Formulation of Model Defects Suitable for the Resonance Regime

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Outline of the Presentation

- Motivation and Scope
- Bayesian Evaluation Technique
- Overview of previous considerations of Model Defects
- Model Defects in the Resonance Regime
- Formulation of a Covariance Matrix for the Model Error
- Summary and Conclusion

Motivation

Why considering model defects?

NO model is perfect!

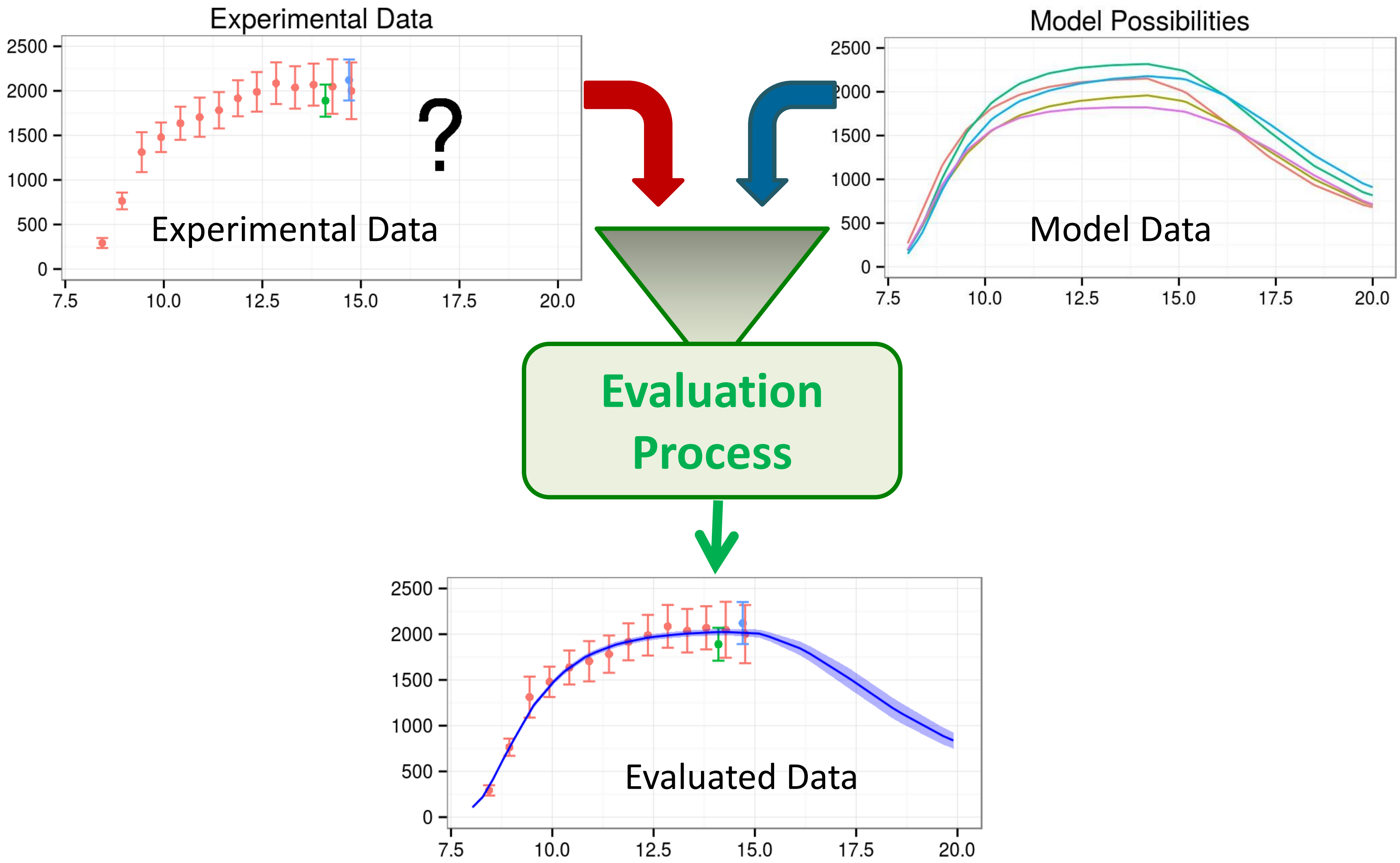
Every model can describe certain apsects of a physical problem, but never the total reality

In nuclear physics:

- Each nucleus consists of nucleons -> Many body problem
- Force between nucleons not exactly known

Up to now there exists no microscopic model that can predict quantitatively resonances in the cross section

Nuclear Data Evaluation



Bayesian Statistics

Bayes Theorem (1761):

$$\pi\left(\vec{p} \mid \vec{\sigma}_{\exp}\right) = \frac{1}{\int d^d p\, \ell\left(\vec{\sigma}_{\exp} \mid \vec{p}\right)\pi\left(\vec{p}\right)}\ \ell\left(\vec{\sigma}_{\exp} \mid \vec{p}\right)\ \pi\left(\vec{p}\right)$$

aposteriori distribution
distribution of parameters taking a-priori and experimental info

Evidence
normalisation

likelihood
Experimental information

apriori distribution
provides the apriori knowledge, e.g. the nuclear model

Evaluation Concept:

Standard Bayesian Evalution Techinque

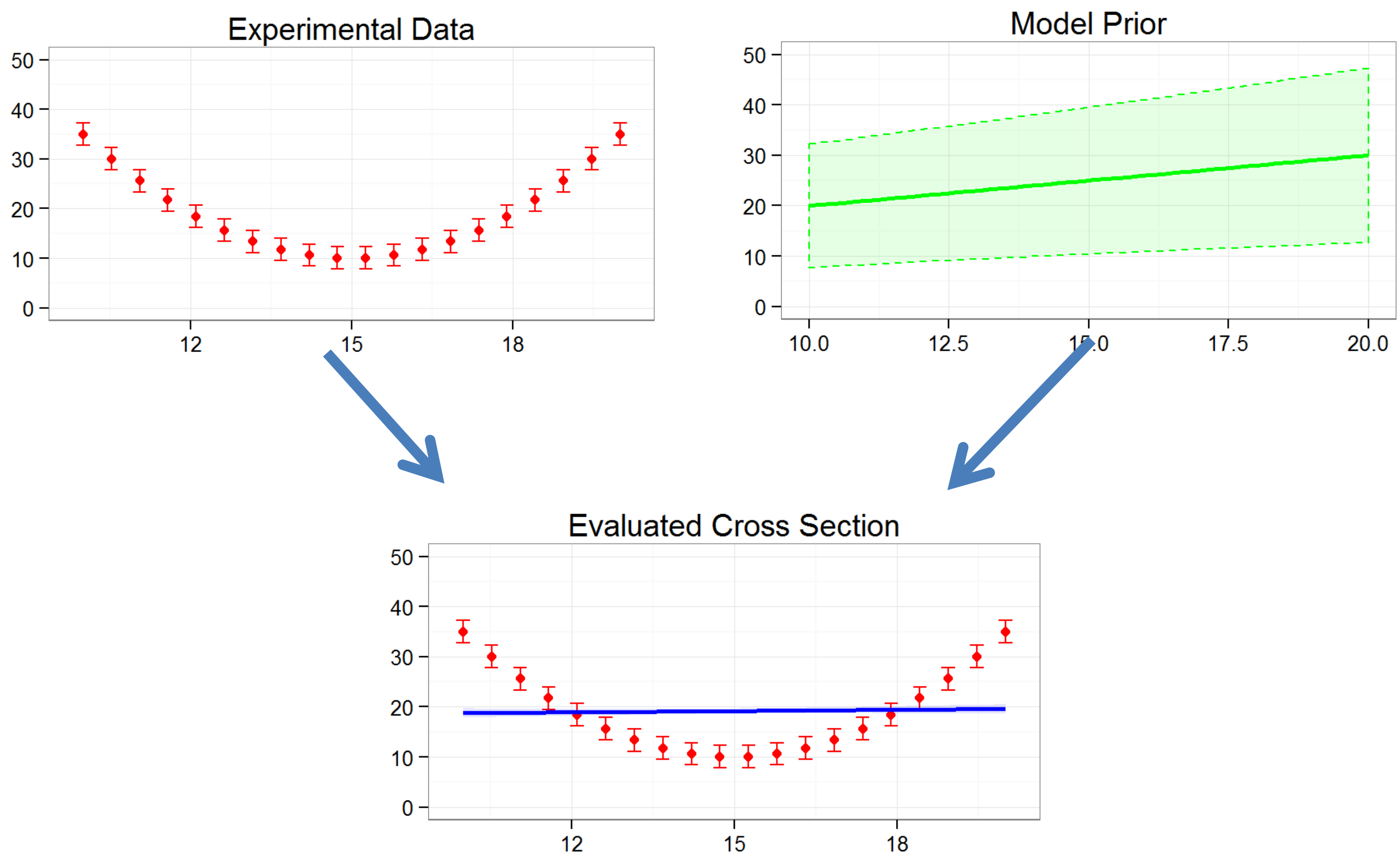
Standard Evaluation:

$$\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$$

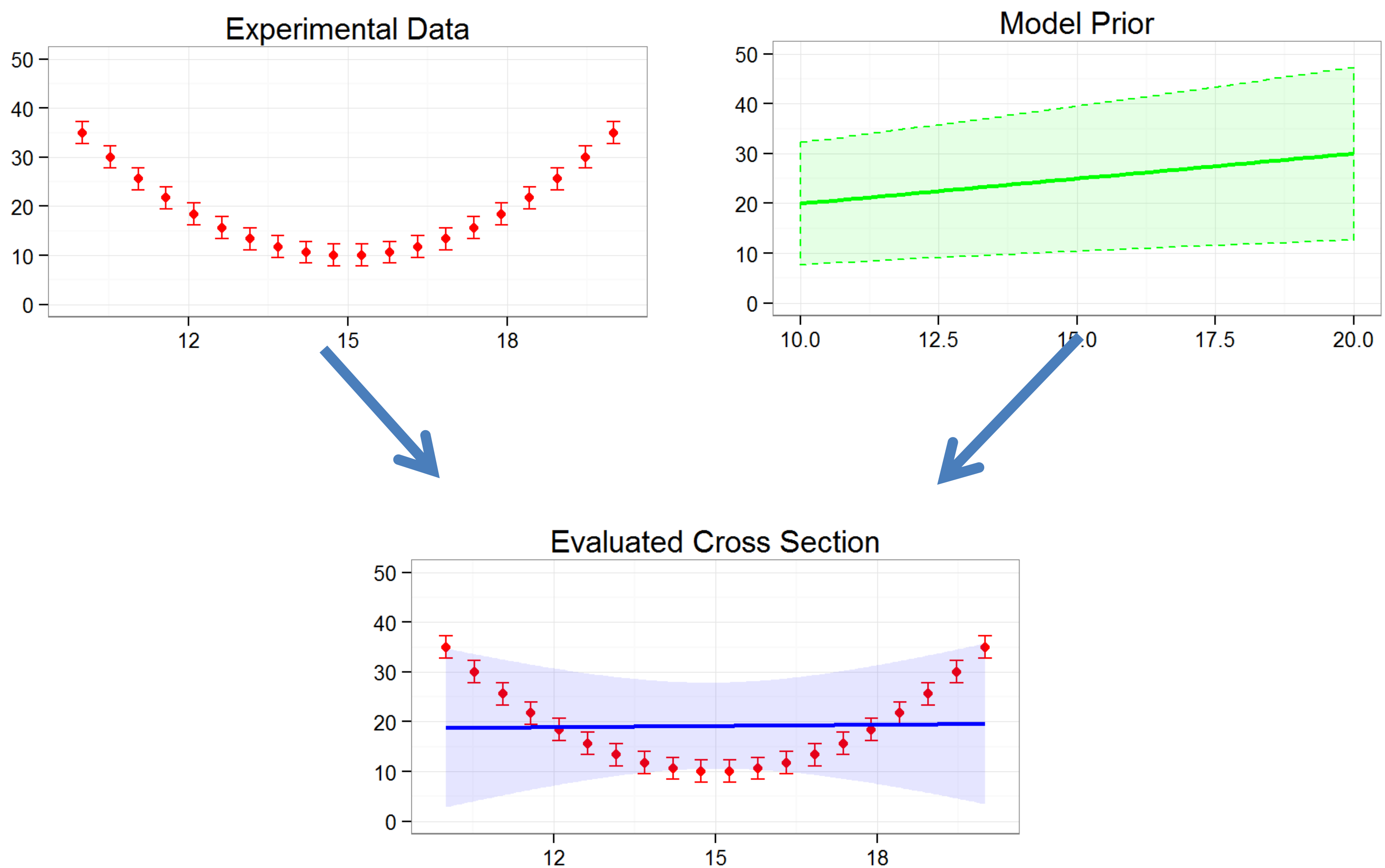
Experiment vector Model vector Uncertainty vector of experiment

Assumption: Model is perfect!

A simple example:
Evaluation without model defects…



…and with model defects



Evaluation Concept:

Statistically consistent Treatment of Model Defects

Standard Evaluation:

$$\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$$

Experiment vector   Model vector   Uncertainty vector of experiment

$$\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$$

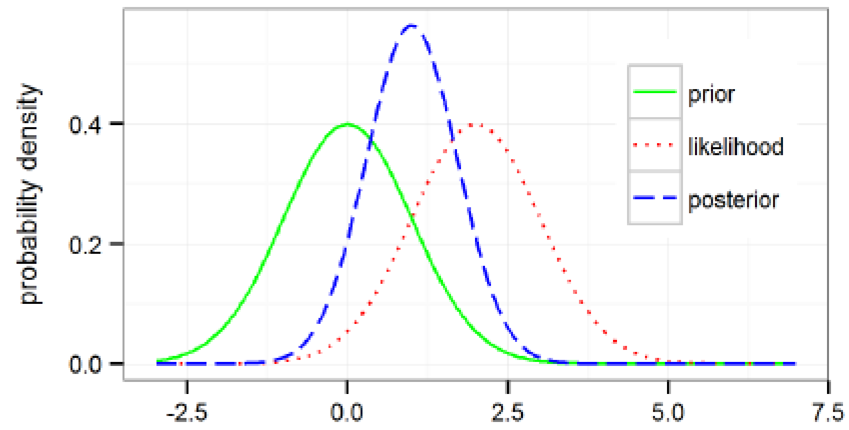
Extended Evaluation: Model defect

PhD thesis of Georg Schnabel (TU Wien, June 2015)

Normal Distributions

$$\rho(t)=\frac{1}{\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(t-\langle t\rangle\right)^2\right]$$

$\langle t\rangle$ mean value of the distribution



Generalisation: Multivariate normal distribution

$$\rho(\vec{t})=\frac{1}{\sqrt{(2\pi)^d\|\mathbf{V}\|}}\exp\left[-\frac{1}{2}\left(\vec{t}-\langle\vec{t}\rangle\right)^T\mathbf{V}^{-1}\left(\vec{t}-\langle\vec{t}\rangle\right)\right] \Rightarrow \begin{array}{l}\vec{t}\sim N\left(\langle t\rangle,\mathbf{V}\right)\\ p(t)\approx N\left(\langle t\rangle,\mathbf{V}\right)\end{array}$$

mean value $\langle t_i\rangle=\int dt_1\cdots\int dt_d\ \rho(\vec{t})\left(t_i-\langle t_i\rangle\right)$

covariance matrix $\mathbf{V}=\left(V_{i,j}\right)=\left(\int dt_1\cdots\int dt_d\ \rho(\vec{t})\left(t_i-\langle t_i\rangle\right)\left(t_j-\langle t_j\rangle\right)\right)$

Multivariate Distributions and Bayesian Evaluation

Basic Assumptions:

$$\vec{\varepsilon}_{\exp} \sim N(0, \mathbf{B})$$

$$\ell(\vec{\sigma}_{\exp} \mid \vec{p}) \sim N(M(\vec{p}), \mathbf{B})$$

$$\pi(\vec{p}) \sim N(\vec{p}_0, \mathbf{A}_0)$$

Multivariate normal distributions for experimental uncertainties, model parameters likelihood assumed

Bayesian Theorem

$$\log \pi(\vec{p} \mid \vec{\sigma}_{\exp}) = \log C + \log \ell(\vec{\sigma}_{\exp} \mid \vec{p}) + \log \pi(\vec{p})$$

$$= \log C - \frac{1}{2}(\vec{\sigma}_{\exp} - M(\vec{p}))^T \mathbf{B}^{-1}(\vec{\sigma}_{\exp} - M(\vec{p}))$$

$$- \frac{1}{2}(\vec{p} - \vec{p}_0)^T \mathbf{A}_0^{-1}(\vec{p} - \vec{p}_0)$$

Bayesian Update including model defects

Basic Assumptions:

$$\vec{\varepsilon}_{\text{exp}} \sim N\left(0, \mathbf{B}\right)$$

$$\ell\left(\vec{\sigma}_{\text{exp}} \mid \vec{p}, \vec{\varepsilon}_{\text{mod}}\right) \sim N\left(M\left(\vec{p}\right) + \vec{\varepsilon}_{\text{mod}}, \mathbf{B}\right)$$

$$\pi\left(\vec{p}\right) \sim N\left(\vec{p}_0, \mathbf{A}_0\right), \quad \pi\left(\vec{\varepsilon}_{\text{mod}}\right) = N\left(\vec{0}, \mathbf{K}_0\right)$$

normal distributions for experimental uncertainties, model parameters likelihood assumed

a-priori independence of model parameters and model deficiency assumed

$$\log\ \pi\left(\vec{p}\vec{\varepsilon}_{\text{mod}} \mid \vec{\sigma}_{\text{exp}}\right) = \log\ \tilde{C} + \log\ \ell\left(\vec{\sigma}_{\text{exp}} \mid \vec{p}\vec{\varepsilon}_{\text{mod}}\right) + \log\ \pi\left(\vec{p}\right) + \log\ \pi\left(\vec{\varepsilon}_{\text{mod}}\right)$$

$$= \log\ \tilde{C} - \frac{1}{2}\left(\vec{\sigma}_{\text{exp}} - M\left(\vec{p}\right) - \vec{\varepsilon}_{\text{mod}}\right)^T \mathbf{B}^{-1}\left(\vec{\sigma}_{\text{exp}} - M\left(\vec{p}\right) - \vec{\varepsilon}_{\text{mod}}\right)$$

$$-\frac{1}{2}\left(\vec{p} - \vec{p}_0\right)^T \mathbf{A}_0^{-1}\left(\vec{p} - \vec{p}_0\right)$$

$$-\frac{1}{2}\left(\vec{\varepsilon}_{\text{mod}}\right)^T \mathbf{K}_0^{-1}\left(\vec{\varepsilon}_{\text{mod}}\right)$$

Surrogate Model: Mapping of Integrated Data

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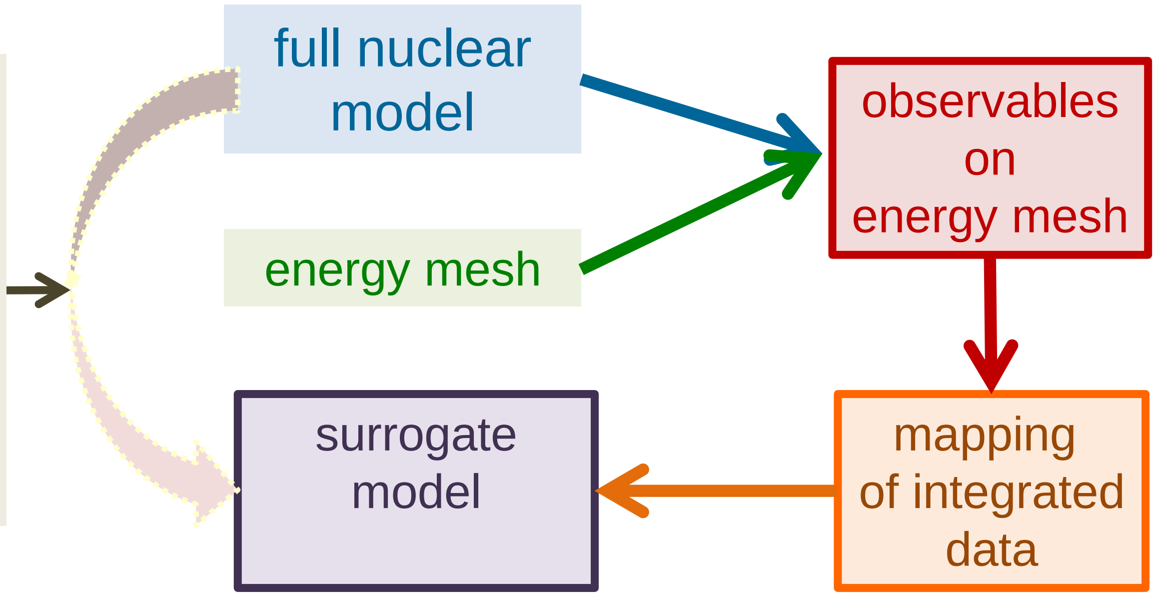
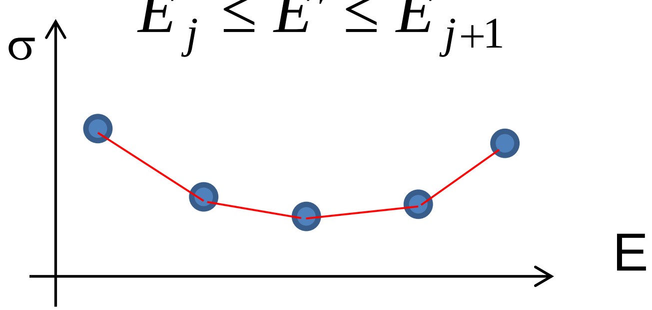
Main properties of nuclear model are transferred
- dominating eigenvalues
- summation properties



Linear mapping relation

$$E_j \le E' \le E_{j+1}$$

$$\sigma^{\mathrm{surr}}(E') = \left(\frac{\mathrm{E}_{\mathrm{j+1}} - E'}{\mathrm{E}_{\mathrm{j+1}} - E_j}\right)\sigma_j^{\mathrm{mod}} + \left(\frac{E' - \mathrm{E}_{\mathrm{j}}}{\mathrm{E}_{\mathrm{j+1}} - E_j}\right)\sigma_{j+1}^{\mathrm{mod}}$$



● value of observable at mesh point

— surrogate model

Overview of Model Defect Treatment

Up to now:

- Model defects formulated as Gaussian processes for cross sections smooth in energy

$$\mathbf{K}_0(E_i,E_j)=\sigma_M(E_i)\sigma_M(E_j)\ \delta_1^{\,2}\cdot\exp\left[-\frac{1}{2\lambda_1^{\,2}}\left(E_i-E_j\right)^2\right]$$

- Modell defects of angle-differential cross sections

But: This covariance matrix cannot be applied to the resonance regime

Model Defects in the Resonance Regime

Setup:

- R-matrix example of n-$^{16}_{8}O$ scattering up to 2.5 MeV
- Single channel R-matrix in three partial waves

$$R^{J\pi}(E) = \frac{{\gamma_\lambda}^2}{E_\lambda - E}$$

with parameters

J^π	E_λ [MeV]	γ_λ $[MeV]$
$1/2^+$	0.70	0.20
$3/2^+$	1.20	0.40
$5/2^-$	2.00	0.30

Model Defects in the Resonance Regime

Generation of experimental data

- Applying an energy dependent deviation function to calculated data

$$d(E) = \alpha_d \cdot \frac{d\sigma_{calc}(E)}{dE}(E)$$

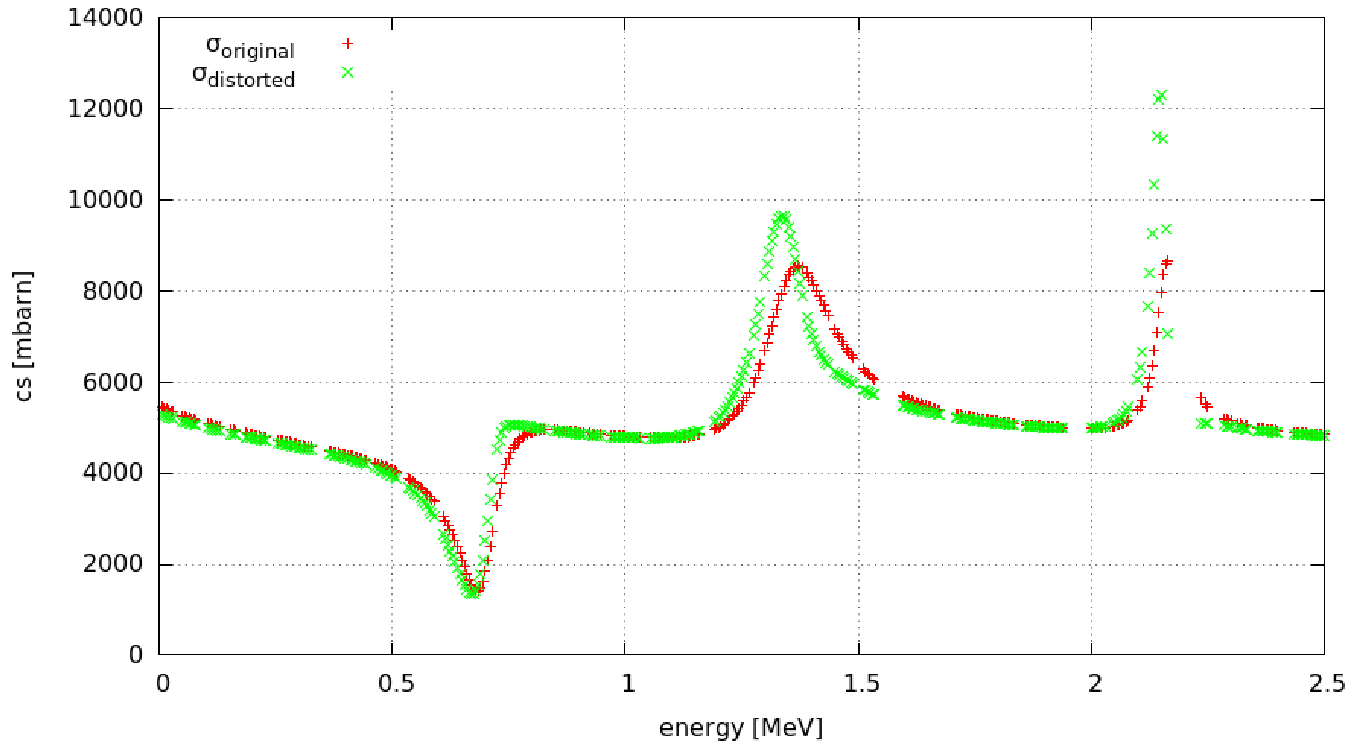
- Experimental data are given by

$$\sigma_{\exp}(E) = [1 + d(E)]\sigma_{calc}(E)$$

on a grid of M energy points $(E_1, E_2, \dots, E_M)$.

Model Defects in the Resonance Regime

Comparison of calculated data and experimental data with $\alpha_d = 7\times 10^{-6}$



Model Defects in the Resonance Regime

- The experimental data are fitted to get a best model parameter set

J^{π}	E_{λ} [MeV]	γ [MeV]
$1/2^{+}$	0.686997	0.202074
$3/2^{+}$	1.171064	0.383547
$5/2^{-}$	1.933526	0.338253

- From these parameters σ_M(E) is calculated on a N-point energy mesh, which contains the experimental grid as a subset

Model Defects in the Resonance Regime

Calculation of the Prior

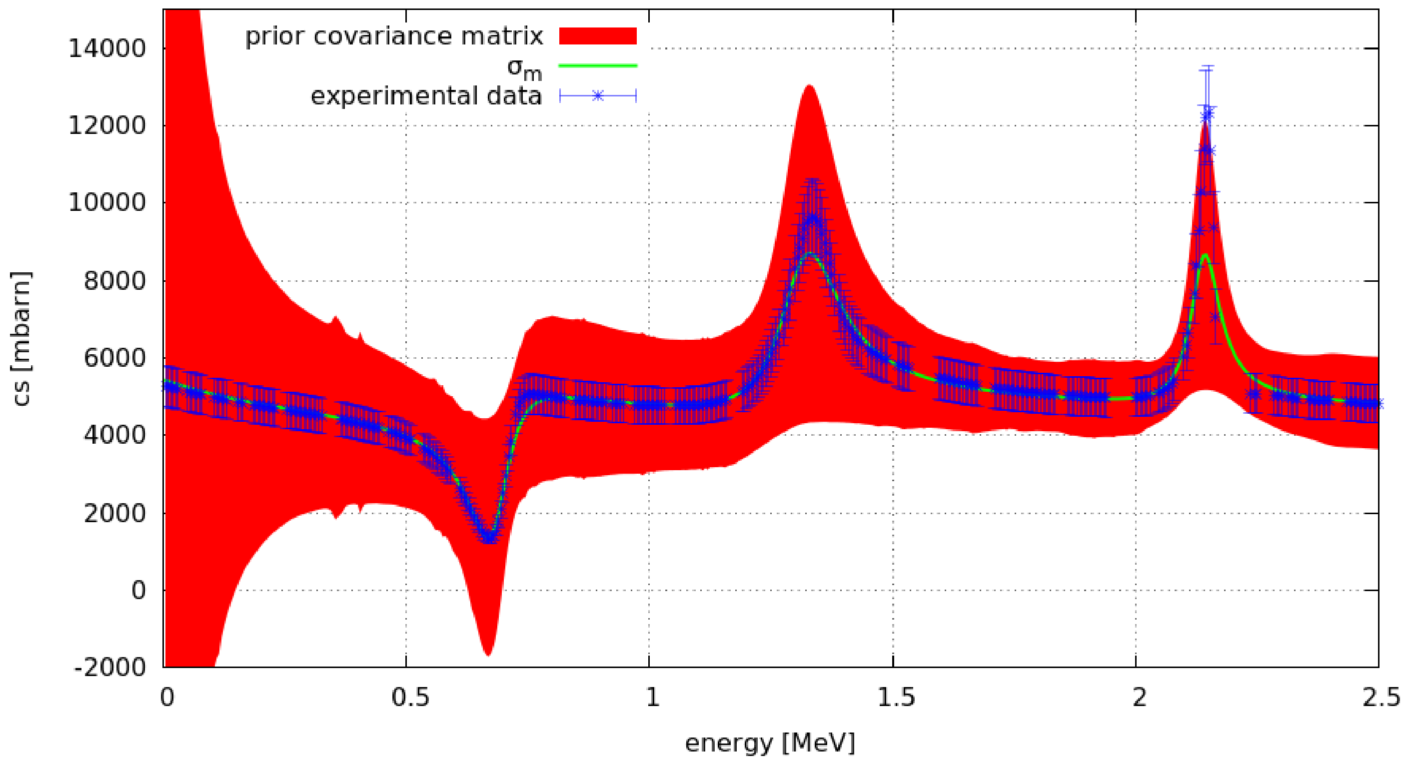
- The six best paramerters $(E_1, \gamma_1, E_2, \gamma_2, E_3, \gamma_3)$ are varied n=200 times according to a normal distribution with $\sigma = 0{,}1$
- With each parameter set, a vector $\vec{x}_k$ with k=1,…,n is calculated
- The prior covarinace matrix is given by

$$\mathbf{A}_0 = \frac{1}{N}\mathbf{U}\mathbf{U}^T$$

with $\mathbf{U} = \left(\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_N\right)$ and $\vec{u}_k = \vec{x}_k - \vec{\sigma}_M$

Model Defects in the Resonance Regime

Best parameter cross section with Prior A_0



All experimental points are contained in error band $\sqrt{A_0(E_i,E_i)}$

Model Defects in the Resonance Regime

Prior covariance matrix of experimental data

- For the experimental data we assume a statistical errror ε_S=0.1 and a normalisation error ε_N=0.05

$$\sigma_{\exp}(E_i) = (1+\varepsilon_N)\sigma_i^{\exp} N(1,\varepsilon_s)$$

with the normal distribution $N(1,\varepsilon_s)$

- This leads to a prior covariance matrix

$$\mathbf{B} = \begin{pmatrix} (\sigma_1^{\exp})^2[\varepsilon_s^2+\varepsilon_N^2] & \sigma_1^{\exp}\sigma_2^{\exp}\varepsilon_N^2 & \cdots & \sigma_1^{\exp}\sigma_M^{\exp}\varepsilon_N^2 \\ \sigma_2^{\exp}\sigma_1^{\exp}\varepsilon_N^2 & (\sigma_2^{\exp})^2[\varepsilon_s^2+\varepsilon_N^2] & \cdots & \sigma_2^{\exp}\sigma_M^{\exp}\varepsilon_N^2 \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_M^{\exp}\sigma_1^{\exp}\varepsilon_N^2 & \sigma_M^{\exp}\sigma_2^{\exp}\varepsilon_N^2 & \cdots & (\sigma_M^{\exp})^2[\varepsilon_s^2+\varepsilon_N^2] \end{pmatrix}$$

Model Defects in the Resonance Regime

Including model error

$$\vec{\varepsilon}_{\text{mod}} \sim N\left(\vec{0}, \mathbf{K}_0\right)$$

Covariance matrix for the model error

$$\mathbf{K}_0(E_i, E_j) = \sigma_M(E_i)\sigma_M(E_j)\ \delta_1^{\ 2} \cdot \exp\left[-\frac{1}{2\lambda_1^{\ 2}}\left(E_i - E_j\right)^2\right]$$

$$+\delta_2^{\ 2} \cdot \alpha \frac{d\sigma_M}{dE}(E_i) \cdot \alpha \frac{d\sigma_M}{dE}(E_j) \cdot \exp\left[-\frac{1}{2\lambda_2^{\ 2}}\left(E_i - E_j\right)^2\right]$$

δ_1	δ_2	$\propto$	λ_1	λ_2
0.05	1.5	0.22	0.5	0.1

Linearized Bayesian Update
including model error

Using multivariate normal distributions allows linearization of Bayesian Theorem for update:

$$\vec{\sigma}_1 = \vec{\sigma}_0 + \mathbf{A}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{S}\mathbf{K}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\left(\vec{\sigma}_{\exp} - \mathbf{S}\vec{\sigma}_M\right)$$

$$\vec{\varepsilon}_1 = \mathbf{K}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{S}\mathbf{K}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\left(\vec{\sigma}_{\exp} - \mathbf{S}\vec{\sigma}_M\right)$$

$$\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{S}\mathbf{K}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\mathbf{S}\mathbf{A}_0$$

$$\mathbf{K}_1 = \mathbf{K}_0 - \mathbf{K}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{S}\mathbf{K}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\mathbf{S}\mathbf{K}_0$$

Linearized Bayesian Update
including model error

We get the best estimate for the cross section

$$\vec{\sigma}_{true} = \vec{\sigma}_1 + \vec{\varepsilon}_1$$

and its covariance matrix

$$\mathbf{U}_1 = \mathbf{U}_0 - \mathbf{C}_0 \left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{S}\mathbf{K}_0\mathbf{S}^T + \mathbf{B} \right)^{-1} \mathbf{C}_0{}^T$$

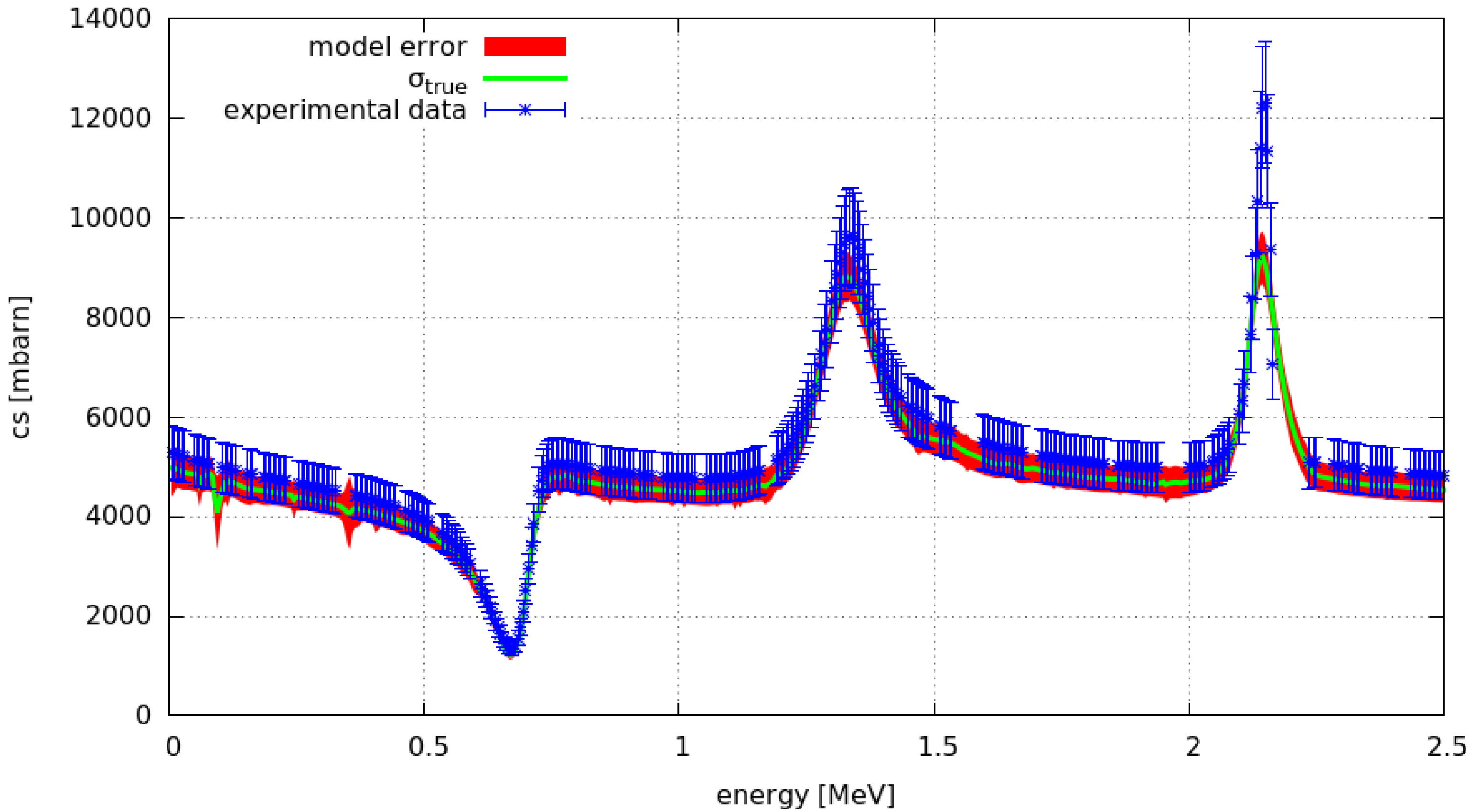
with

$$\mathbf{U}_0 = \mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{K}_0$$

$$\mathbf{C}_0 = \mathbf{A}_0\mathbf{S}^T + \mathbf{K}_0\mathbf{S}^T$$

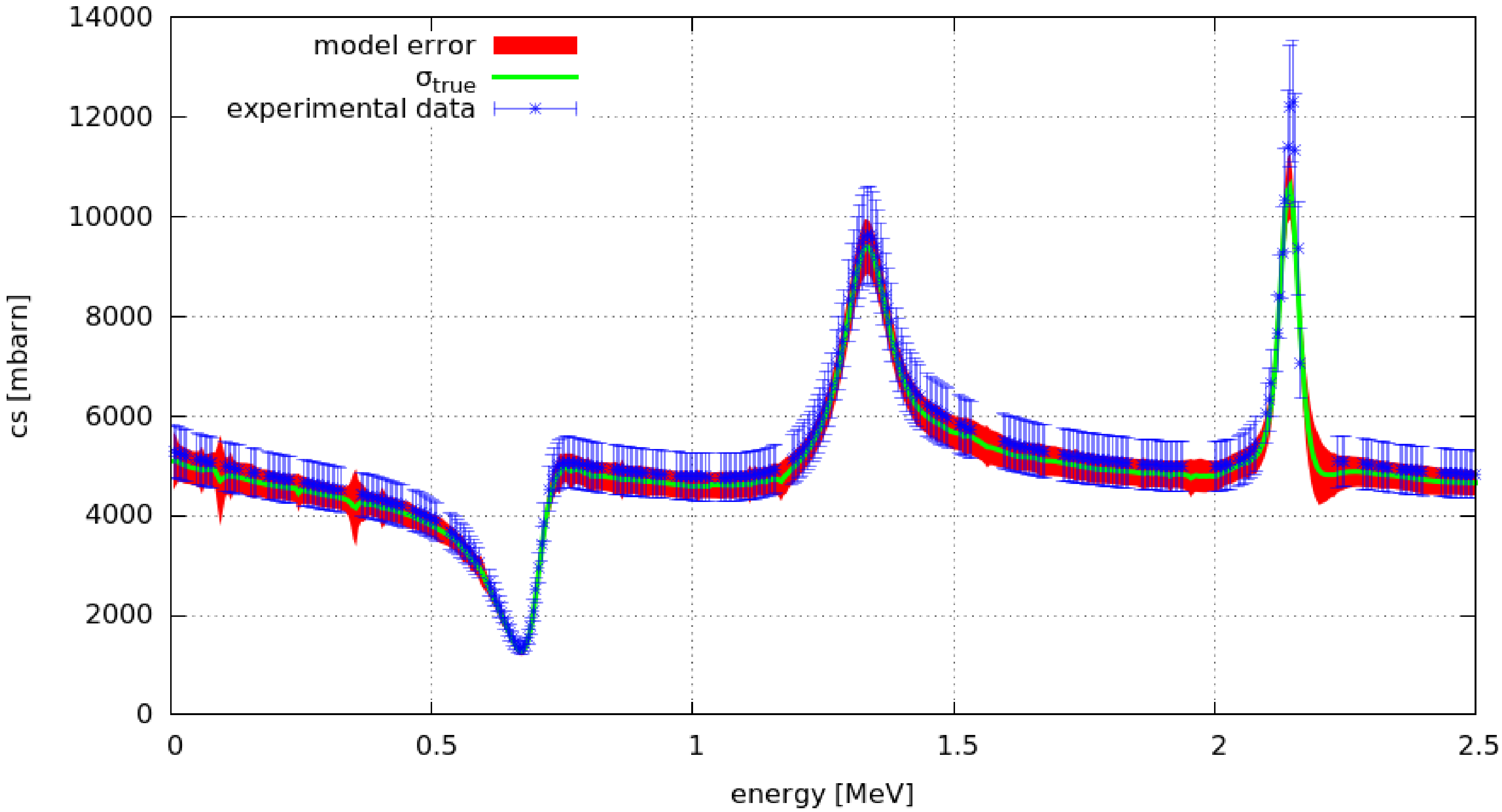
Results

Updated cross section without including model defects



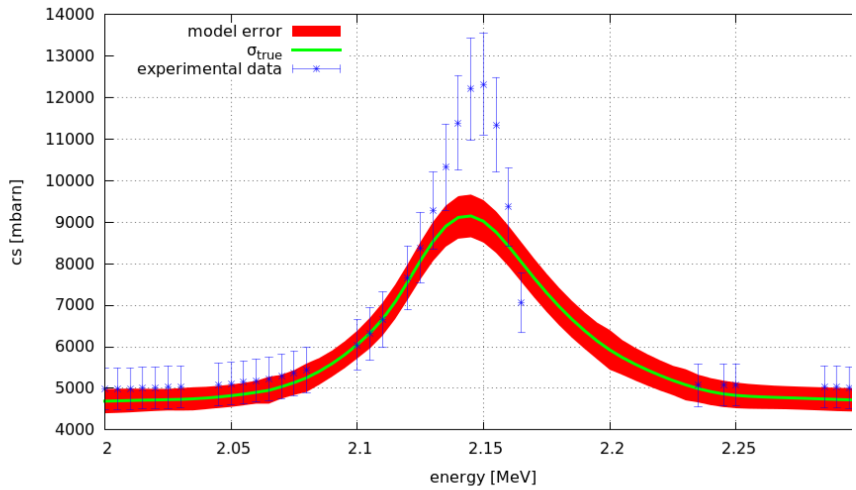
Results

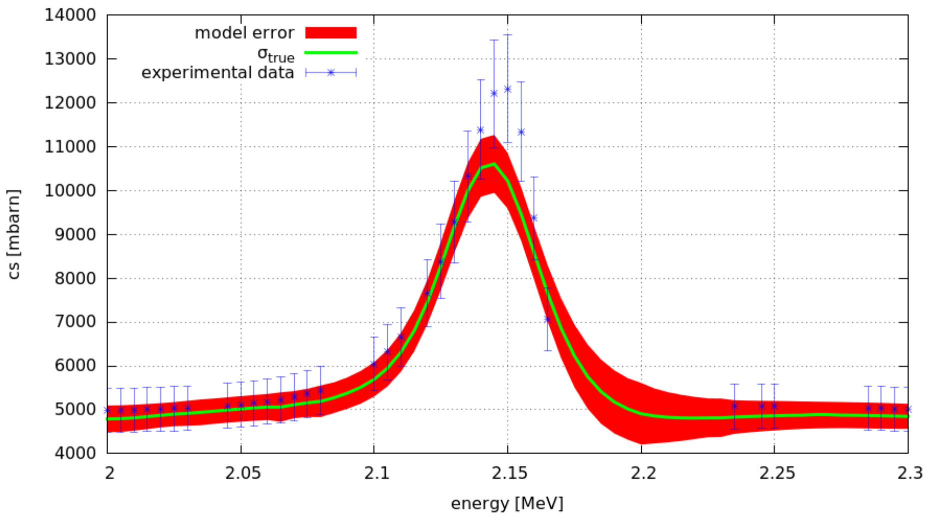
„True“ cross section with model defects



Results

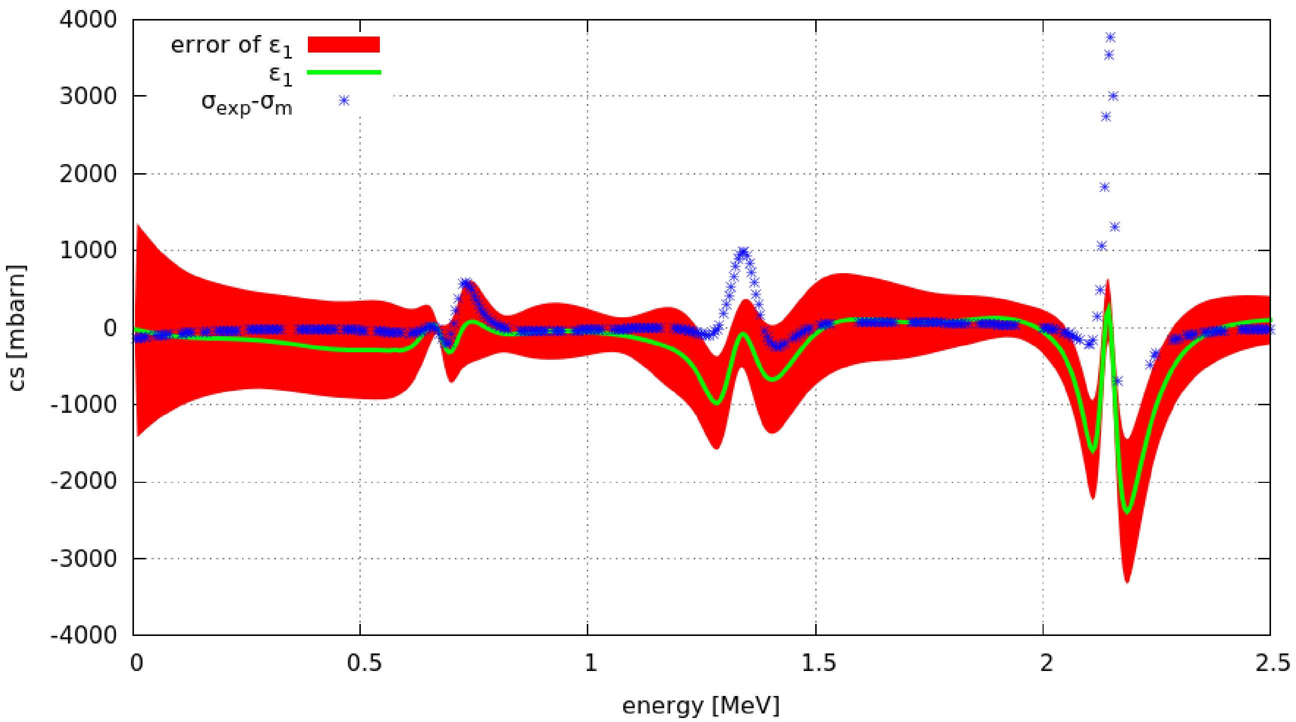
Without model defects - With model defects





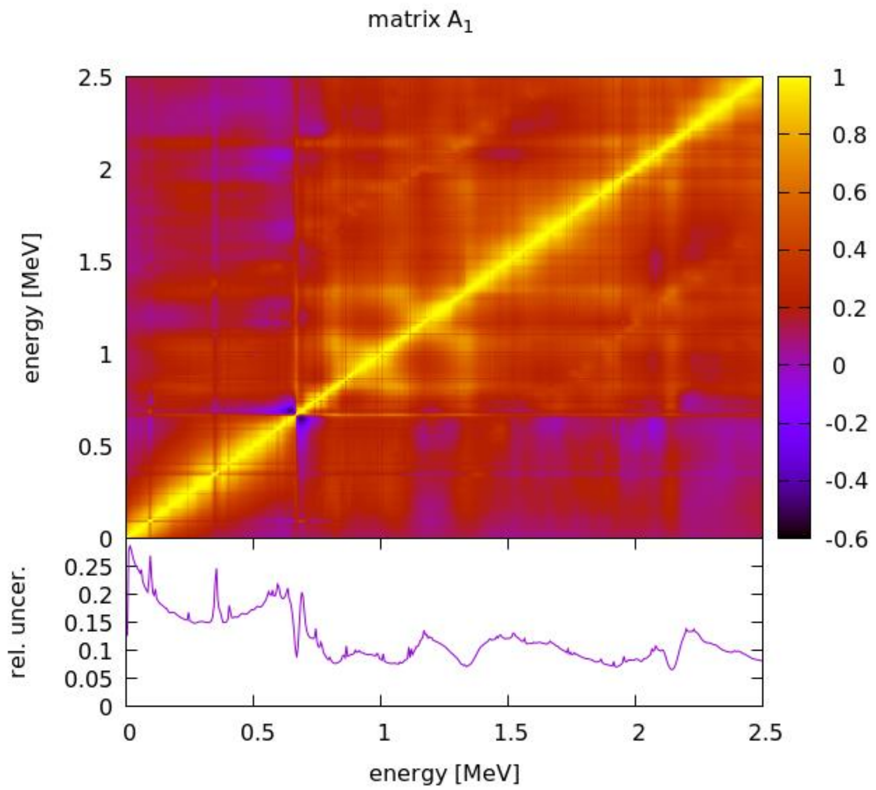
Results

The model error – a comparison

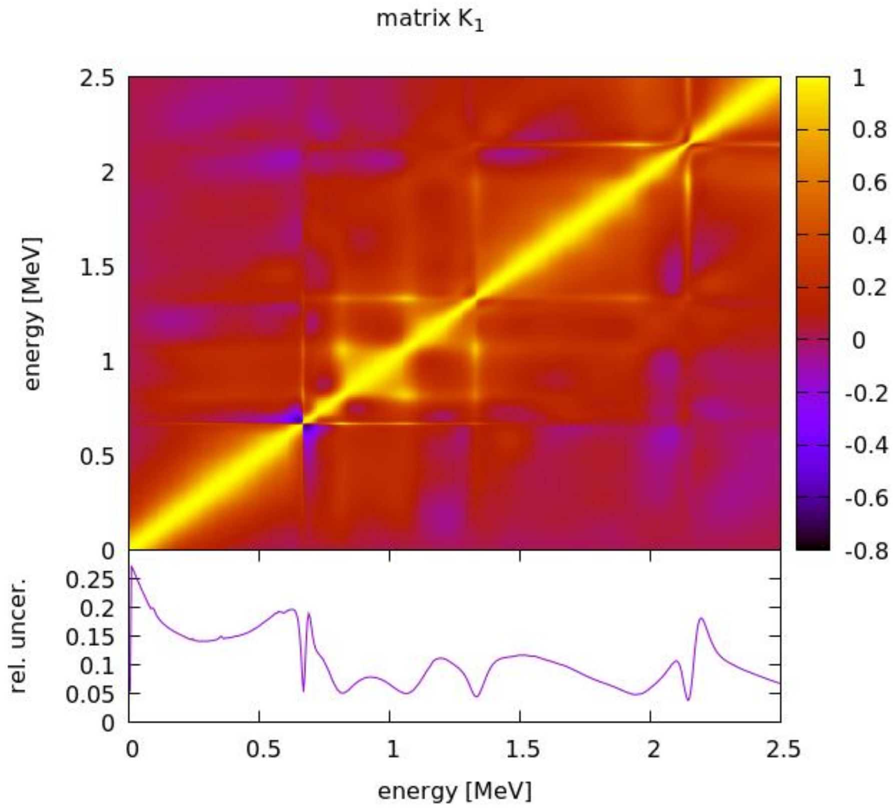


Correlation matrices

$$\mathbf{A}_1(E_i,E_j)/\sqrt{\mathbf{A}_1(E_i,E_i)}$$

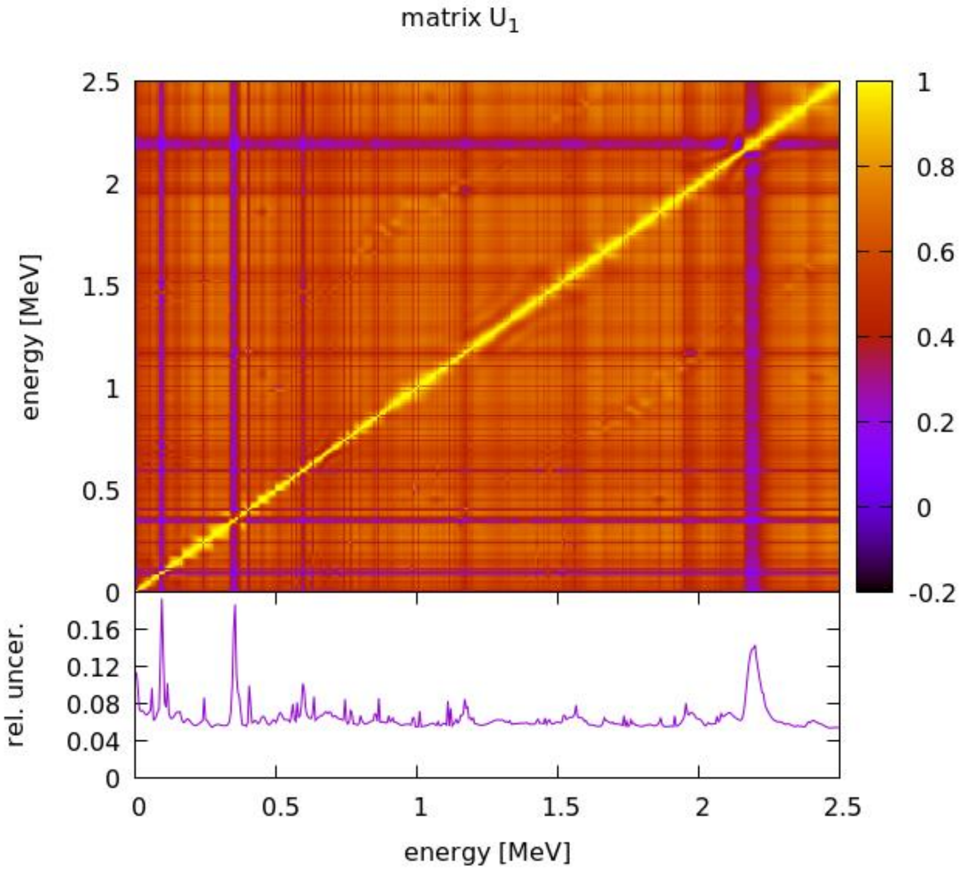


$$\mathbf{K}_1(E_i,E_j)/\sqrt{\mathbf{K}_1(E_i,E_i)}$$



Correlation matrices

$$\mathbf{U}_1(E_i, E_j)/\sqrt{\mathbf{U}_1(E_i, E_i)}$$



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Summary and Conclusions

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- We proposed a prior covariance matrix for the model error in the resonance regime for the first time.
- This is one possible form (but not the only one).
- Makes it possible to perform an evaluation with model defects for the total energy range up to 200 MeV including resonances at lower energies.
- The magnitude of the model error can explicitly be estimated.

Thank you for your attention