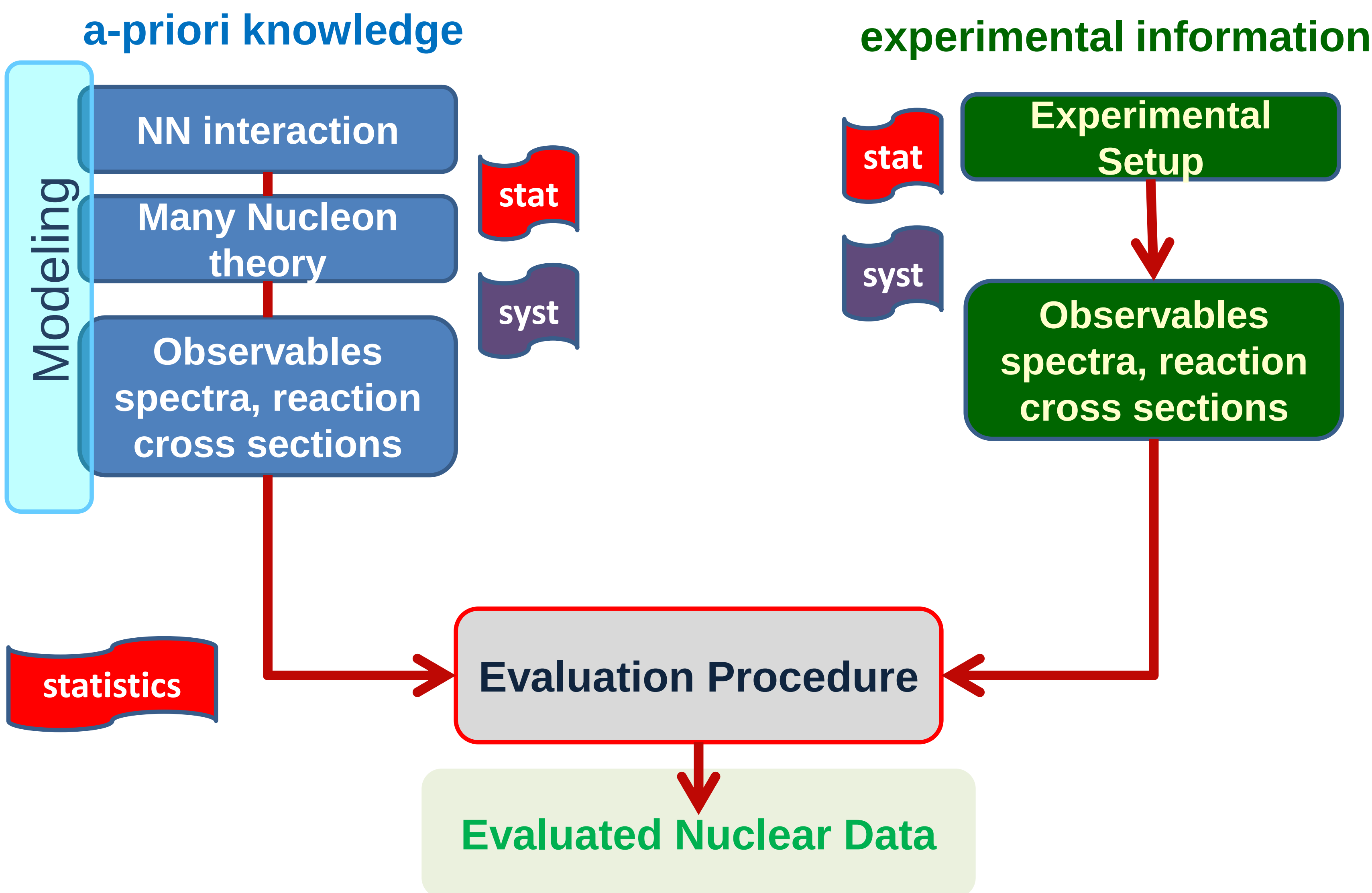
- design and construction of nuclear facilities (reactor, waste,fusion)
- accelerator applications (medicine, materials science, ADS)
- Safety issues and control systems (non-destructive testing, …)

Uncertainties: driven by



Requests: reliability of evaluation

Concept of Evaluation



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Bayesian Statistics

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Bayesian statistics:

sum rule: $p(\underline{x}|M) + p(\overline{\underline{x}}|M) = 1$

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

Bayes Theorem (1763):

$$p(\underline{x}|\underline{\sigma}\,M) = \frac{1}{p(\underline{\sigma}|M)}\,p(\underline{\sigma}|\underline{x}\,M)\,p(\underline{x}|M)$$

updated probability distribution of the set of parameters

likelihood function, from experiment

PRIOR

$p(\underline{x}|\underline{\sigma}\,M)$ .... probability distribution of parameters $\underline{x}$ for a given model M and data $\underline{\sigma}$

$p(\underline{\sigma}|\underline{x}\,M)$ .... probability distribution of data $\underline{\sigma}$ for a model M with parameters $\underline{x}$

$p(\underline{x}|M)$ .... probability for the ocurence of $\underline{x}$ when M is true

Nuclear Data Evaluation within Bayesian Statistics

Prior: obtained by variation of nuclear model parameters.
(nuclear models for n-^{181}Ta as given in TALYS 1.4 by default)

- physically reasonable boundaries defined
- homogenous distributions of parameters
- no correlation between parameters assumed

negative eigenvalues eliminated by regularization

Experimental Data for n-^{181}Ta:
Total cross sections, elastic differential cross sections

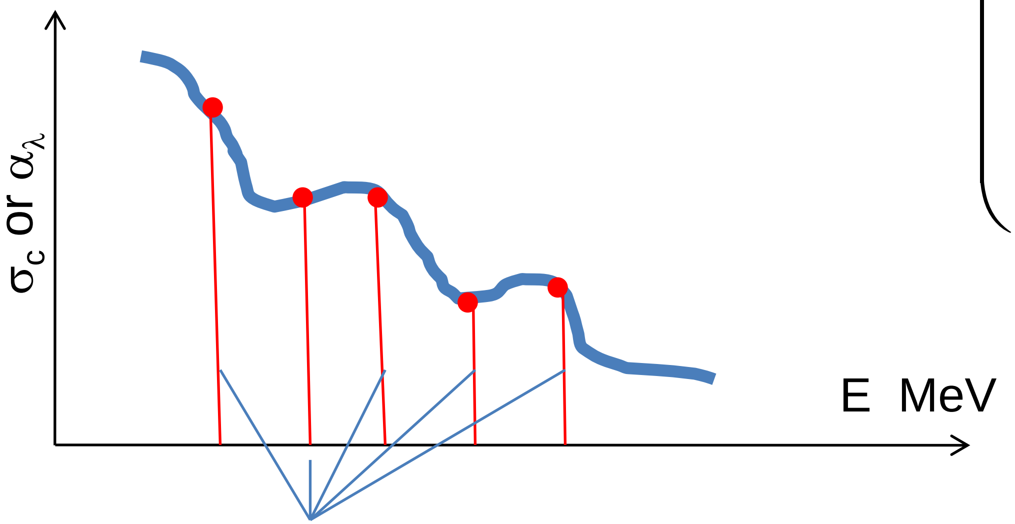
Evaluation:
Linearized Update Procedure (assumption: normal distribution)

Representation of energy dependence

Use of cubic spline interpolation to represent $\sigma_c(E)$ and $\alpha_\lambda(E)$

Properties are conserved:
especially sum rules

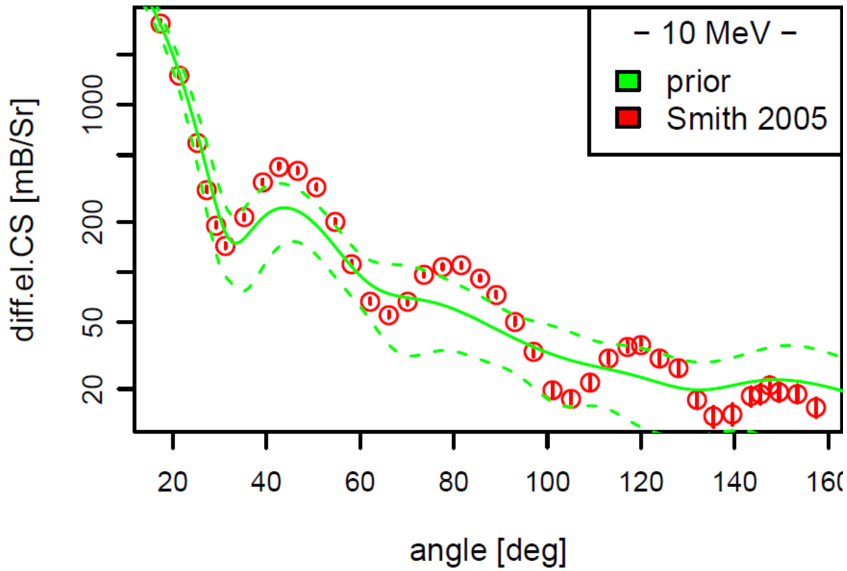
$$\begin{pmatrix} \sigma_c(E'_1) \\ \sigma_c(E'_2) \\ \vdots \\ \sigma_c(E'_J) \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} \sigma_c(E_1) \\ \sigma_c(E_2) \\ \vdots \\ \sigma_c(E_M) \end{pmatrix}$$



$\underline{\underline{S}}$ is a *JxM* matrix

values p_i for $\sigma_c(E_i)$ or $\alpha_\lambda(E_i)$ at the mesh points E_i are parameters of the cubic spline representation

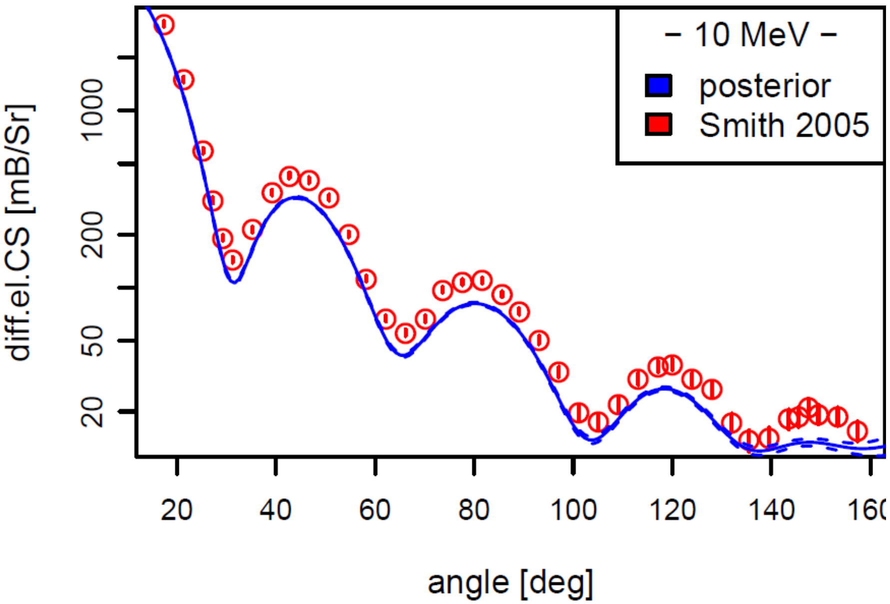
Evaluated differential elastic n-^{181}Ta cross section at E=10 MeV



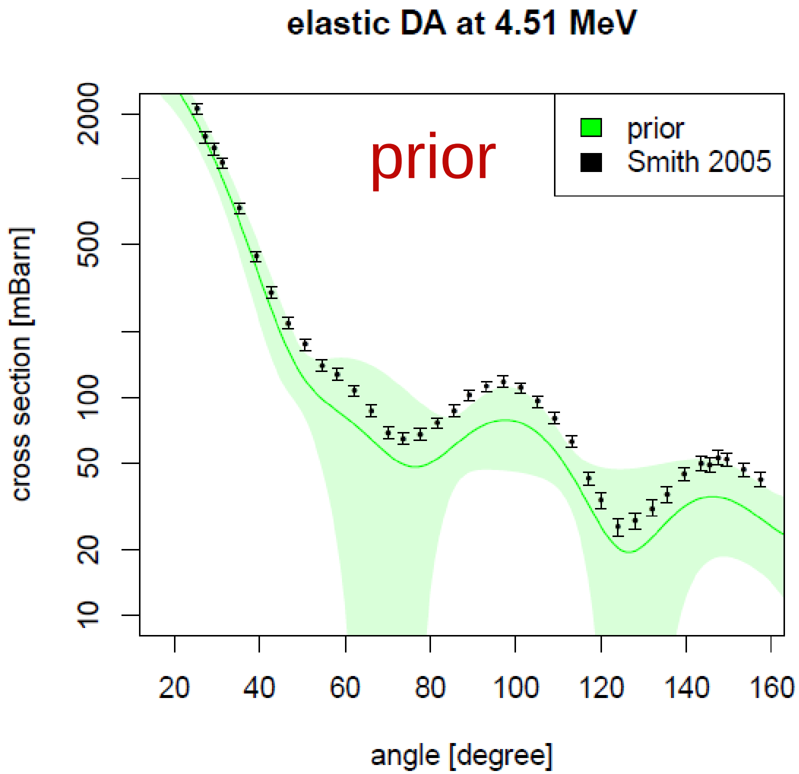
<u>Problem:</u>
The evaluated values are lower and the variances of the evaluated cross sections are too small.

Model defects negligible for total cross section

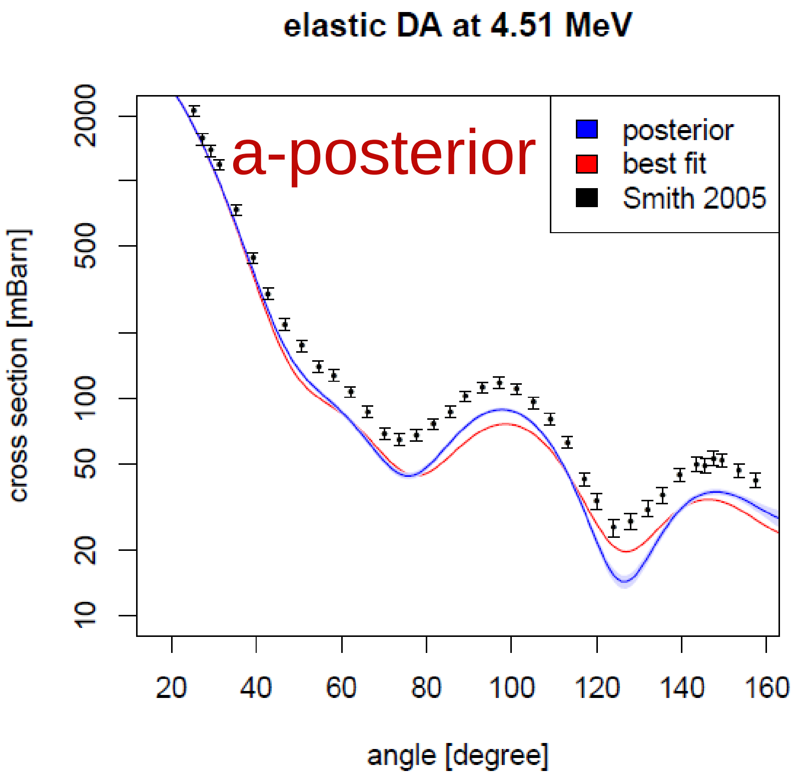
<u>Question:</u>
Is this specific for the energy or a general problem?



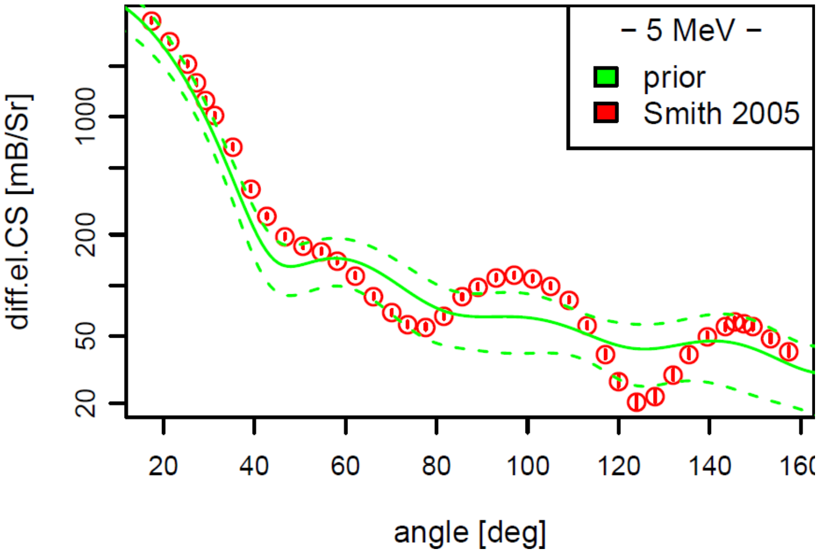
Evaluated differential elastic n-^{181}Ta cross section at E=4,51 MeV

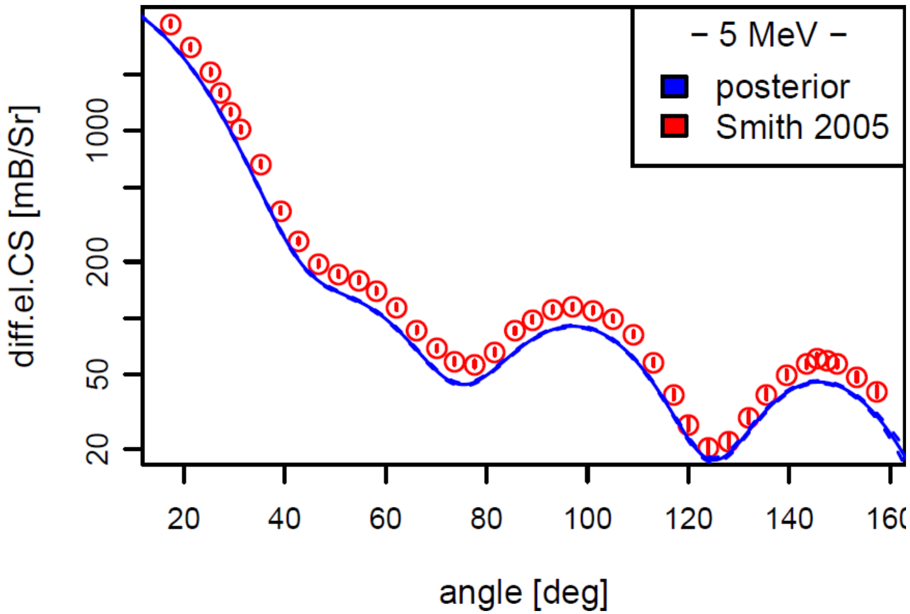


The effect is similar at all energies considered



Evaluated differential elastic n-^{181}Ta cross section at E=5 MeV

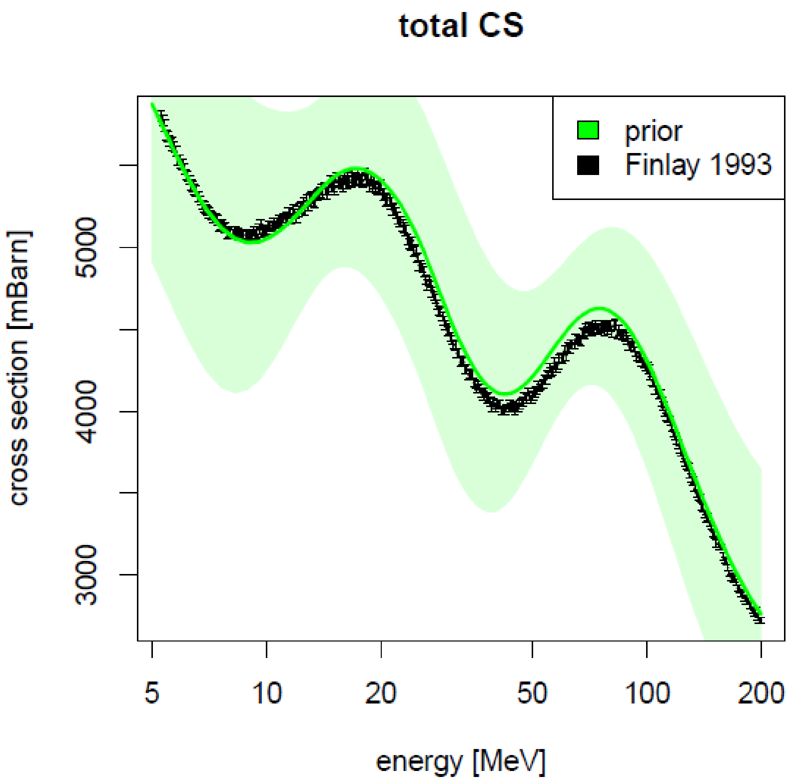




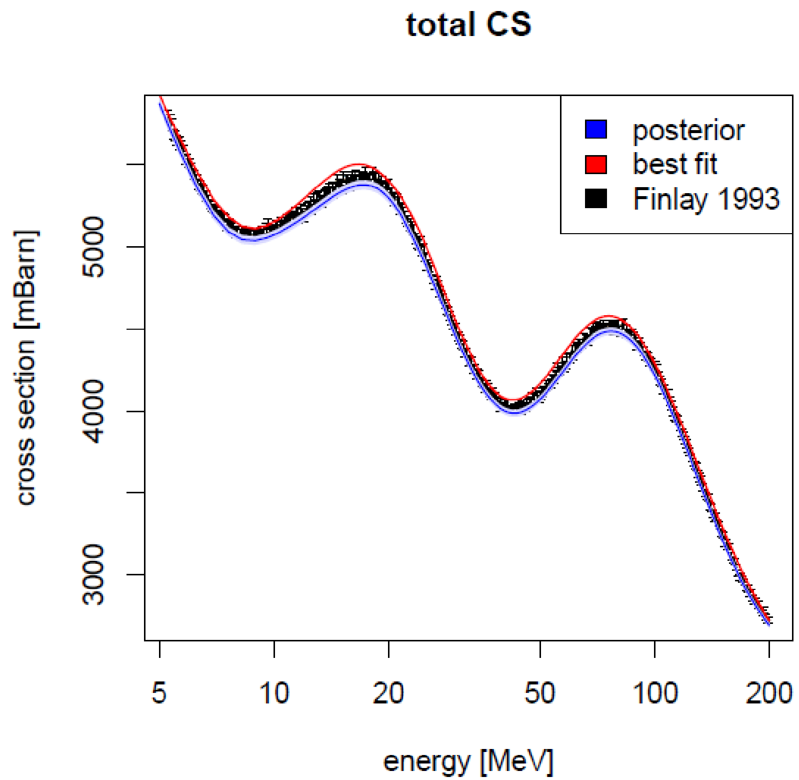
<u>Question:</u>
Is this an effect of the well known total cross section?

No, the same only with exp. diff. cross sections.

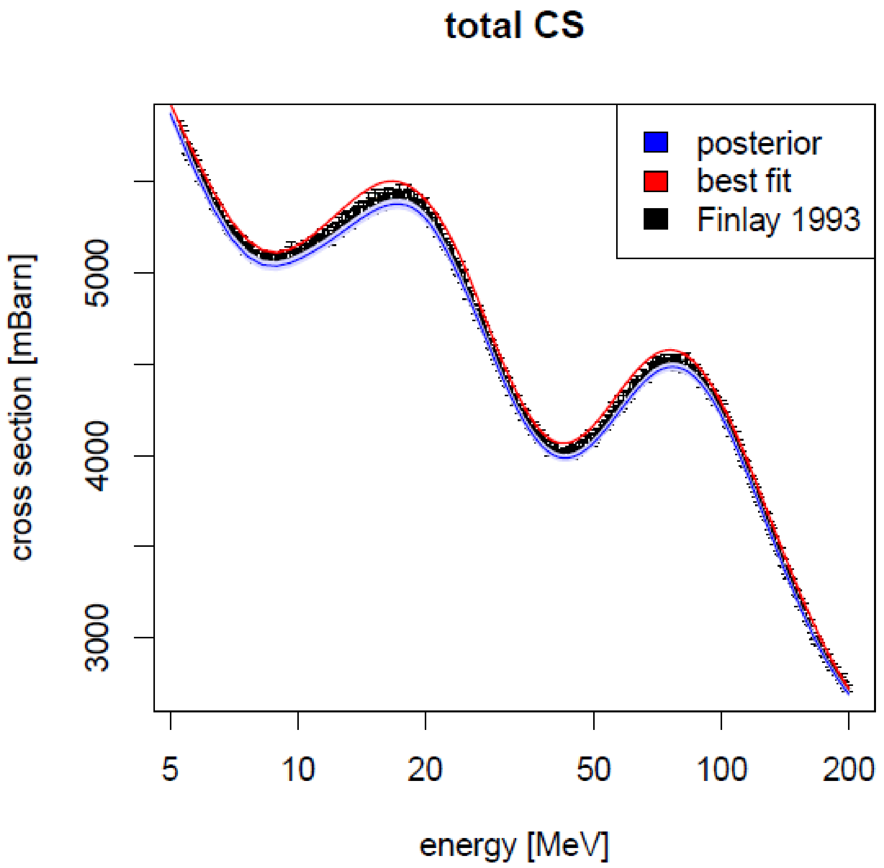
Evaluated total n-^{181}Ta cross section



Evaluation of total cross sections only

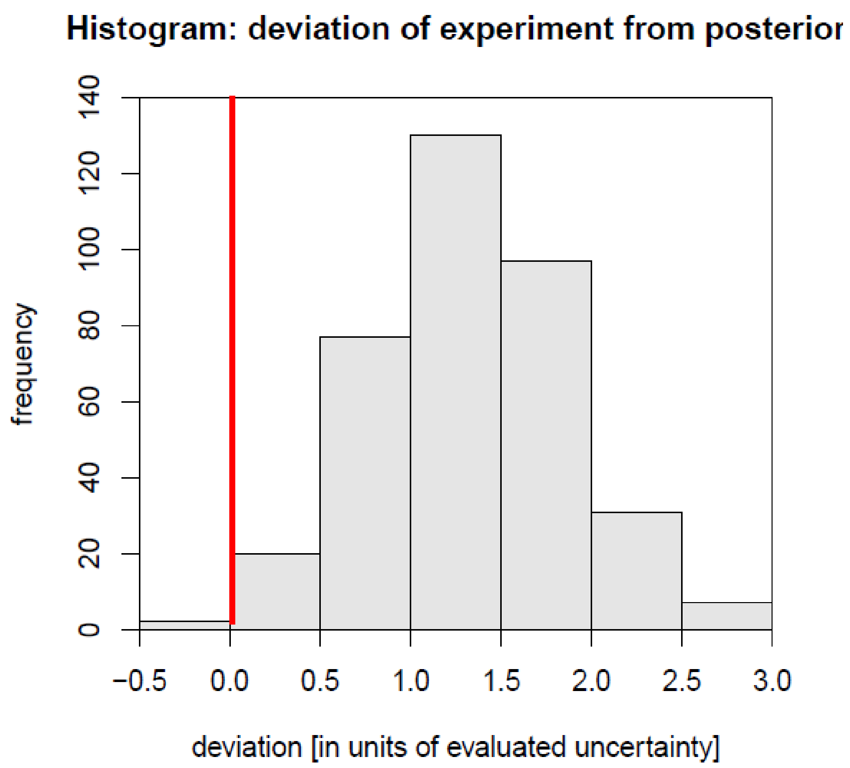


Posterior for total cross section



Evaluation of total n-^{181}Ta cross section only

- The posterior is systematically lower
- Uncertainties too small



Problems of the evaluation

Outcome of test evaluation

prior: accounts for parameter uncertainties only

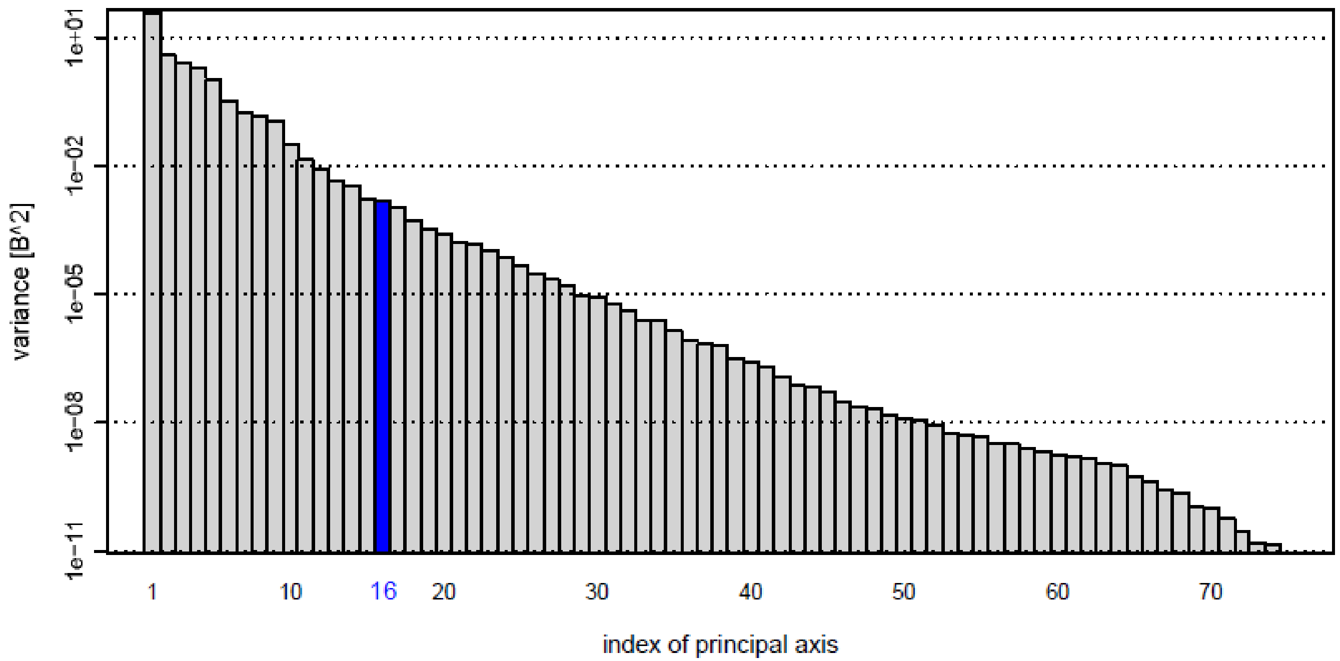
data: n-^{181}Ta including either $\sigma_{\mathrm{tot}}, \left(d\sigma/d\Omega\right)_{\mathrm{el}}$ or both between 0.3 and 150 MeV

- Inclusion of normalisation necessary — ok
- Evaluation of σ_{tot} is too small !
- Uncertainties of σ_{tot} are too small !
- Evaluation of diff.data systematically too low !
- Uncertainties of evaluated diff.data unrealistically small !

Principal component analysis

K. Pearson, Philosophical Magazine 2(11),559 (1901)

Eigenvalues and Eigenvectors of covariance matrix A^{PU}

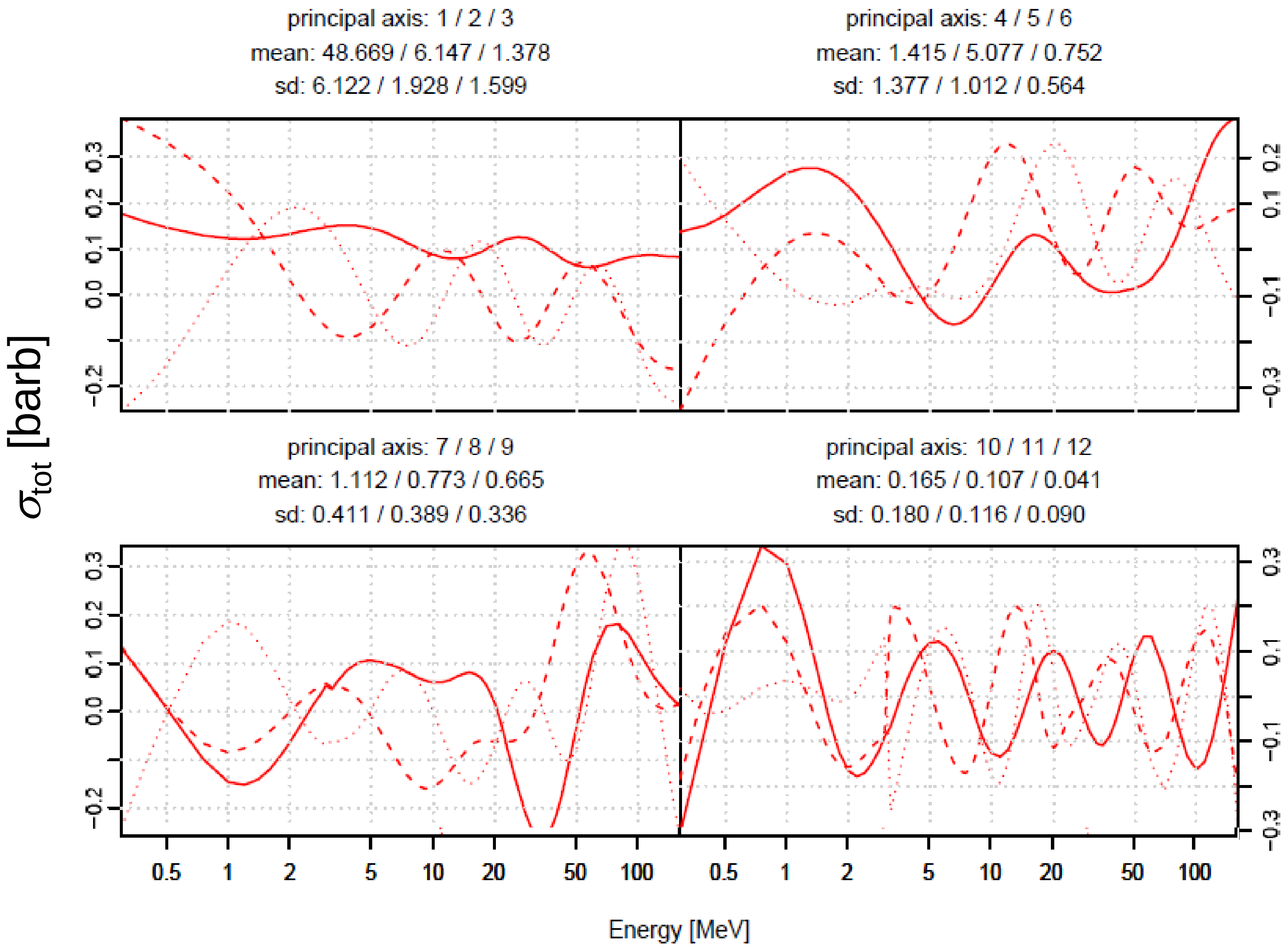


σ_{tot} depends on 16 optical model parameters → 16 dof of cross section subspace

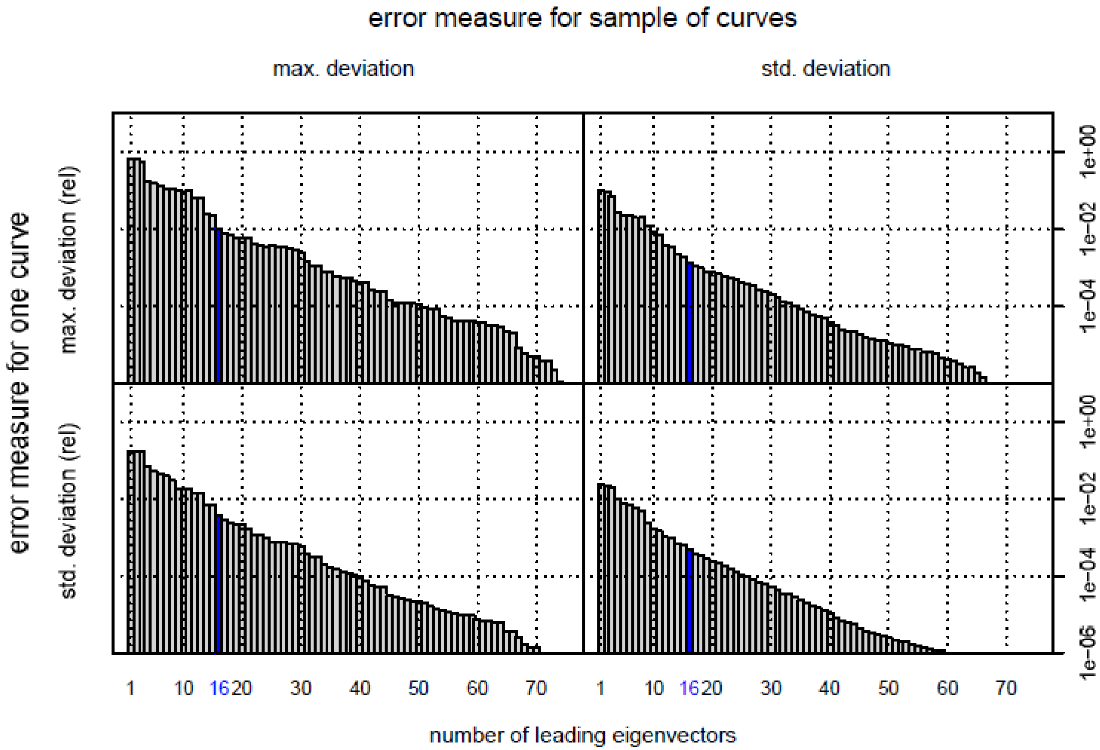
Eigenvalues = variances in direction of axes

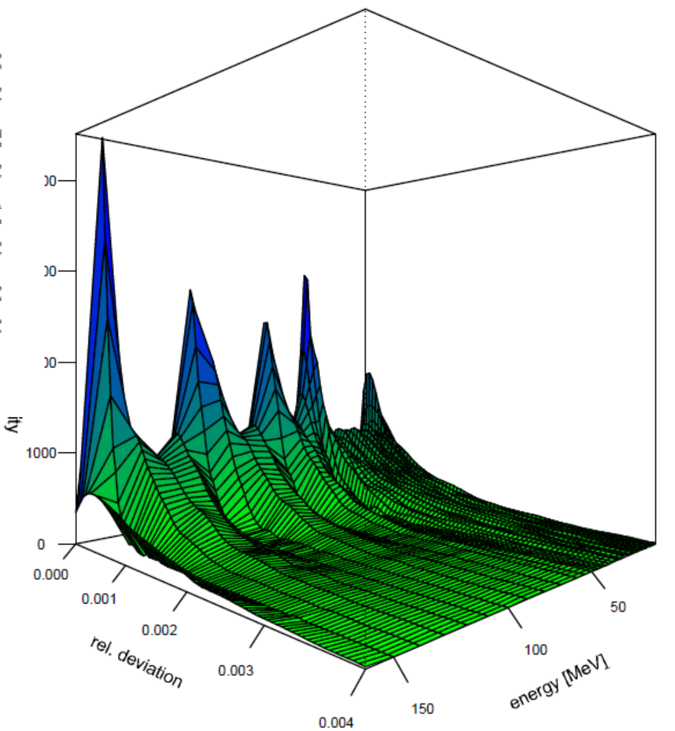
Largest eigenvalue = most significant information

Principal component analysis



Principal component truncation

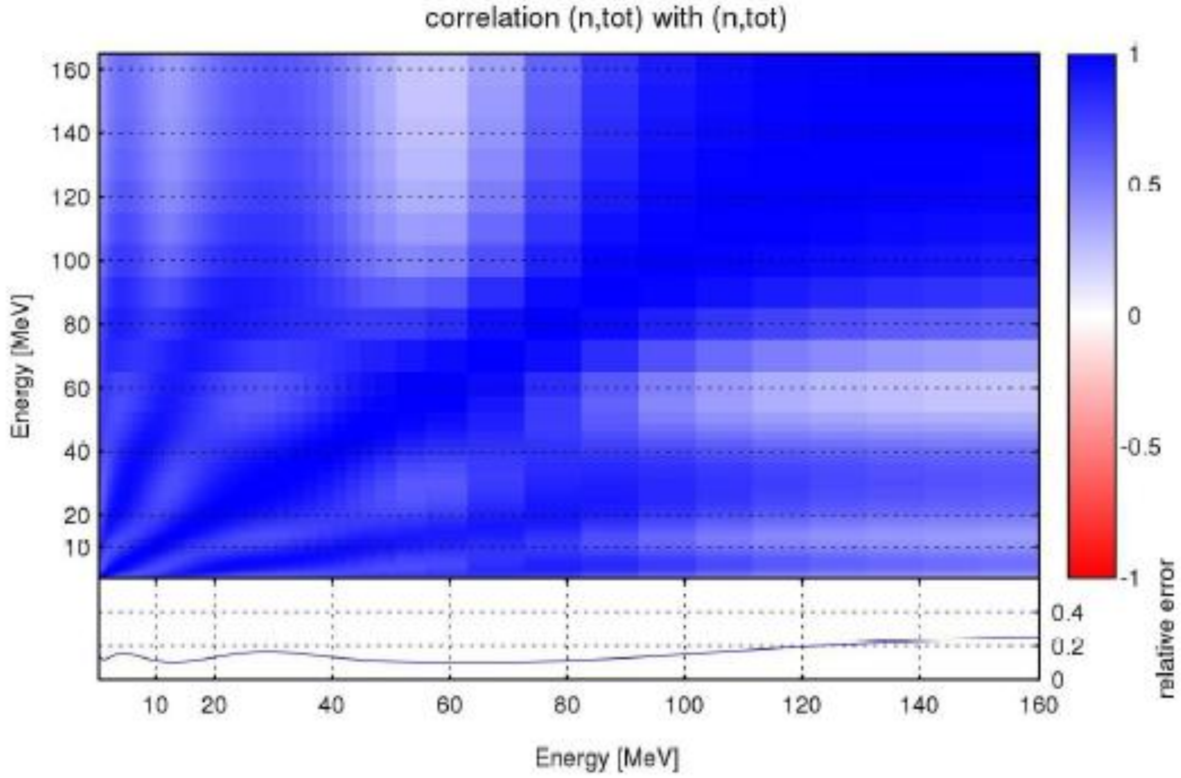




Spectral representation of the covariance matrix by the first 16 eigenvectors leads to accuracy better than 0.3% for $\sigma_{tot}(E)$

Truncated correlation matrix for σ_{tot}

Restricting to 16 eigenvectors leads to an almost perfect reproduction of the correlation matrix for total xsections



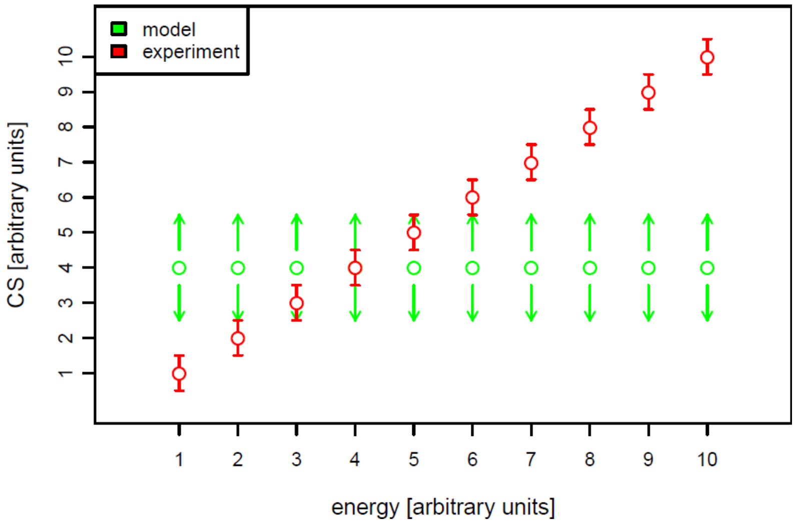
Proof of interpretation

Problem: Quality of the model is essential

Experimental Data

Primitive schematic model

(only one finite eigenvalue)



$$\underline{x}_{post} = \frac{x_{prior} + \bar{y}\dfrac{n\delta^2_{prior}}{\Delta^2_{stat} + n\Delta^2_{syst}}}{1 + \dfrac{n\delta^2_{prior}}{\Delta^2_{stat} + n\Delta^2_{syst}}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix} \qquad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

$$\underline{\underline{A}}_{post} = \frac{\delta^2_{prior}}{1 + \dfrac{n\delta^2_{prior}}{\Delta^2_{stat} + n\Delta^2_{syst}}} \underline{\underline{J}}_n \quad \text{mit} \quad \underline{\underline{J}}_n = \frac{1}{n}\begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & \cdots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & \cdots & 1 & 1 \end{pmatrix}$$

If model strongly correlates, but excludes the shape of the experiments → the posterior becomes arbitrary (bad)

Analysis of the problem

The a-posterior can only be constructed from basis functions available in the covariance matrix

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

⇓

The experimental cross section data for ^{181}Ta contain only eigenfunctions with very small variances and are contained in the ensemble of cross sections only in a very small fraction

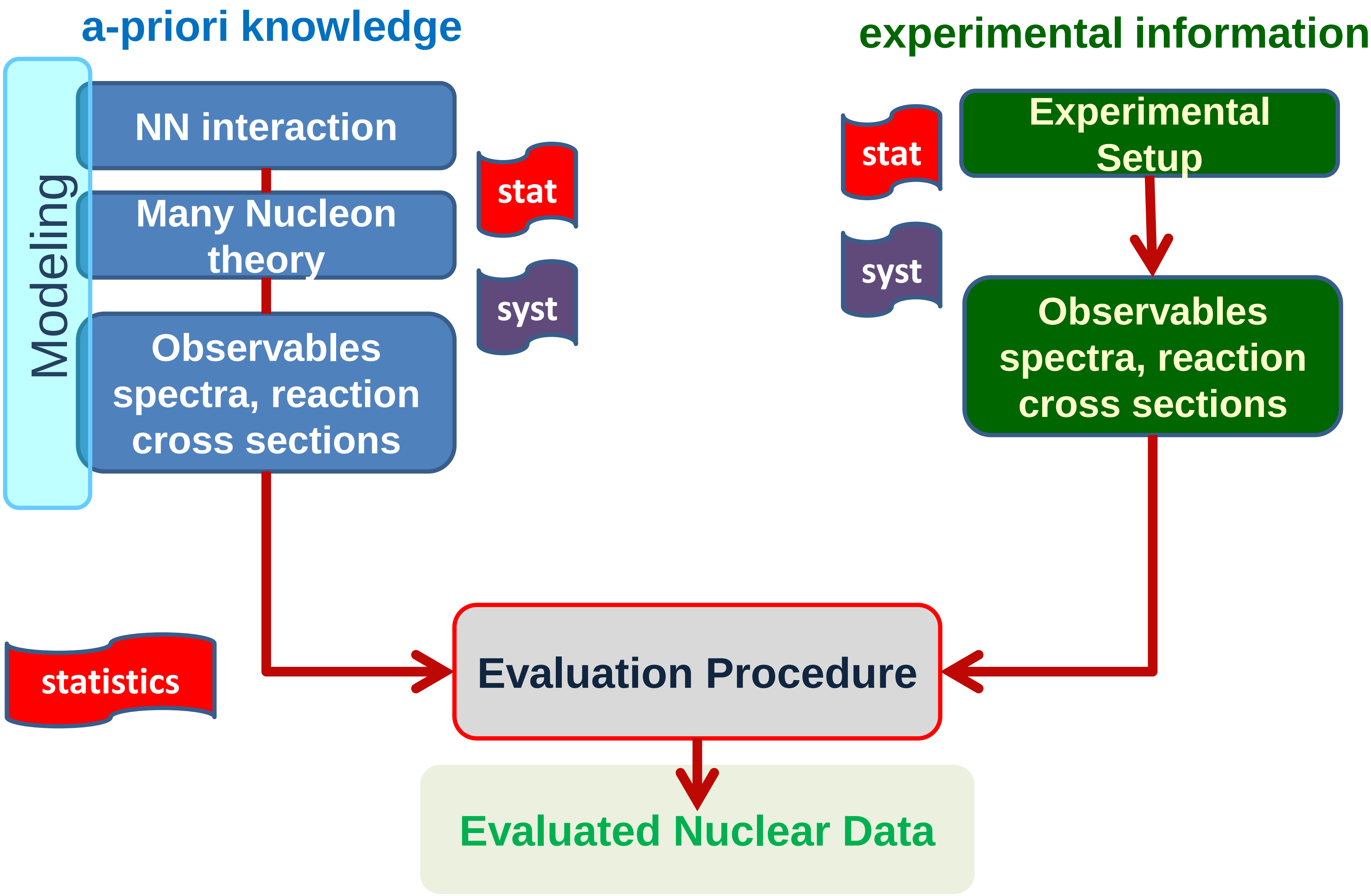
⇓

the a-posterior uncertainties are only given by this small fraction by the parameter uncertainties of the nuclear model

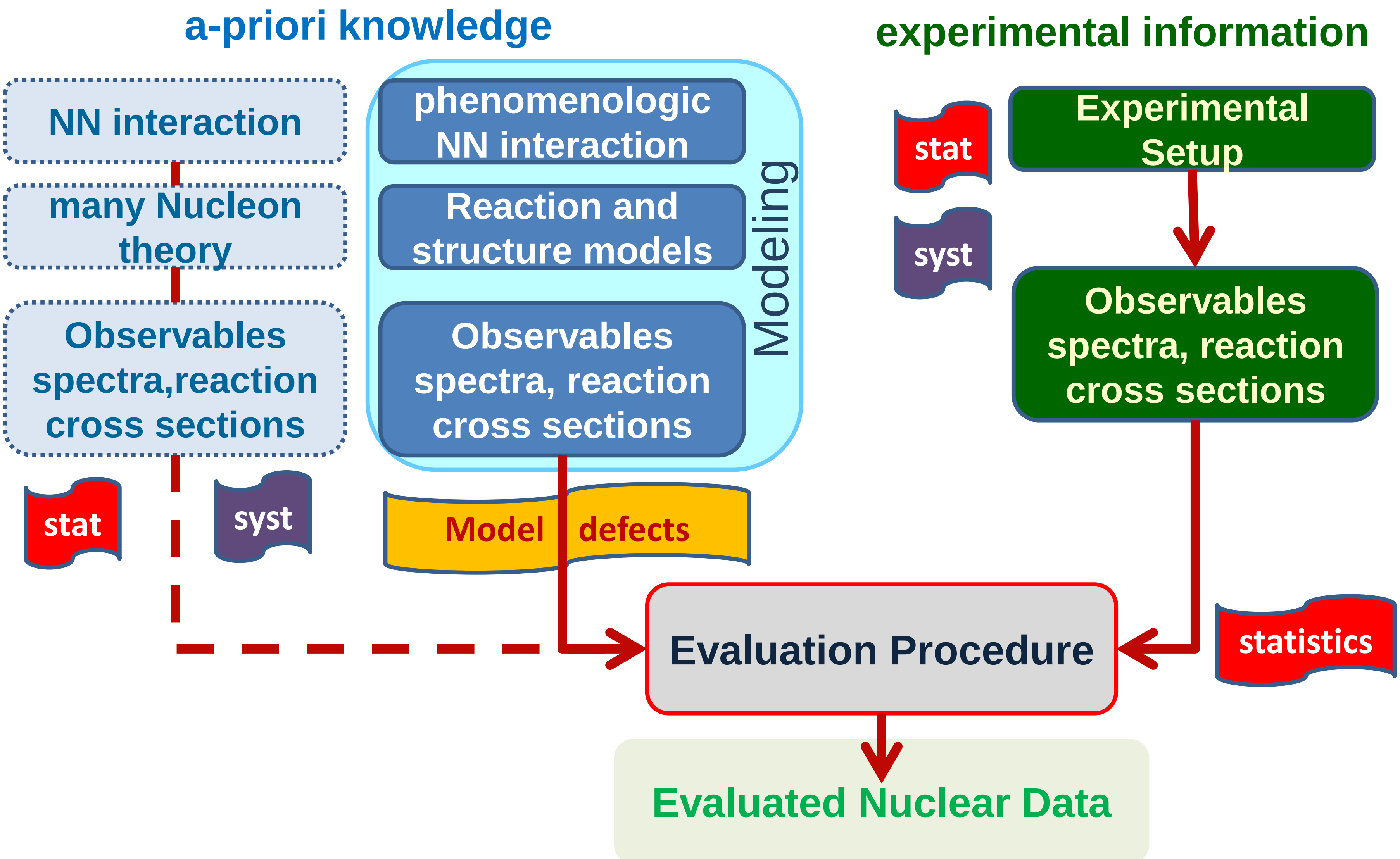
⇓

The strong correlations of the prior must become weaker

Concept of Evaluation



Concept of Evaluation



Model Defects

Systematic deviation of nuclear model values from experimental value which cannot be accounted for within the model by variations of parameters.

D. Neudecker, H. Leeb, R. Capote, NIM A (2013)

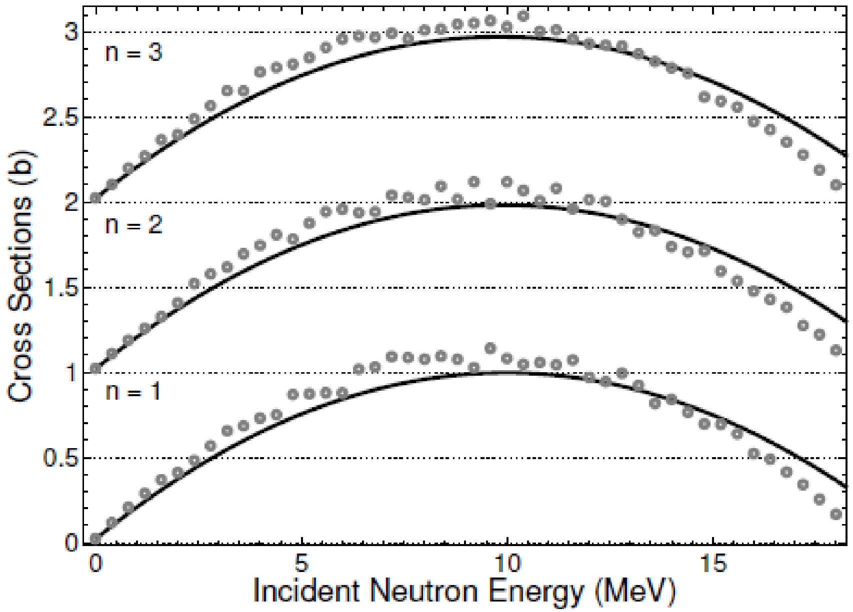


Figure 1: Schematic example of model data (black lines) which deviate systematically from experimental data (gray circles) for $n = \{1, 2, 3\}$ isotopes above 14 MeV.

Determination of prior

Nuclear model calculations are used to determine the PRIOR:

The contributions to the covariance matrix of the model are:

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

Parameter uncertainties

Numerical implementation errors

neglected

Deficiencies of the model, is of non-statistical nature

Method and code based on complete ignorance and transformation group invariance developed by Pigni and Leeb

Improved method developed and first application to ^{55}Mn

Model Defects

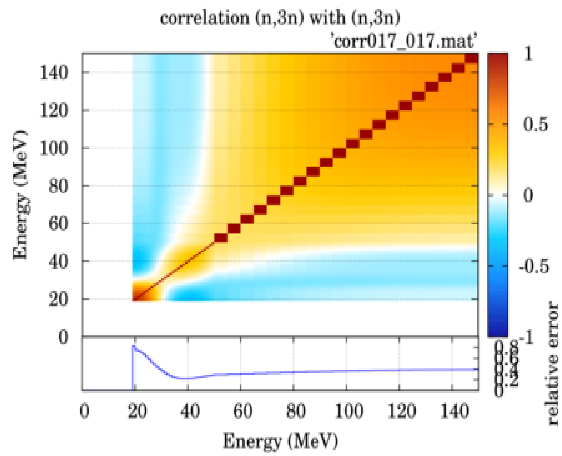
H. Leeb et al., Nucl.Data Sheets 109, 2762 (2008)

$$D^c = \sum_{n=1}^{N^c} w^{c,n} \sum_{m=1}^{M} w_m^{c,n} \sum_{j \in Ebin} w_j^{c,n,m} \frac{\sigma_{ex}^{c,n}(E_j)}{\sigma_{th}^{c,n}(E_j)}$$

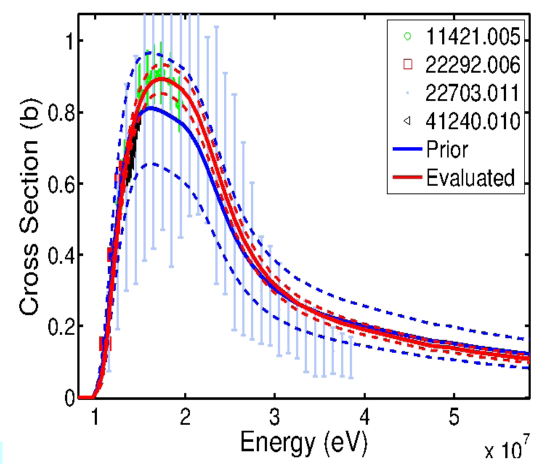
$$\mathrm{cov}\left(\Delta\sigma^c(E), \Delta\sigma^{c'}(E')\right) = A_0^{MD}(E_m, E_{m'})$$

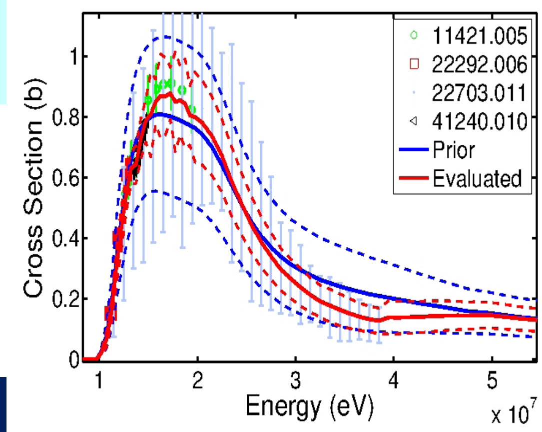
$$= \frac{\sigma_{th}^c(E_m)\sigma_{th}^{c'}(E_{m'})}{\sqrt{N^c(E_m)}\sqrt{N^{c'}(E_{m'})}}$$

$$\times \left\{ \sum_{n=1}^{N^c} \left[\left\langle D_n^c(E_m)\right\rangle - D^c\right]\left[\left\langle D_n^{c'}(E_{m'})\right\rangle - D^{c'}\right] + \sum_{n=1}^{N^c} \delta_{cc'} g_{mm'} \sqrt{\mathrm{var}\left(D_n^c(E_m)\right)\mathrm{var}\left(D_n^{c'}(E_{m'})\right)} \right\}$$



without model defects



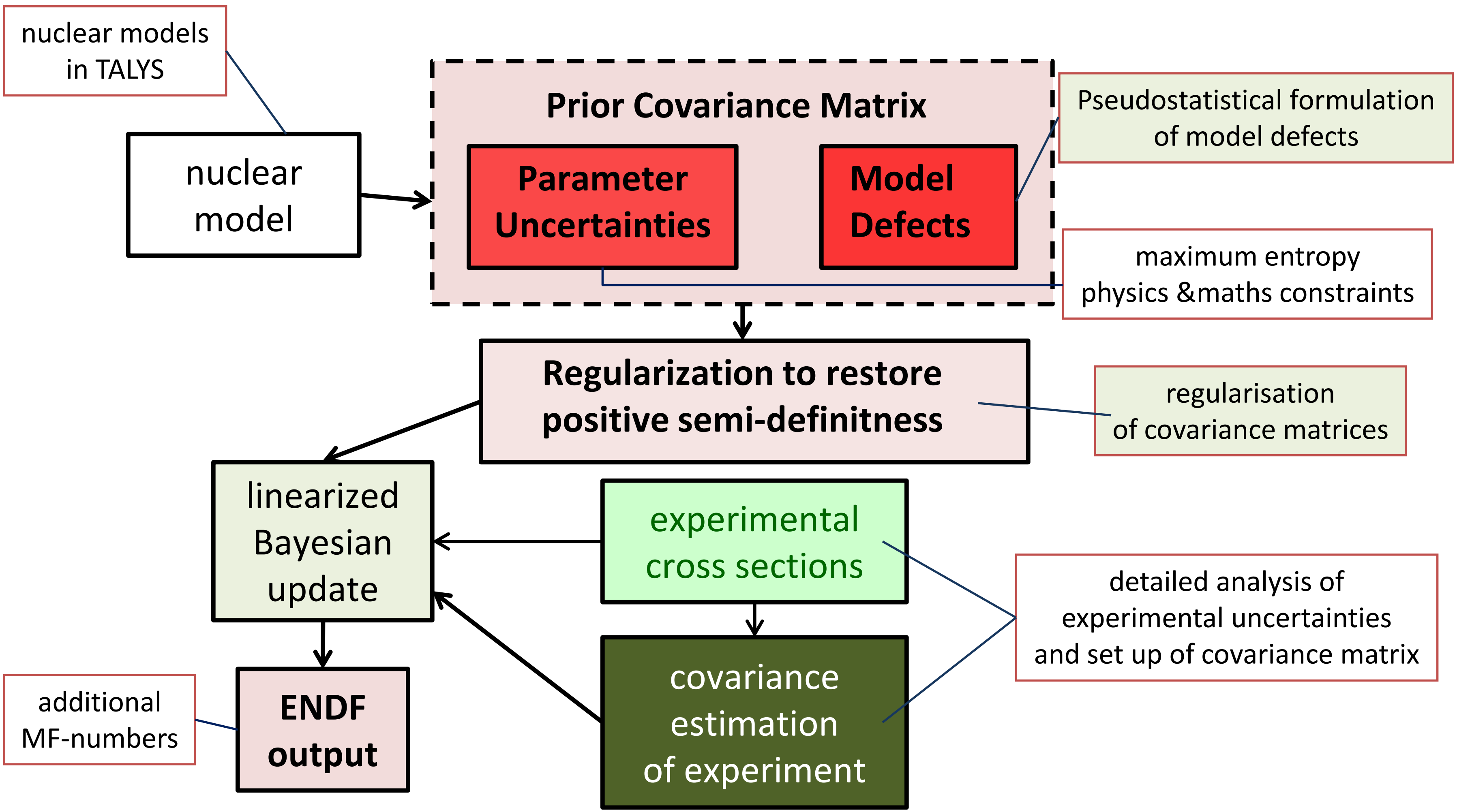


without model defects

Other Procedures for model defects:
Trkov, R. Capote, Soukhovitsii et al.,
NIM A212 (2011) 3098

model defects are essential if model deviates significantly from experiment

Layout of Full Bayesian Evaluation Technique



The importance of model defects

D. Neudecker, H. Leeb, R. Capote, NIM A (2013)

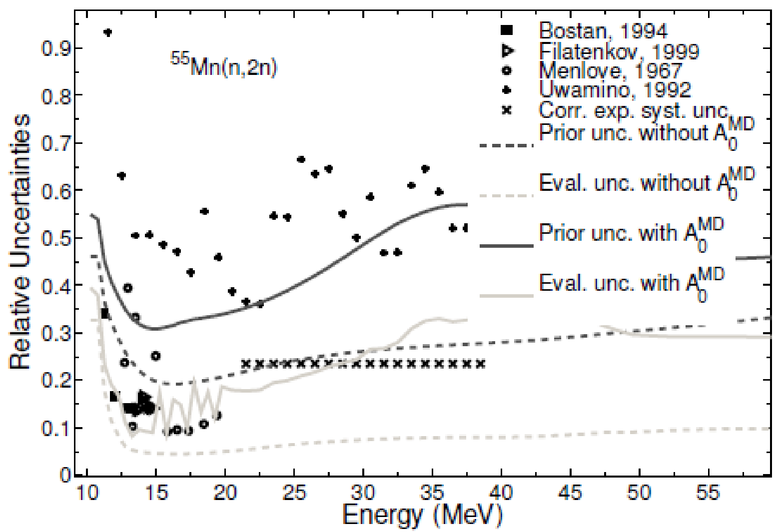
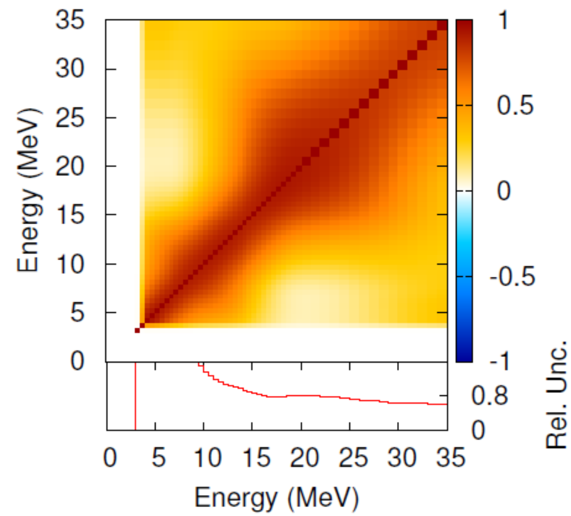
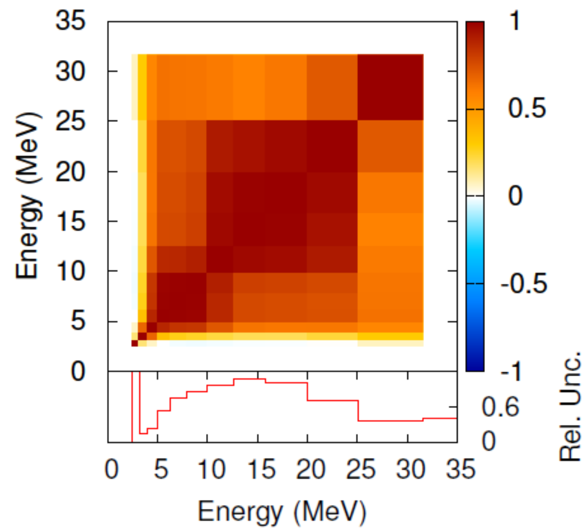


Figure 4: Dimensionless evaluated and prior ^{55}Mn(n,2n) relative uncertainties including and omitting model defect uncertainties are compared to experimental relative uncertainties of [26–28, 30] as well as to the correlated experimental uncertainty above 20 MeV.

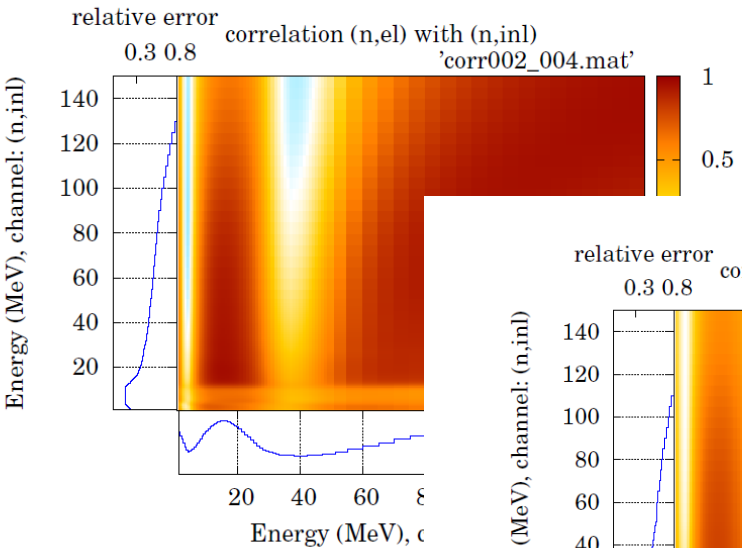


Model defects of Leeb et al., NDS 109 (2008)2762

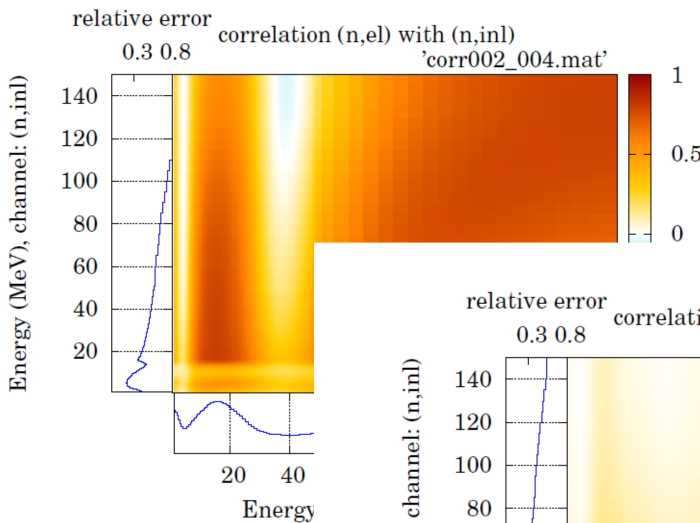


Model Defects of Trkov, Capote et al., NDS 112 (2011)3098

Cross channel correlations

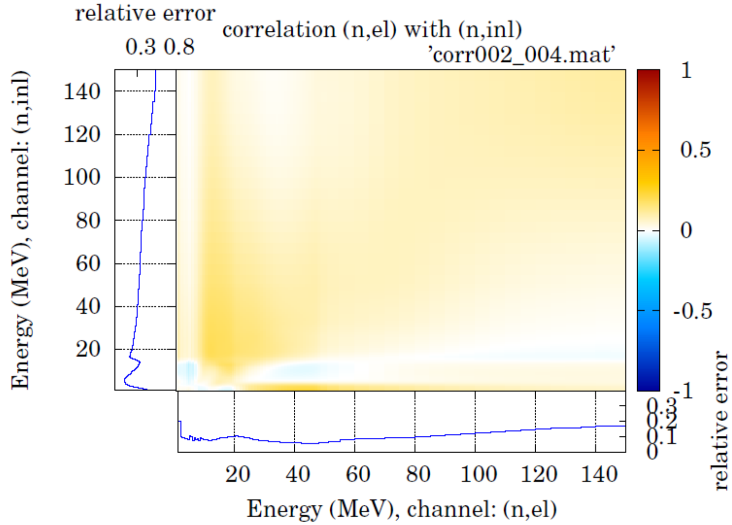


parameter uncertainties



prior

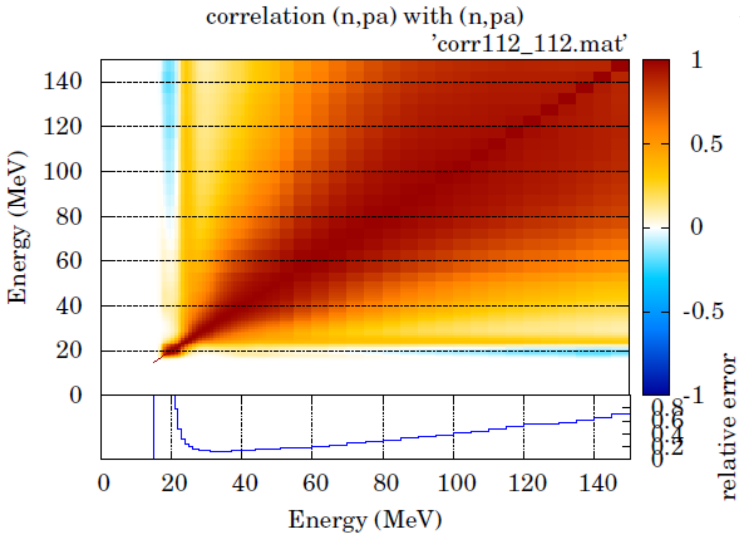
full evaluation

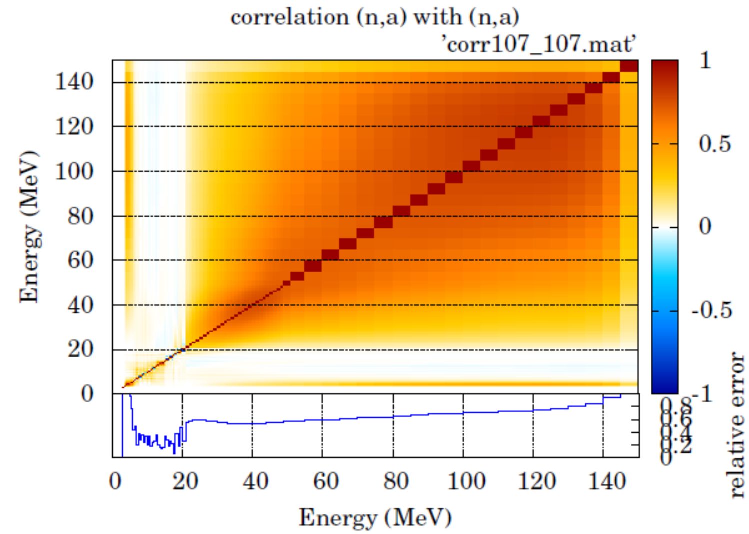


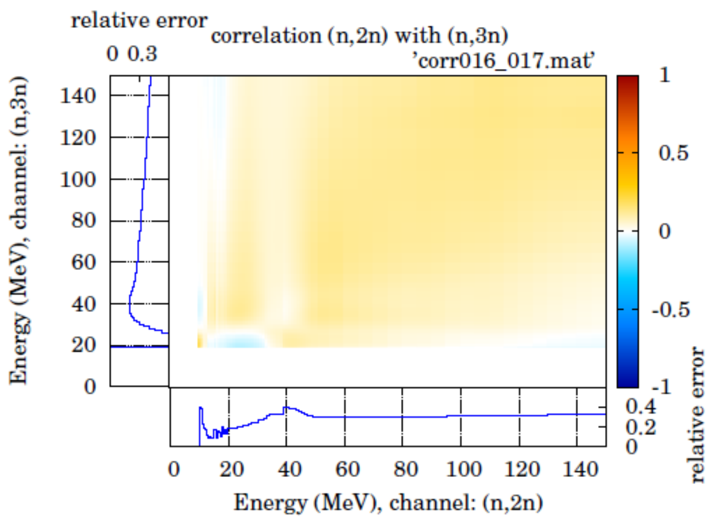
$<\sigma_{ela}(E)\ \sigma_{inl}(E')>$

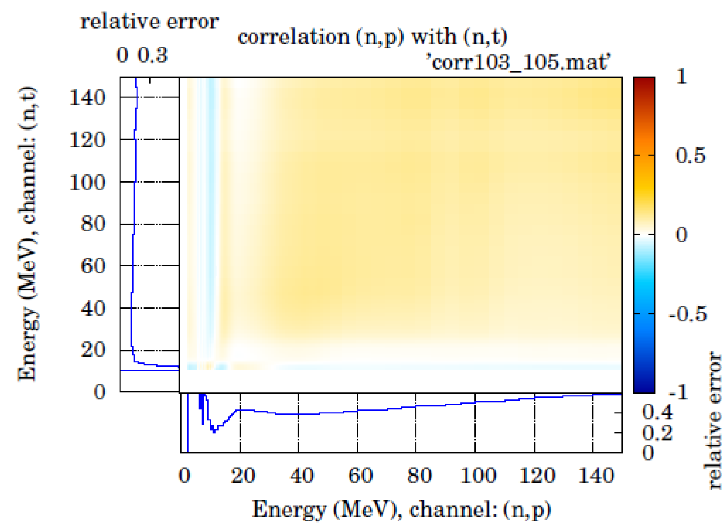
Cross channel correlations

^{55}Mn

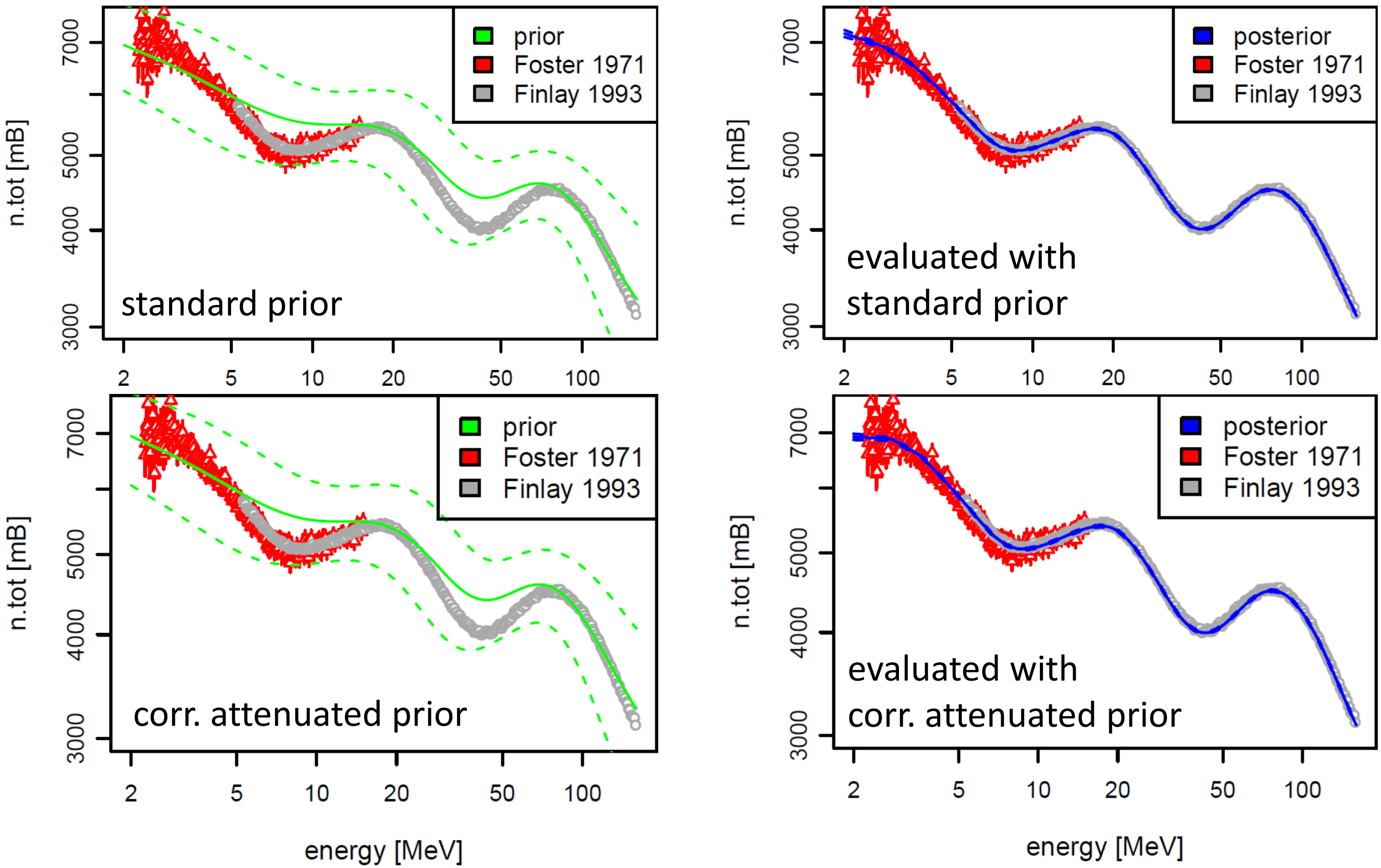




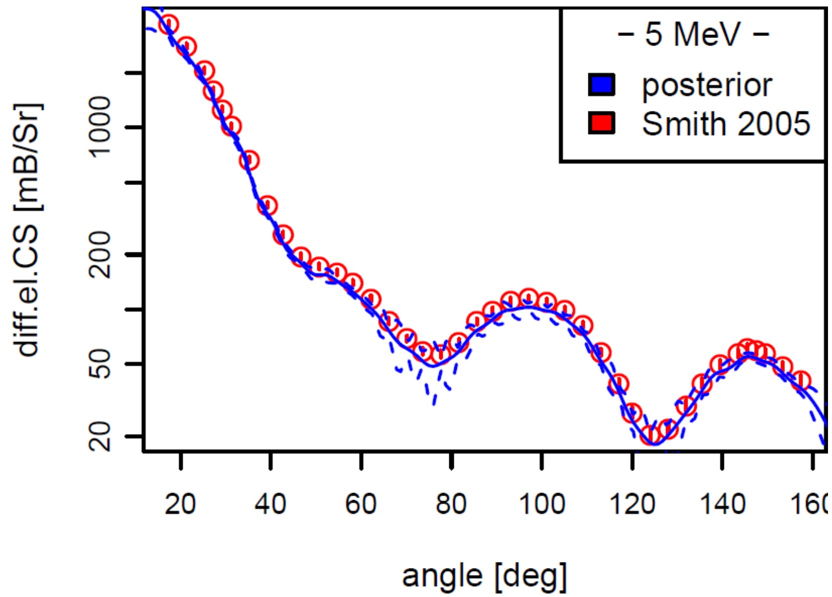




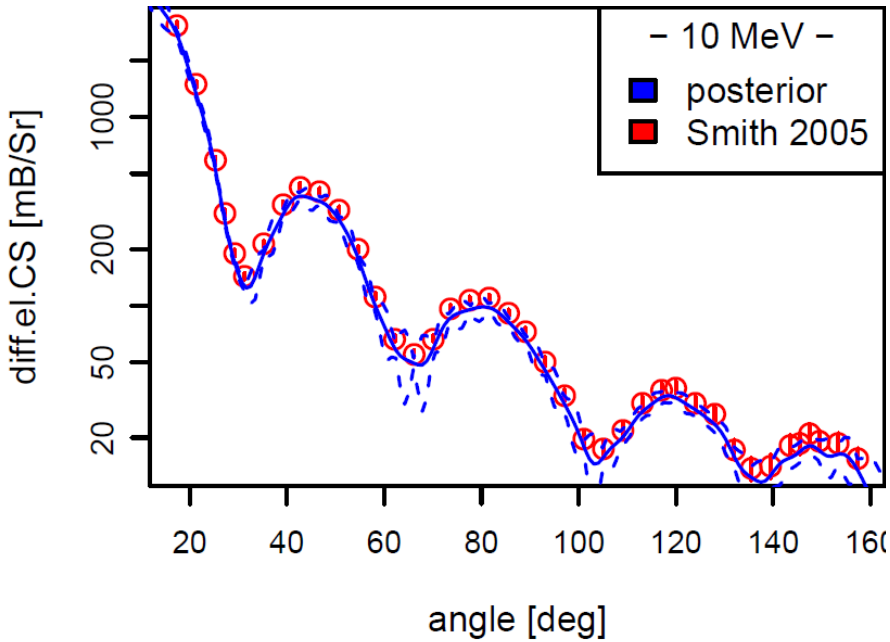
Example: n–^{181}Ta total cross section



Example: differential n–^{181}Ta elastic cross section



As expected the uncertainties remain in the order of the systematic errors



Problem:

The pseudostatistical inclusion of model defect covariances violates sum rules, unitarity …

Summary and Outlook

Basics of Evaluation Procedures

- The Bayesian evaluation – prerequisite is a perfect model
- Systematic uncertainties – correlated in one step
- Model defects are essential for a realistic evaluation
- Best physics model is required for a proper evaluation

Future Steps Required

- Inclusion of model defects without violation of sum rules, …
- Define meaning of covariance matrices – definition of validation procedure
- Continuous improvement of modeling

The Hen-Egg Problem

Observable: $\sigma = \sigma(x, \underline{p})$ parameter p_i, $i=1,\ldots,N$

$$\langle \Delta\sigma(x)\Delta\sigma(x')\rangle = \sum_{i,j=1}^{N} \frac{\partial\sigma(x)}{\partial p_i} \langle \Delta p_i \Delta p_j \rangle \frac{\partial\sigma(x')}{\partial p_j}$$

<u>observables:</u> <u>parameters:</u>

correlated ← uncorrelated

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uncorrelated → correlated

General criterion for covariances required !!!

e.g. for application, comparison

What is the true Covariance Matrix

Observable: $y(x) = f(x, \vec{p}) = g(x, \vec{q})$ $p_i \quad i = 1, \cdots, N$

exact description   model $q_j \quad j = 1, \cdots, M$

introduce grid in $x_i \quad i = 1, 2, \cdots, M$ $\left(\underline{\underline{S}}\right)_{i,j} = \frac{\partial f(x_i, \underline{p})}{\partial p_j}$

$$\underline{\underline{F}} = \left(\langle \Delta p_i \Delta p_j \rangle\right) \qquad \underline{\underline{G}} = \left(\langle \Delta q_i \Delta q_j \rangle\right)$$

$$\left(\langle \Delta y(x_i) \Delta y(x_j) \rangle\right)^{ph} = \underline{\underline{Y}}^{ph} = \underline{\underline{S}}\,\underline{\underline{F}}\,\underline{\underline{S}}^T$$

$$\left(\langle \Delta y(x_i) \Delta y(x_j) \rangle\right)^{mo} = \underline{\underline{Y}}^{mo} = \underline{\underline{R}}\,\underline{\underline{G}}\,\underline{\underline{R}}^T$$

Assumption:

$$\underline{\underline{Y}}^{ph} = \underline{\underline{Y}}^{mo}$$

If *M>N* : for diagonal $\underline{\underline{F}}$, $\underline{\underline{G}}$ contains dependencies

If *M=N* : corresponds to a rotation in parameter space

If *M<N* : covariance $\underline{\underline{G}}$ is projection of $\underline{\underline{F}}$

Requests on Nuclear Theory

NN interaction

NN-interaction
3N-interaction
…….. ???

many Nucleon theory

Nuclear Structure Theory
mean field - RPA, QRPA - ?
Inclusion of continuum, …
novel approaches ???

Nuclear Reaction Theory
consistency, actual nucl.structure, …
reactions with composite particles, …
fission, breakup, … ???

Observables
spectra,reaction
cross sections, …

Additional Observables ???

Conclusion

- Model defects are essential for a realistic evaluation
- Best physics model is required for a proper evaluation

Nuclear Data Evaluation is a Challenge for Nuclear Theory

Thank you for your attention