The Full Bayesian Evaluation Technique

Properties and Developments

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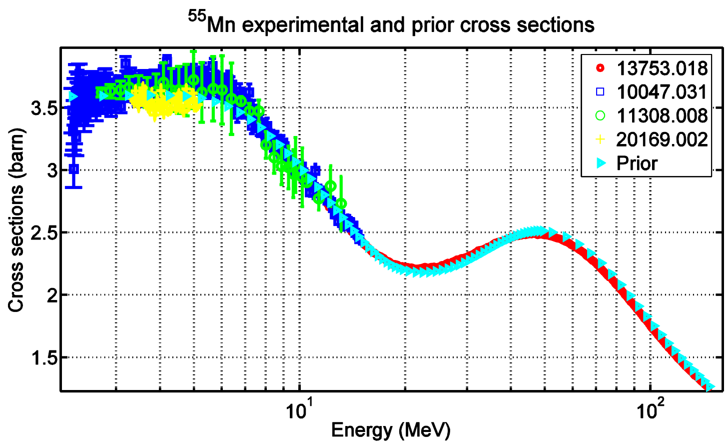
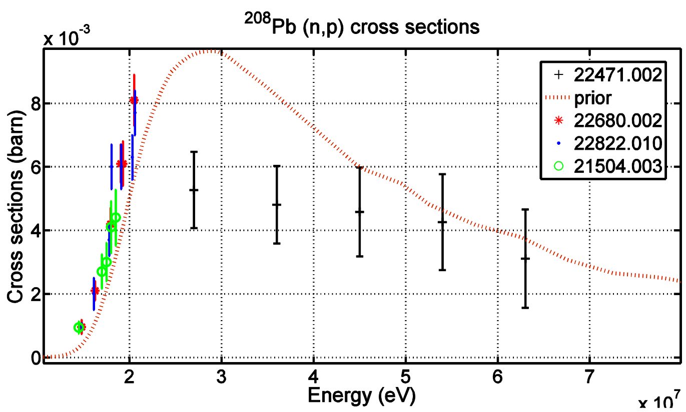
Introduction

Aims of the Full Bayesian Evaluation Technique





Aims

Consistent combination of experimental and model cross sections σ_i

?

Estimation of related uncertainties in form of covariance matrices

$$\mathrm{Cov}(\sigma_i,\sigma_j) = \left\langle \left(\sigma_i - \langle\sigma_i\rangle\right)\left(\sigma_j - \langle\sigma_j\rangle\right)\right\rangle$$

??

Are needed for the design and development of novel nuclear technologies (Nuclear waste incineration, Fusion and GenerationIV reactor,...).

2 fundamental principles of Statistics:

x … model cross sections
M … model
σ … experimental cross sections

$$p(x|M) + p(\overline{x}|M) = 1$$ Normalization Condition

$$p(\sigma, x|M) = p(\sigma|x, M)p(x|M)$$ Product Rule

BAYES THEOREM

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

Likelihood function
Measures the prob. that σ is measured if x and M are correct.

Prior distribution
Measures the prob. to obtain the correct model cross sections x if M is true.

TU WIEN

BAYES THEOREM

Likelihood function

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

Prior distribution

Assumption: normal distribution of x around x_0 and σ around y(x)

In exponential form

$$p(x\,|\,\sigma, M) = N \exp\left\{ -\frac{1}{2}(\sigma - y(x))^T B^{-1} (\sigma - y(x)) - \frac{1}{2}(x_0 - x)^T A_0^{-1} (x_0 - x) \right\}$$

BAYES THEOREM in exponential form

Assumption: normal distribution of x around x_0 and σ around y(x)

$$p(x \mid \sigma, M) = N \exp\left\{ -\frac{1}{2}(\sigma - y(x))^T B^{-1} (\sigma - y(x)) - \frac{1}{2}(x_0 - x)^T {A_0}^{-1} (x_0 - x) \right\}$$

σ around y(x) normally distributed, if considering

x_0 around x normally distributed, if considering

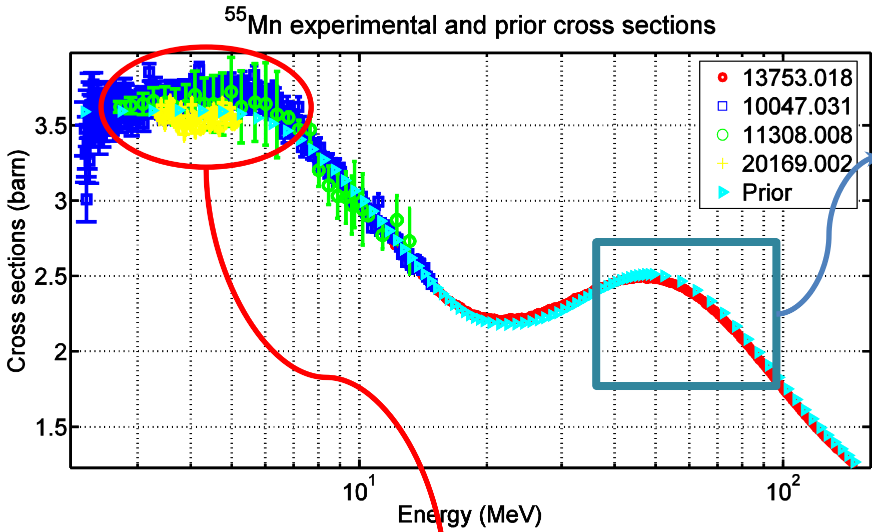
Uncertainties of experiment | **Model Defects** | **Parameter Uncertainties**

B | **A_0^{MD}** | **A_0^{PU}**

$$A_0 = A_0^{MD} + A_0^{PU}$$

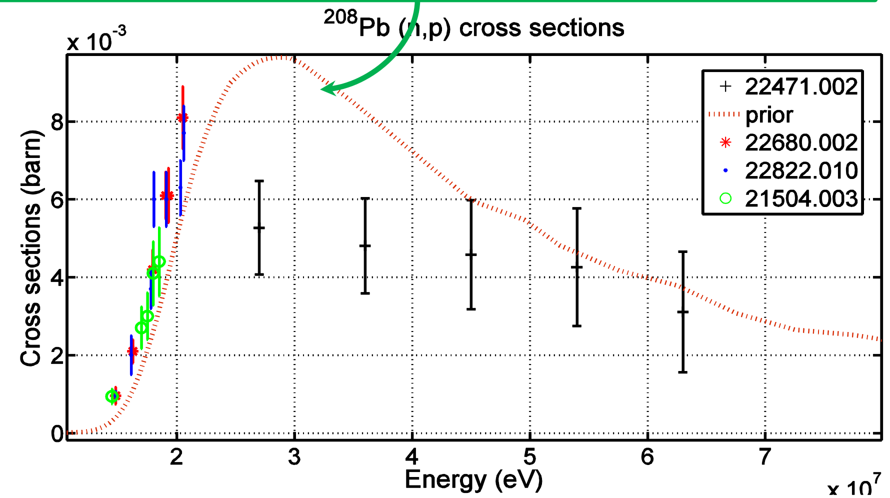
$$\mathrm{Cov}(\sigma_i, \sigma_j) = \int d\sigma_i \int d\sigma_j \int d\sigma_k\, p(\ldots\sigma_i, \sigma_j \ldots)(\sigma_i - \langle\sigma_i\rangle)(\sigma_j - \langle\sigma_j\rangle)$$

Theory - *Experimental uncertainties, Parameter Uncertainties and Model Defects*



Model deviates from experimental data due to limited knowledge of model parameters, considered in **Parameter Uncertainties A_0^{PU}**

Model deviates from experimental data considered in **Model Defects A_0^{MD}**



Three different experimental data sets which deviate systematically from each other, considered in **uncertainties of experiment B**

Theory

Parameter Uncertainties and Model Defects

Parameter Uncertainties A_0^{PU}:

- account for the limited knowledge of the model parameters a_k
- are calculated by means of Monte Carlo variation of parameters a_k within defined boundaries following different distribution functions

$$A_0^{PU} = \left\langle \left(\sigma_i(a_k) - \sigma_i \right) \left(\sigma_j(a_l) - \sigma_j \right) \right\rangle$$

- parameter boundaries are chosen relatively broad to conform to the required complete ignorance of prior knowledge.

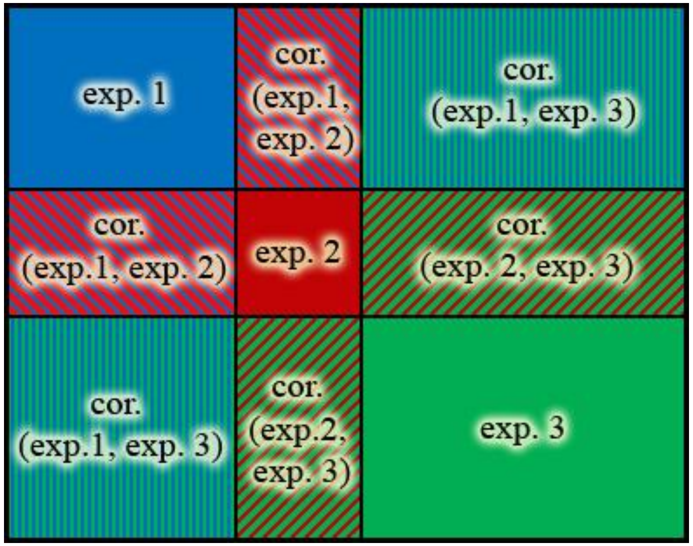
Model Defects A_0^{MD}:

- account for systematic deviations of the model from the experiment which cannot be corrected by exploiting the whole model parameter space
- formulation should neither be based on experimental data of the isotope in question nor on model information

Theory

Experimental uncertainties

Systematic and statistical uncertainties are considered for the ***single experiments***.
Systematic uncertainties are considered as well ***between different experiments*** depending on their correlation.
All experiments which are correlated to each other, are part of one **large block covariance matrix.**



$$B(\sigma_i,\sigma_j) = \langle \Delta\sigma_i, \Delta\sigma_j \rangle + \frac{\partial\sigma}{\partial E}\Big|_{E_i} \langle \Delta E_i, \Delta E_j \rangle \frac{\partial\sigma}{\partial E}\Big|_{E_j} + \frac{\partial\sigma}{\partial\sigma_S}\Big|_{E_i} \langle \Delta\sigma_{Si}, \Delta\sigma_{Sj} \rangle \frac{\partial\sigma}{\partial\sigma_S}\Big|_{E_j}$$

Errors in terms of cross sections | energy | cross section of standard material

Theory

Experimental uncertainties

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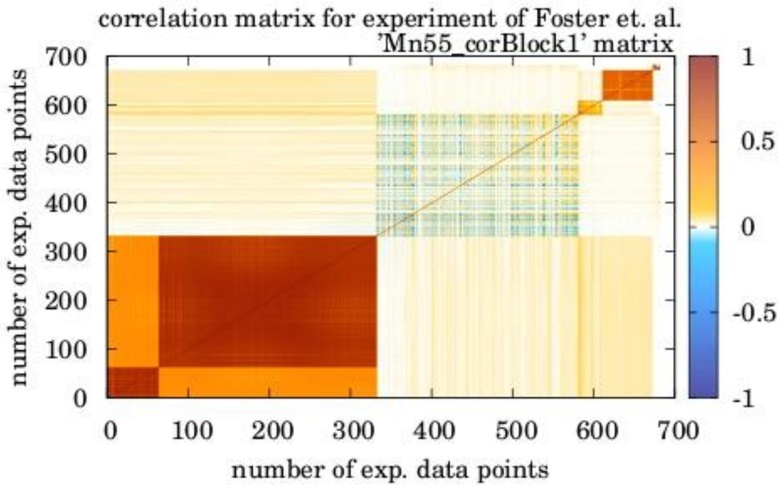


$$B(\sigma_i,\sigma_j) = \langle \Delta\sigma_i, \Delta\sigma_j \rangle + \frac{\partial\sigma}{\partial E}\Big|_{E_i} \langle \Delta E_i, \Delta E_j \rangle \frac{\partial\sigma}{\partial E}\Big|_{E_j} + \frac{\partial\sigma}{\partial\sigma_s}\Big|_{E_i} \langle \Delta\sigma_{si}, \Delta\sigma_{sj} \rangle \frac{\partial\sigma}{\partial\sigma_s}\Big|_{E_j}$$

Errors in terms of cross sections | energy | cross section of standard material

Theory

The Full Bayesian Technique

In Geneus, **the linearized version of the Bayes theorem** is implemented

$$A_1 = A_0 - A_0 S^T \left(S A_0 S^T + B\right)^{-1} S A_0,$$

$$\sigma_1 = \sigma_0 + A_0 S^T \left(S A_0 S^T + B\right)^{-1} \left(\sigma_{Exp} - \sigma_0\left(E_{Exp}\right)\right),$$

$$S = \frac{\partial \sigma_0\left(E_{Exp}\right)}{\partial \sigma_0}$$

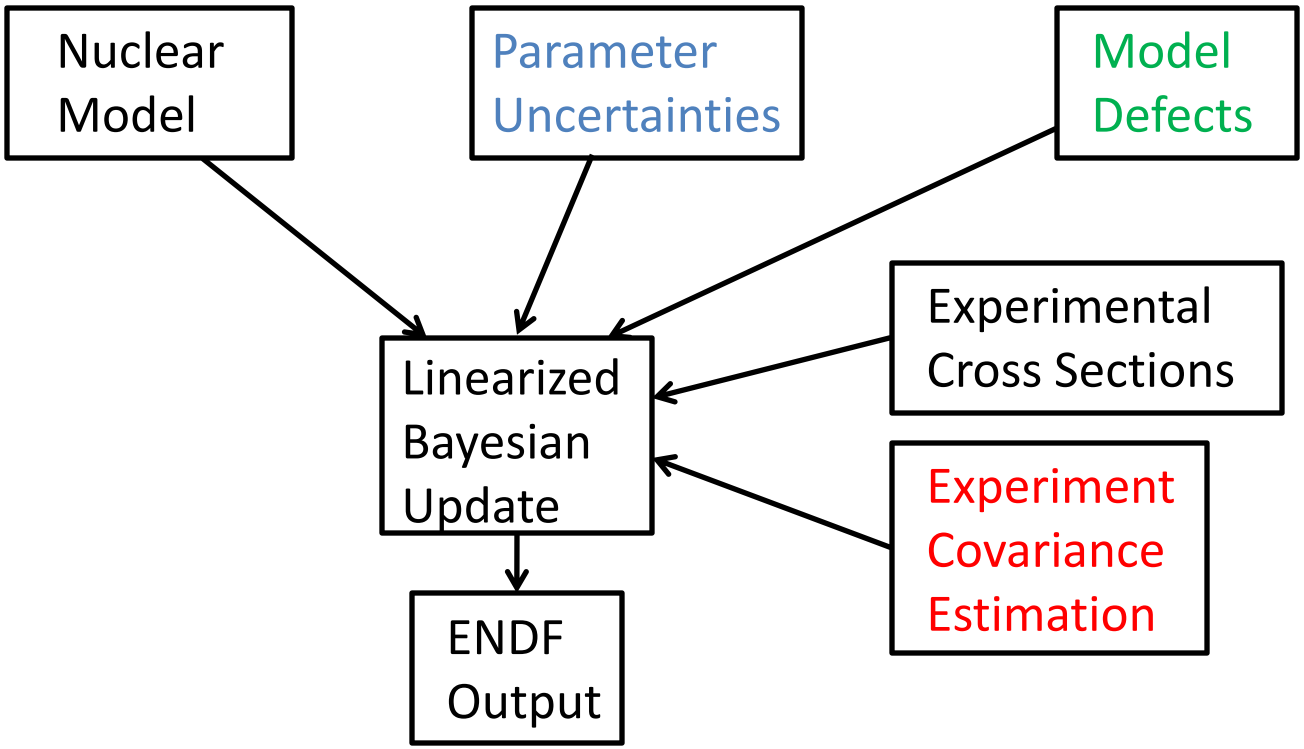
Every update step corresponds to the inclusion of one large experimental block covariance matrix B.

Theory

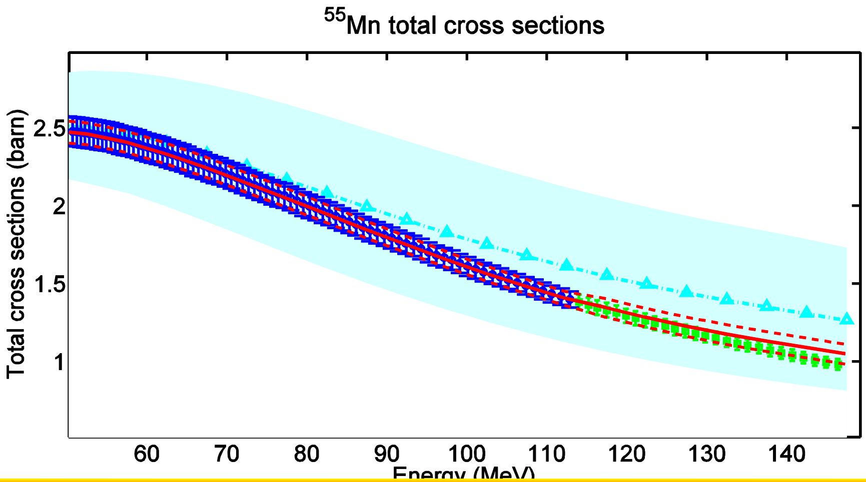
The Full Bayesian Evaluation Technique

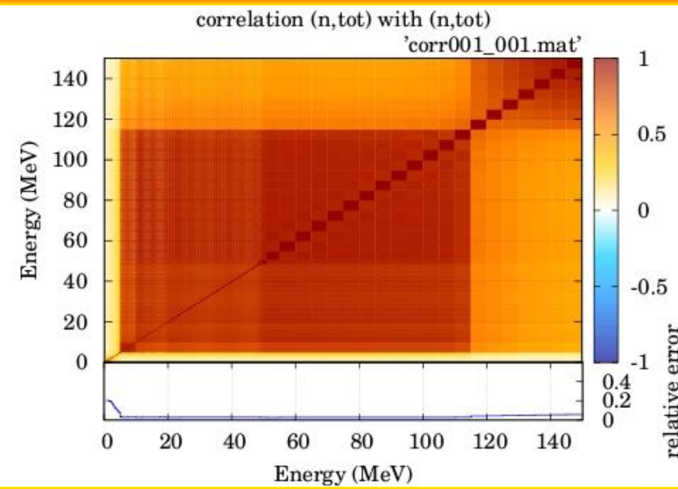
GENEUS

GEneral Nuclear data Evaluation and Uncertainty System



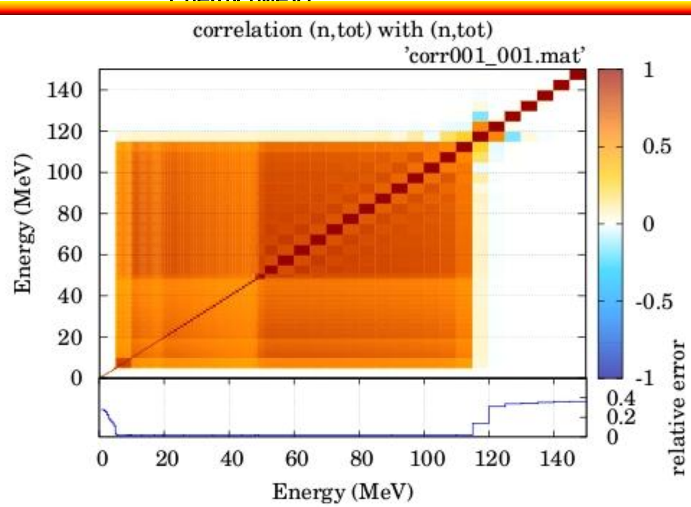
Properties
Predictive Power of the Full Bayesian Technique

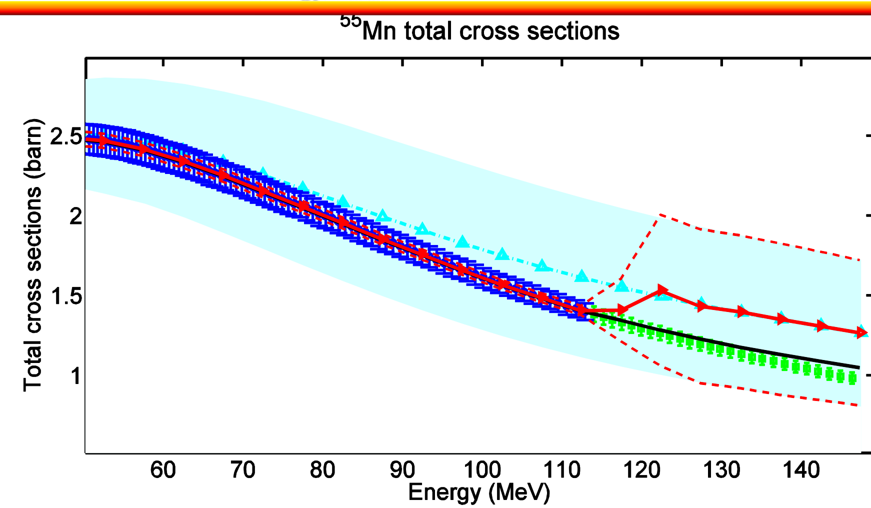




Eval. with full prior

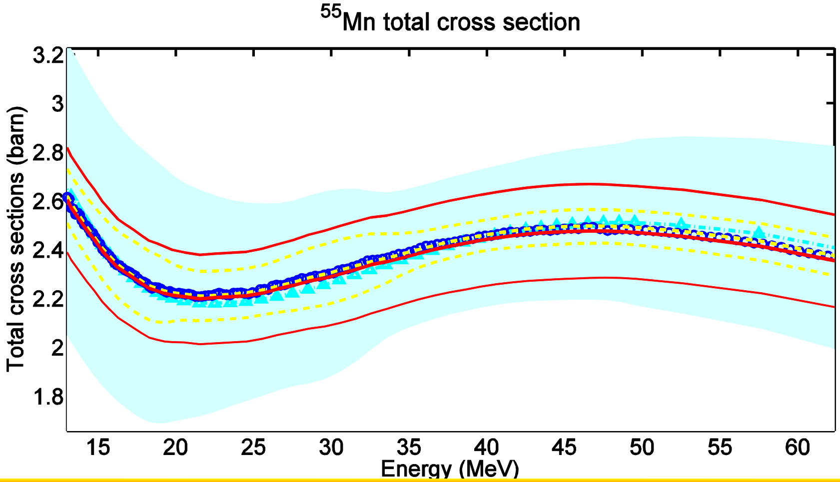
Eval. with diagonal prior



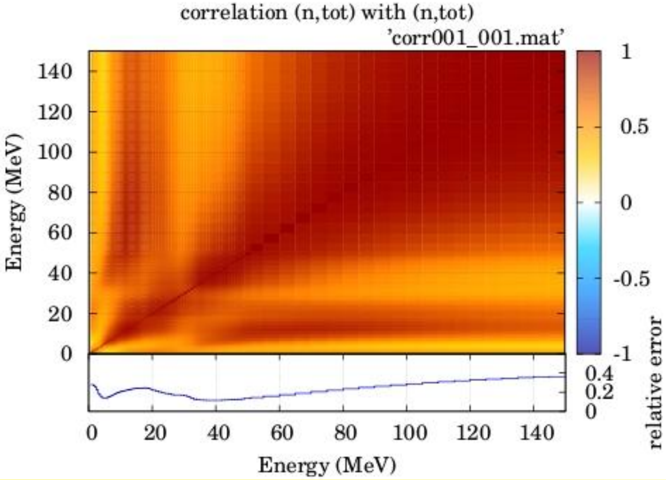


Properties

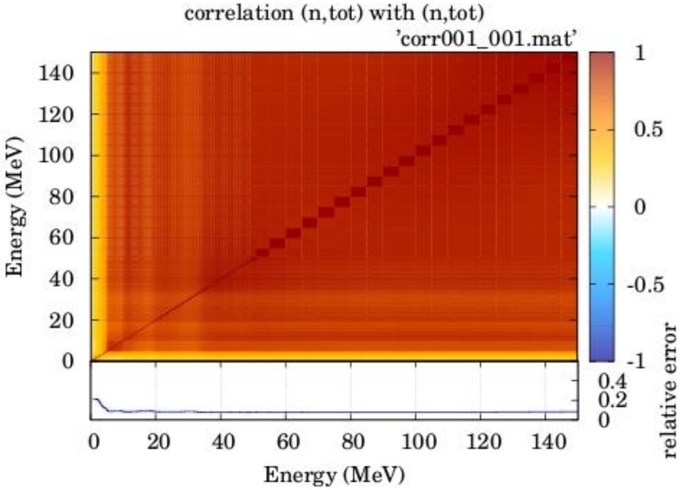
Impact of experimental uncertainties



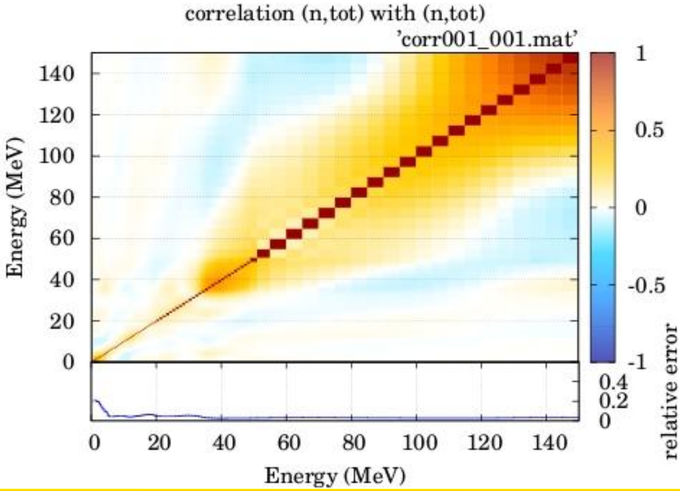
Cross sections



Prior



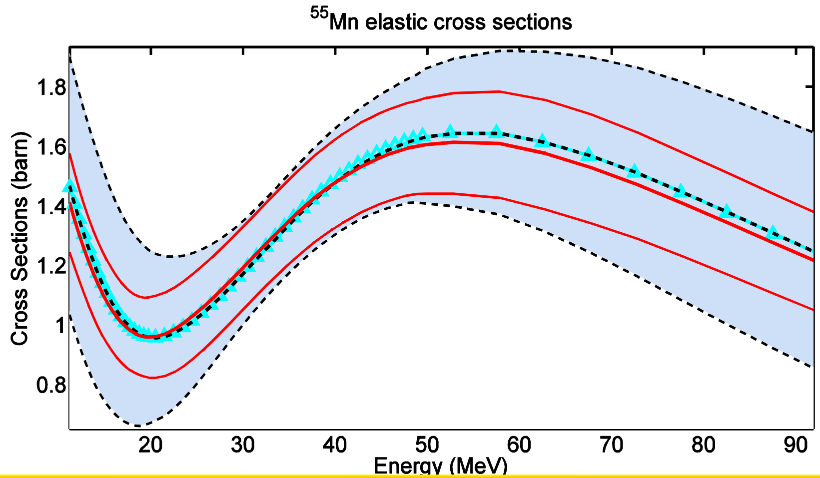
Eval. with full exp. Cov



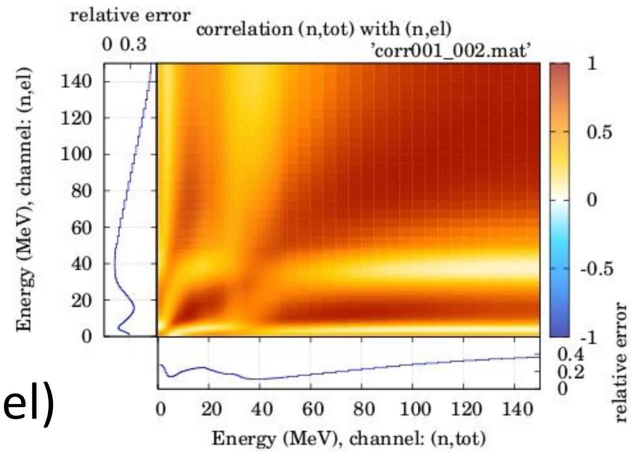
Eval. with diagonal experimental Cov

Properties

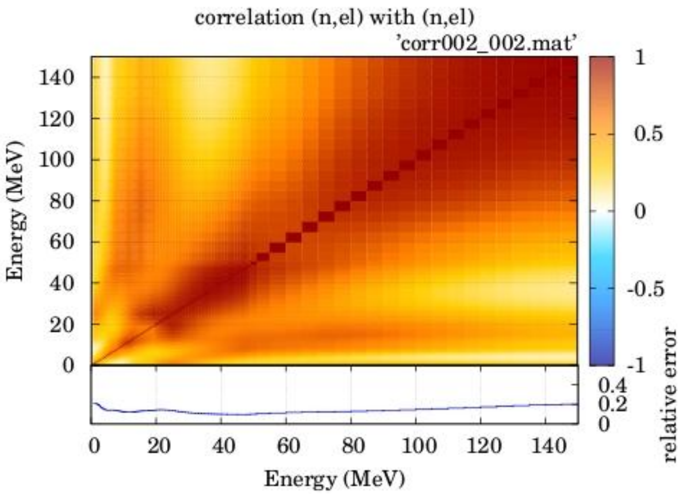
Impact of cross channel correlations



Cross sections

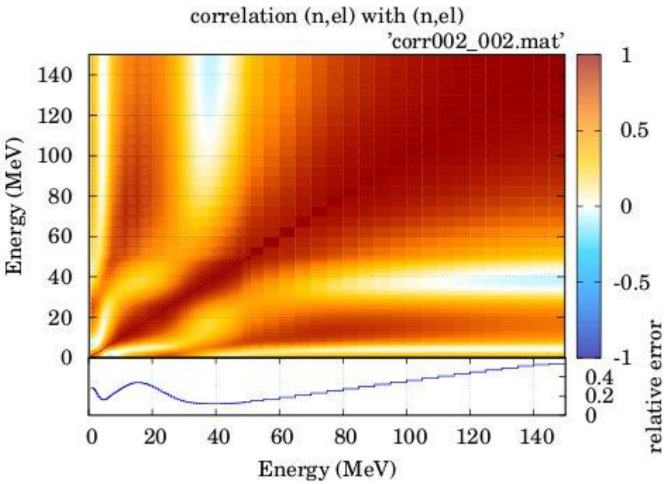


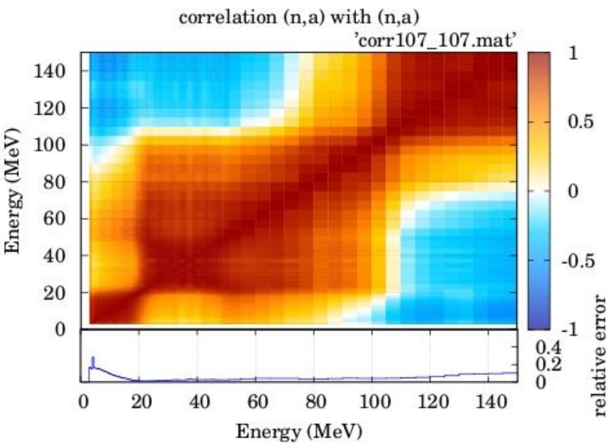
Prior (n,tot;n,el)



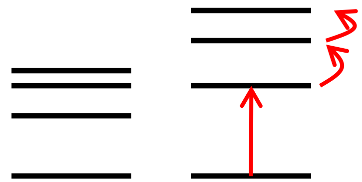
Eval. with full prior

Prior and eval. without prior corr. between channels

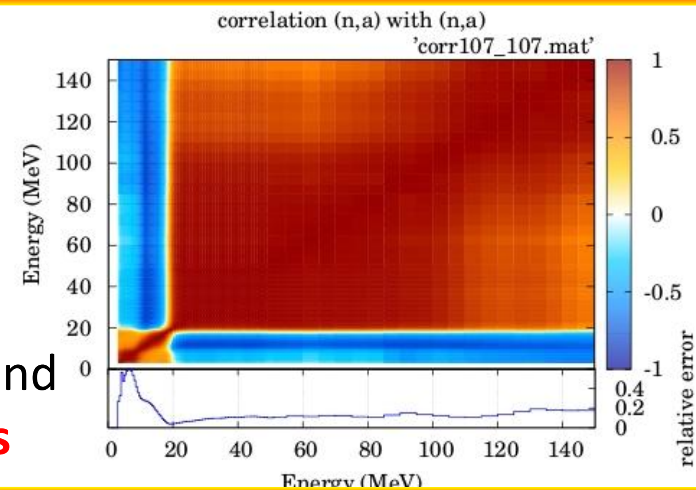




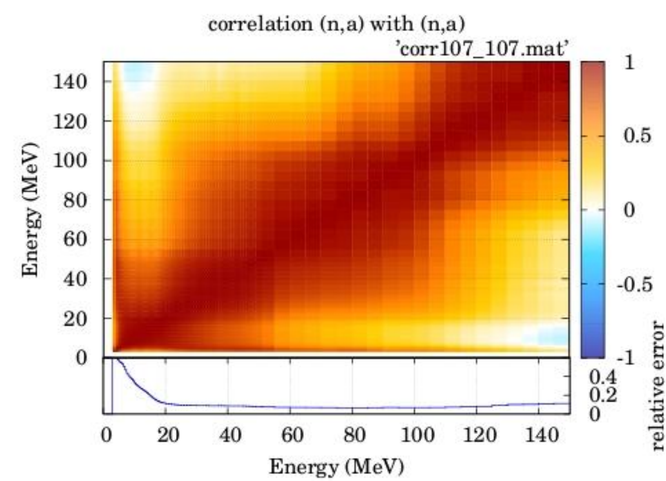
varied n-potential



Varied n-pot and **level densities**



Varied n- and **p-potential**

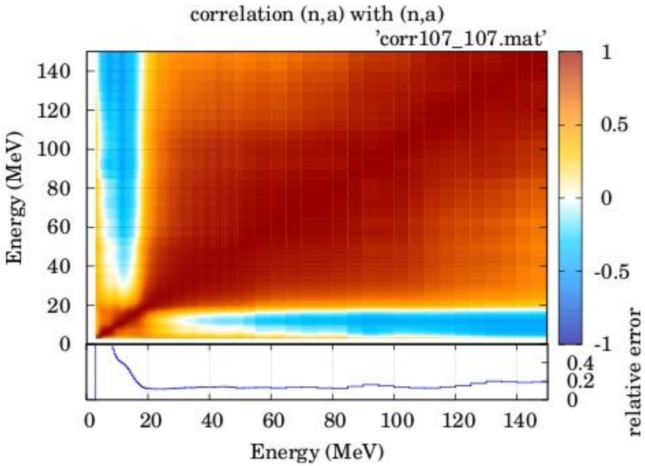


<u>Approximative α-potential of TALYS:</u>

$$V_V{}^{\alpha}(E) = \left(2V_V{}^{n}(E/4) + 2V_V{}^{p}(E/4)\right) v_1{}^{\alpha}$$

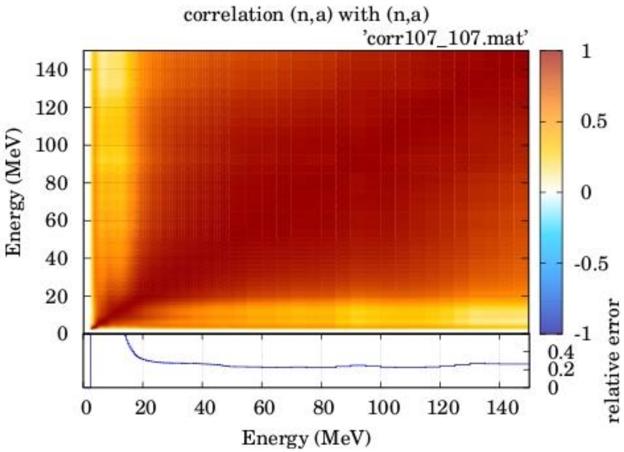
Recent Developments

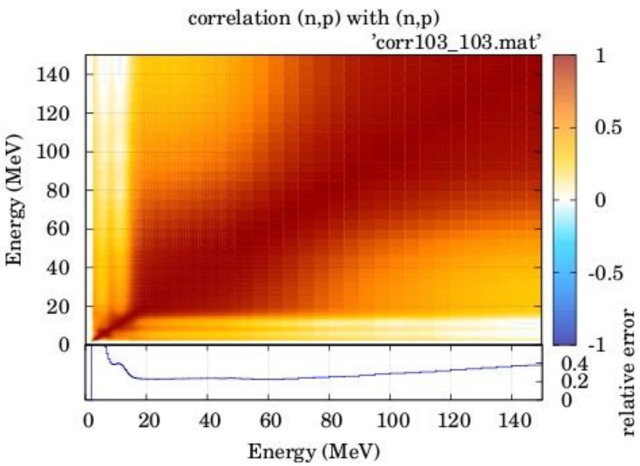
Different contributions to Parameter Uncertainties



varied n-, p-pot. and lev. dens.

Additional variation of α-parameters





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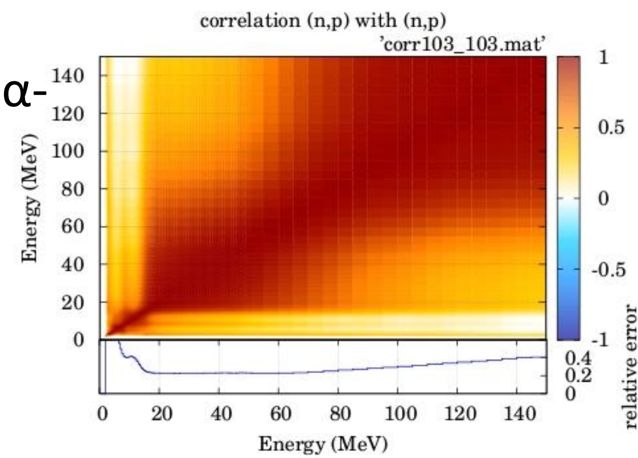
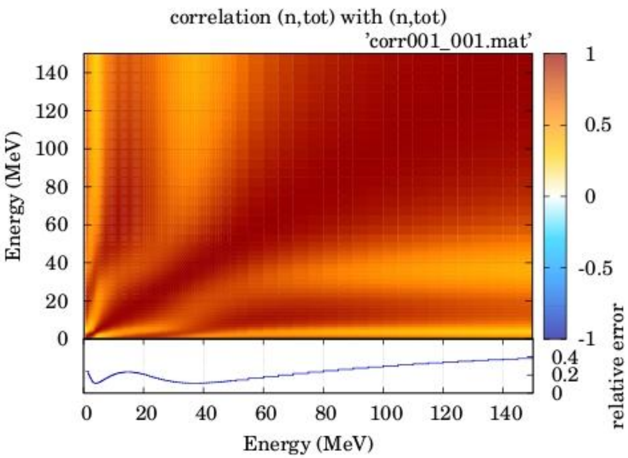
Additional variation of α-parameters



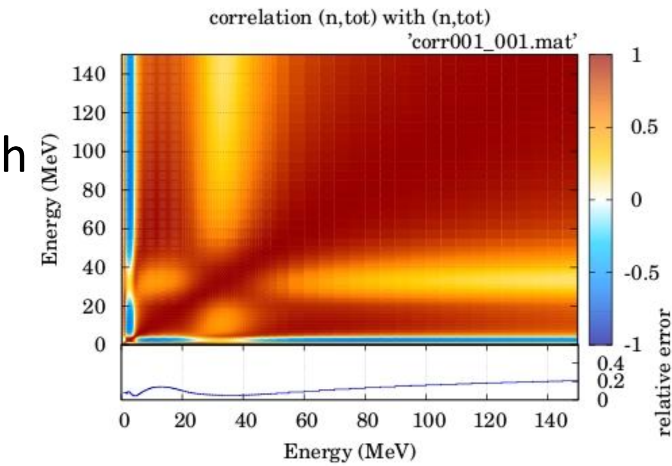
Recent Developments

Distribution fuctions for Parameter Uncertainties



Uniformly distributed parameters.

Uniformly distributed parameters with half of the par. intervals.

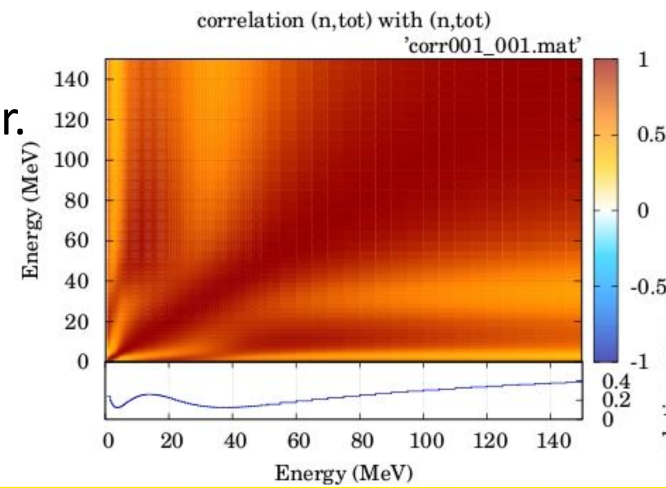


<u>Maximum entropy distribution:</u>

Can be derived by maximizing

$$S = -\int_{\xi_1^<}^{\xi_1^>} d\xi_1 \dots \int_{\xi_k^<}^{\xi_k^>} d\xi_k\, p(\vec{\xi}) \ln\left(\frac{p(\vec{\xi})}{m(\vec{\xi})}\right) - \sum_{l=0}^{K} \lambda_l G_l[p]$$

Maximum entropy distr.



Summary and Outlook

Summary:

- The Full Bayesian Evaluation Technique provides consistent cross sections and uncertainties even beyond the energy range of the actually included experimental data by means of sound prior covariance matrices.
- Experimental uncertainties limit the evaluated ones and have a large impact on the evaluated covariance matrices.
- Considering cross-channel covariance matrices enables experimental data to change cross sections and covariance matrices of different reaction channels.

Outlook:

- Inclusion of fission channel.
- Treatment of differential data.

The GENEUS-team

Gundacker Stefan

Model Defects

Leeb Helmut

Parameter Unc.

Neudecker Denise

Experiment Est.
Bayesian Updat.

Srdinko Thomas

Parallelization
(for Par. Unc.)

Wildpaner Volker

ENDF-Output

Thank you for your attention!