UPPSALA UNIVERSITET

Recent ND developments and plans at UU

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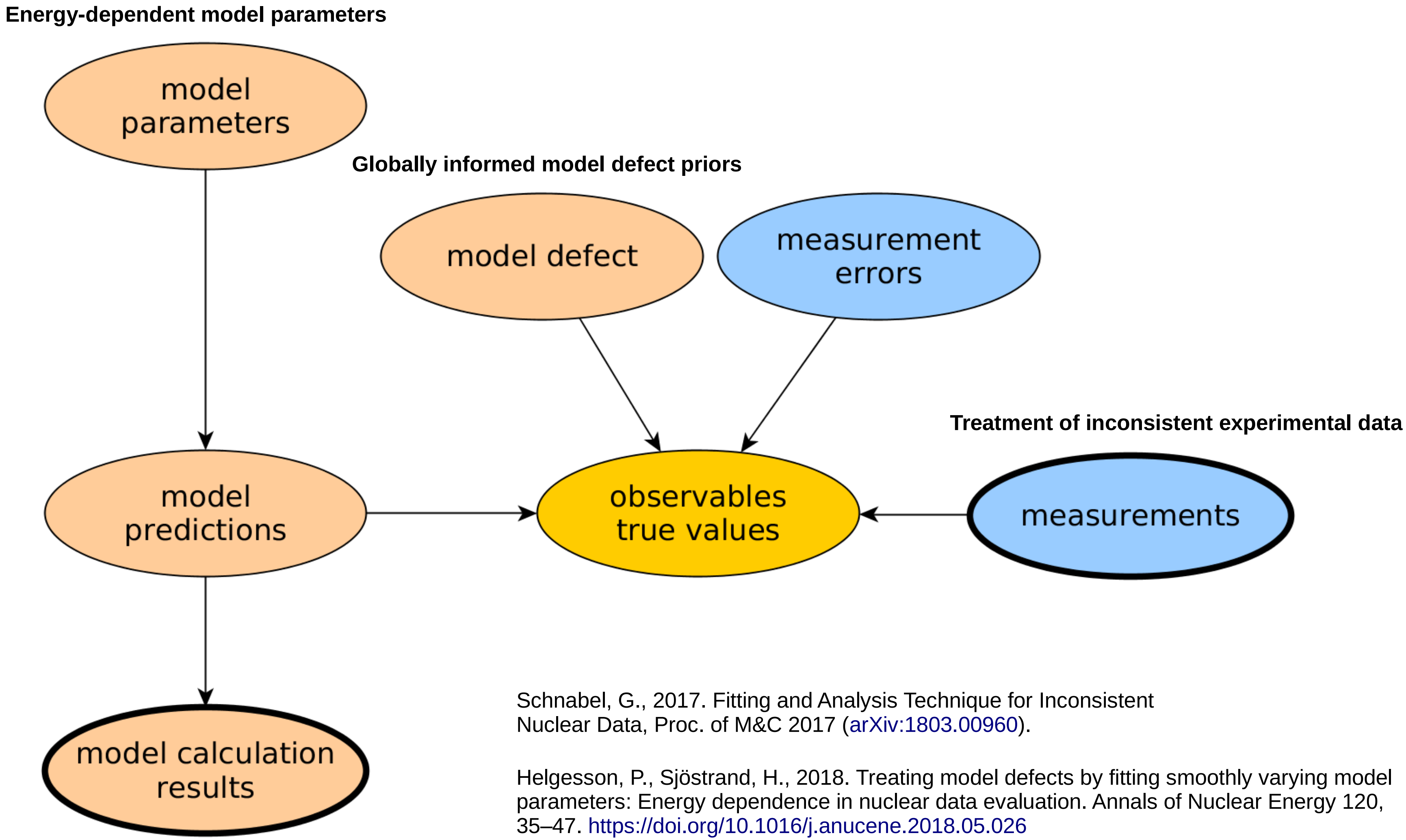
Parameters & Complexity

Outline



Schnabel, G., 2017. Fitting and Analysis Technique for Inconsistent Nuclear Data, Proc. of M&C 2017 (arXiv:1803.00960).

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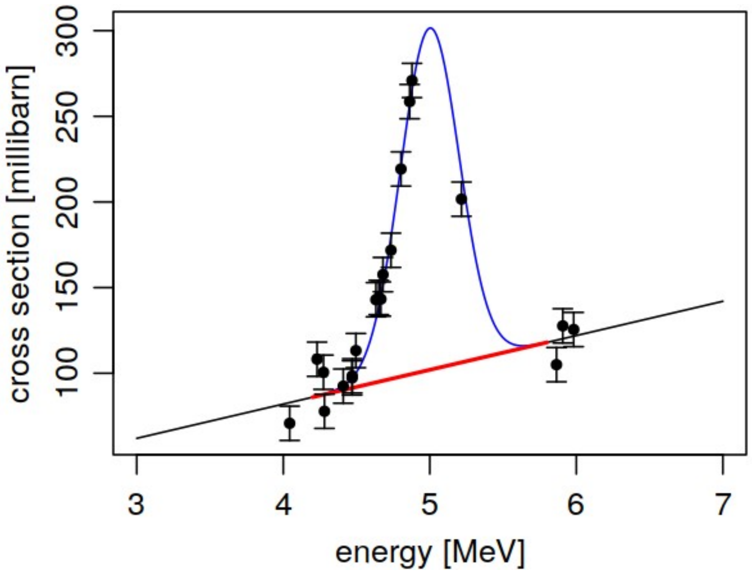
Schnabel, G., Sjöstrand, H., Construction of model defect priors inspired by dynamic time warping, WONDER 2018

Motivation of GP regression



Background + Signal

$$f(E) = a_1 + a_2 E + a_3 \exp\left(-\frac{(\mu - E)^2}{2\sigma^2}\right)$$

More general

$$f(E) = \sum_{k=1}^{\infty} a_k \sin(2\pi c k\, E)$$

Prior / Regularization

$$a_k \sim \mathcal{N}(0, 1/k)$$

Model + Defect

$$f(E) = \mathcal{M}_{\vec{p}}(E) + \delta(E) = \mathcal{M}_{\vec{p}}(E) + \boxed{\sum_{k=1}^{\infty} a_k \sin(2\pi c k\, E)}$$

Gaussian process
- infinite series
- normal prior on coeffs

Covariance matrix

<u>Covariance matrices</u> can represent a variety of things such as normalization uncertainties, linear trends, splines, Fourier series, polynomial expansions, white noise, etc.

$$\boxed{y(x) = kx + d,} \quad k \sim \mathcal{N}(0, \delta_k^2),\ d \sim \mathcal{N}(0, \delta_d^2)$$

$$\text{Observations} \quad (\vec{y}_{\text{exp}}, \vec{x}_{\text{exp}})$$

$$S_{\text{exp}} = \left(\vec{x}_{\text{exp}}, \vec{1}\right)$$

$$\vec{p} = \begin{pmatrix} k \\ d \end{pmatrix} = AS^T \left(SAS^T + B\right)^{-1} \vec{y}_{\text{exp}}$$

$$A = \begin{pmatrix} \delta_k^2 & 0 \\ 0 & \delta_d^2 \end{pmatrix}$$

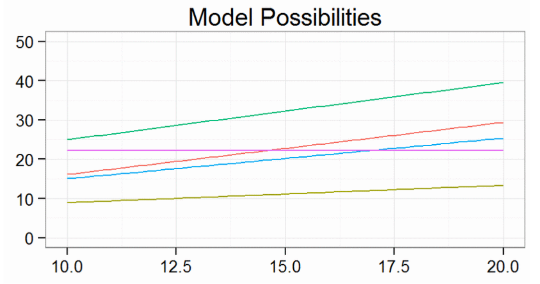
$$\vec{y}_{\text{pred}} = S_{\text{pred}}\vec{p} = \left(\vec{x}_{\text{pred}}, \vec{1}\right) \begin{pmatrix} k \\ d \end{pmatrix}$$

$$B = \begin{pmatrix} \varepsilon_1^2 & 0 & 0 \\ 0 & \varepsilon_2^2 & 0 \\ 0 & 0 & \ddots \end{pmatrix}$$

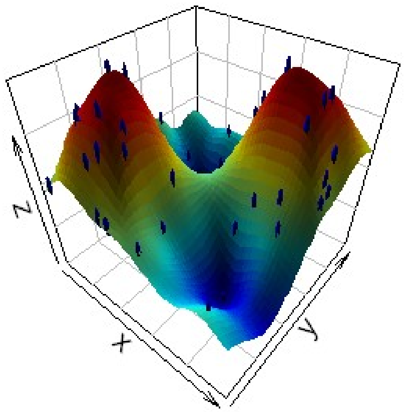
$$\boxed{\kappa(x_1, x_2) := Cov[y(x_1), y(x_2)] = \delta_k^2 x_1 x_2 + \delta_d^2}$$

$$K_{\text{pred,exp}} = \kappa(\vec{x}_{\text{pred}}, \vec{x}_{\text{exp}}) \quad K_{\text{exp,exp}} = \kappa(\vec{x}_{\text{exp}}, \vec{x}_{\text{exp}})$$

$$\vec{y}_{\text{pred}} = K_{\text{pred,exp}} K^{-1}_{\text{exp,exp}} \vec{y}_{\text{exp}}$$



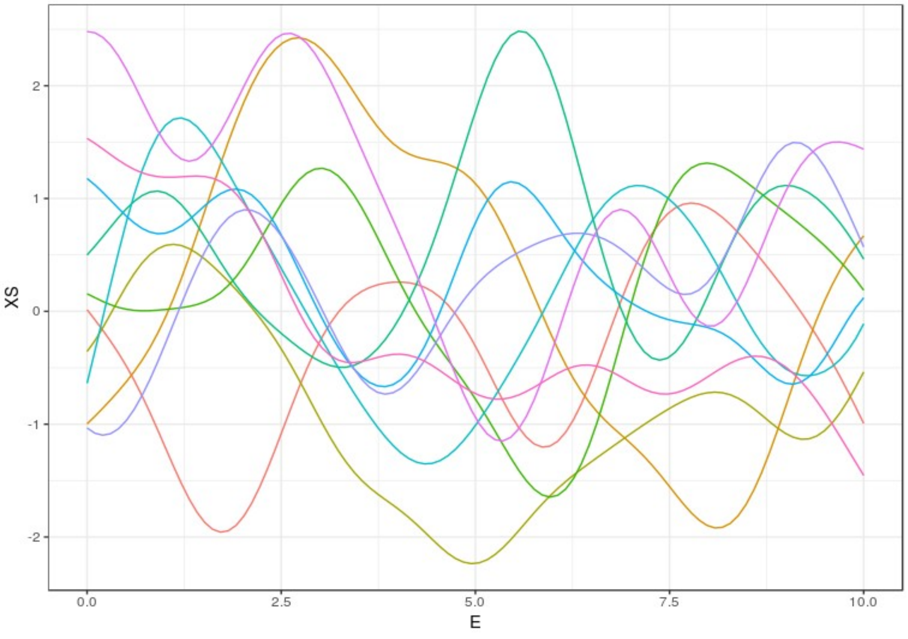
Power of GP



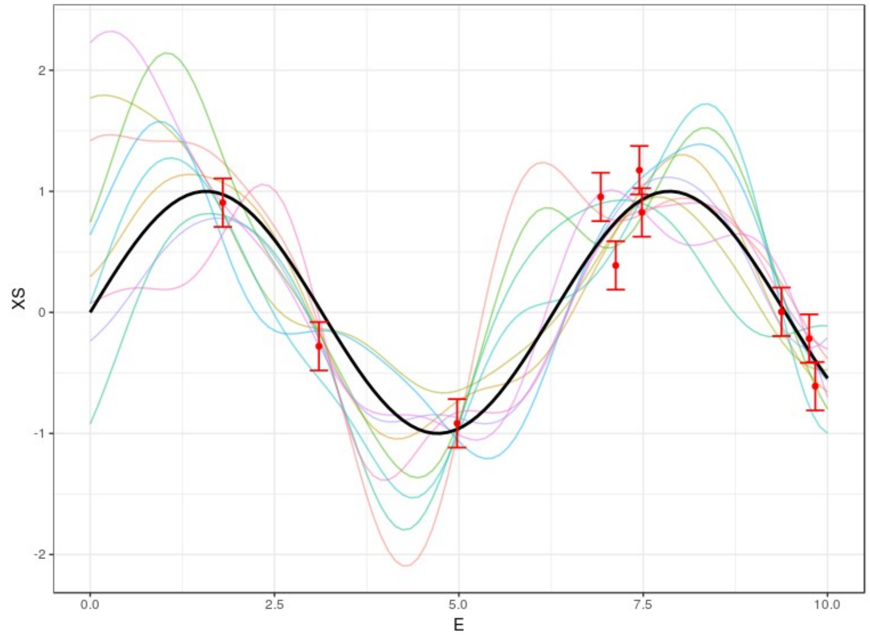
Powerful concept
Directly parametrize covariance matrix and work implicitly with an infinite number of parameters/basis functions!

$$\kappa(\boldsymbol{x}_1, \boldsymbol{x}_2) = \delta^2 \exp\left(-\frac{(\boldsymbol{x}_1 - \boldsymbol{x}_2)^2}{2\lambda^2}\right)$$

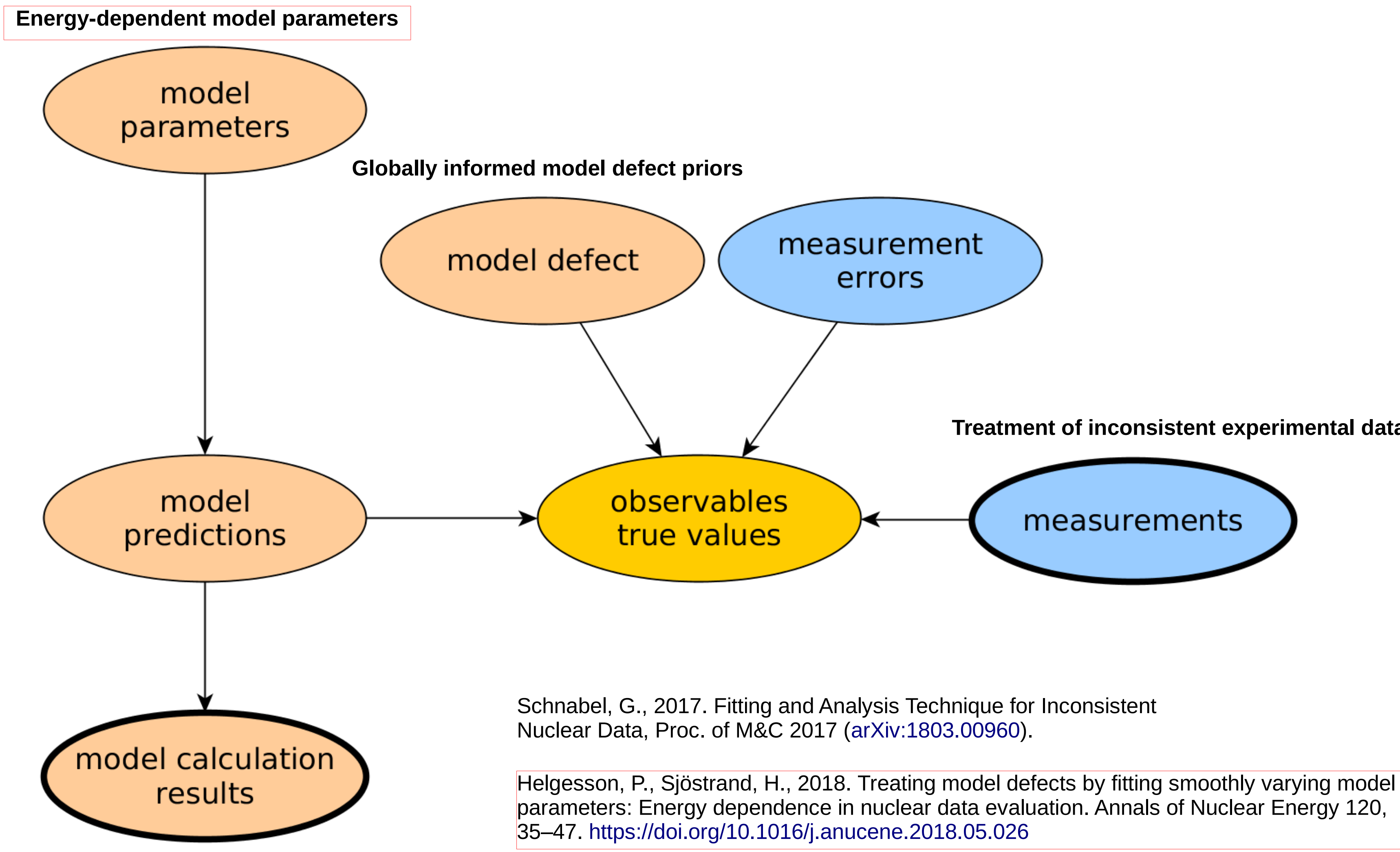
Sample from prior (δ=λ=1)



Sample from posterior



Energy-dependent parameters



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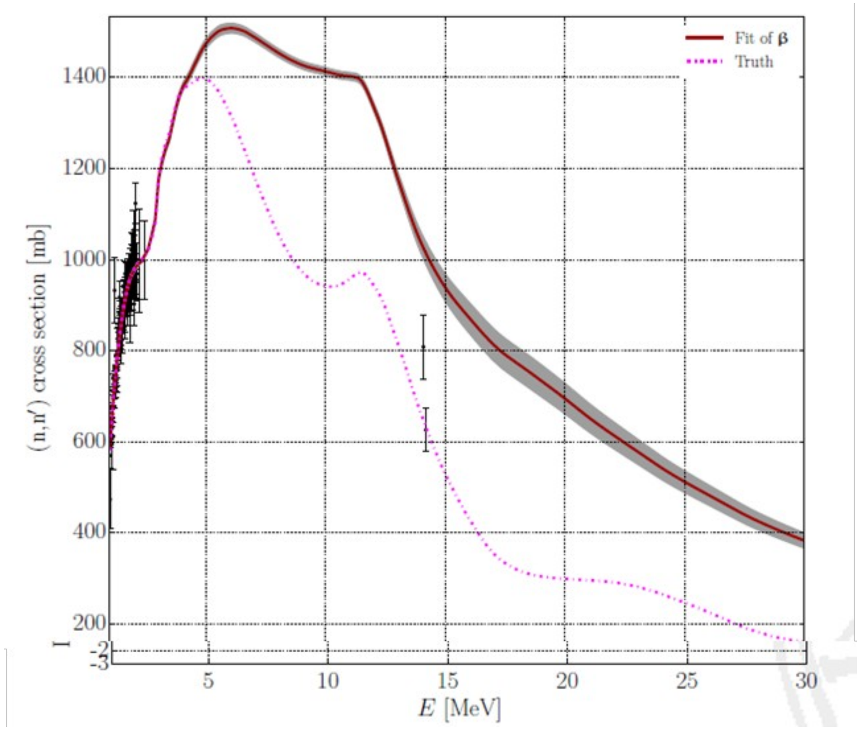
Energy-dependent model parameters

- Some parameters energy dependent (e.g., optical potential)
- Use GPs to fine-tune energy dependence to get a better reproduction of data
- Better physics or <u>vehicle to treat model defects</u>



$$f(E) = \mathcal{M}(E \mid \vec{p}(E')) \longrightarrow \mathcal{M}(E \mid \vec{p}(E') + \vec{\delta}(E'))$$

Gaussian process

$$k(E, E') = \delta^2 \exp\left(-\frac{1}{2}\frac{(E-E')^2}{\lambda^2}\right)$$

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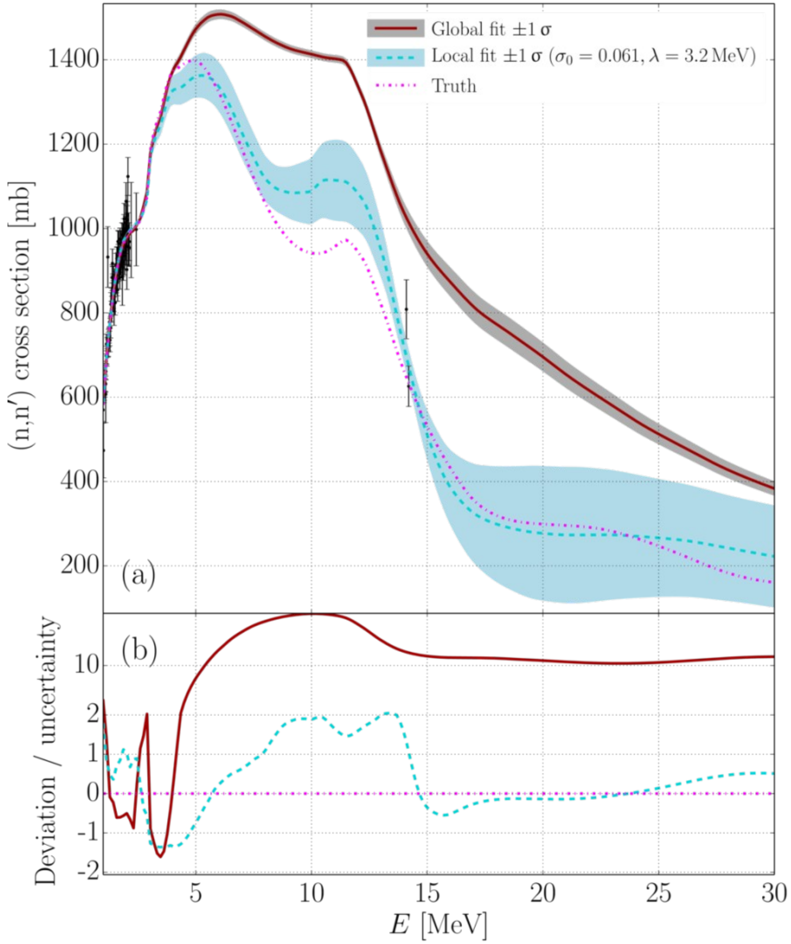
Synthetic data study

- Model: “Pseudo-TALYS” (^{56}Fe like data)
- Sampled truth:
- $f_{\mathrm{true}}(x) = f(x, \boldsymbol{\beta})\,(1 + \xi(x))$
  - – $\boldsymbol{\beta}$ and $\xi(x)$ sampled
  - $\Rightarrow$ Varying model defect, $\xi(x)$
- Sampled experimental data

Found: Energy-dependent much more reasonable uncertainties.



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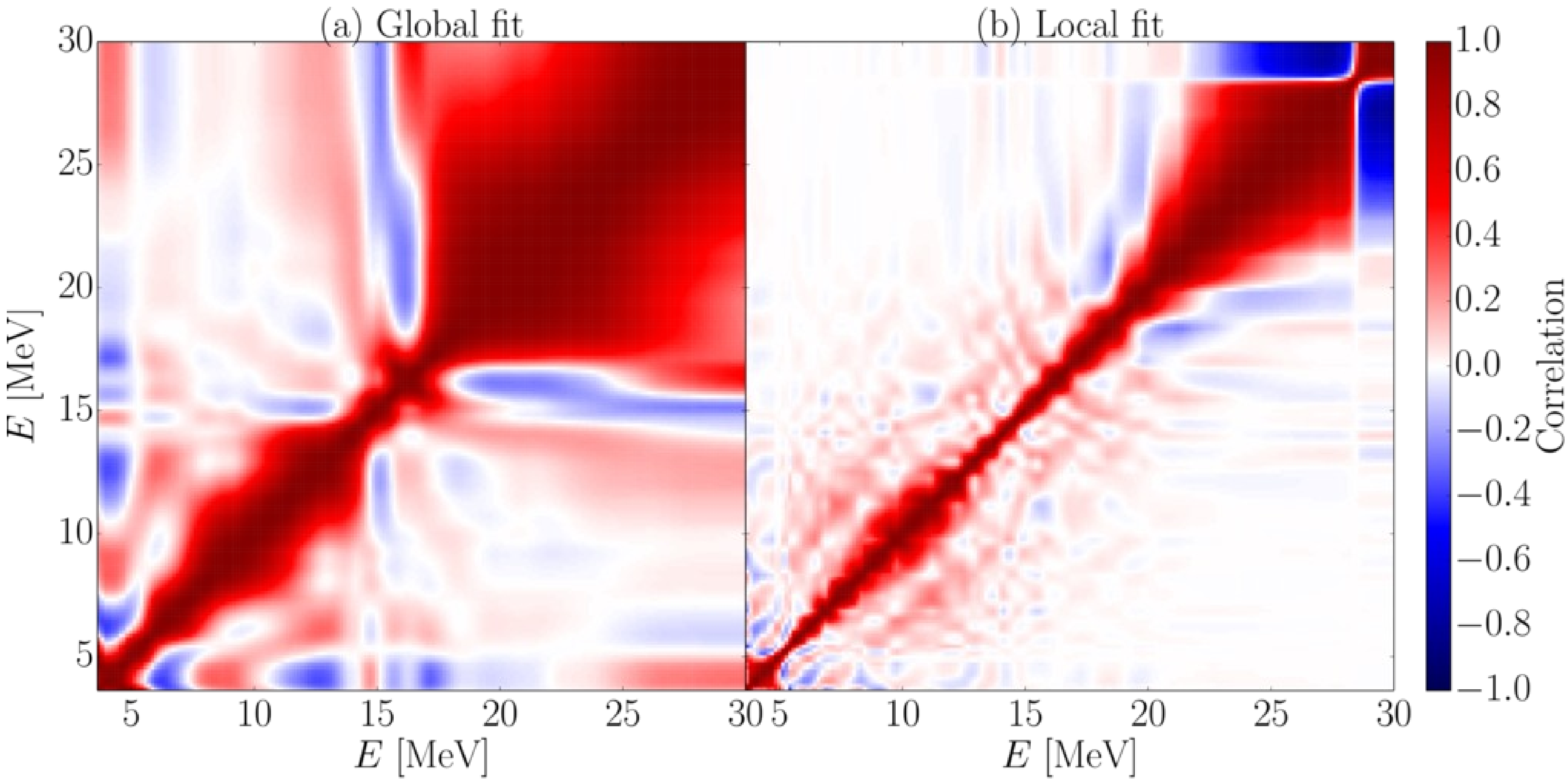
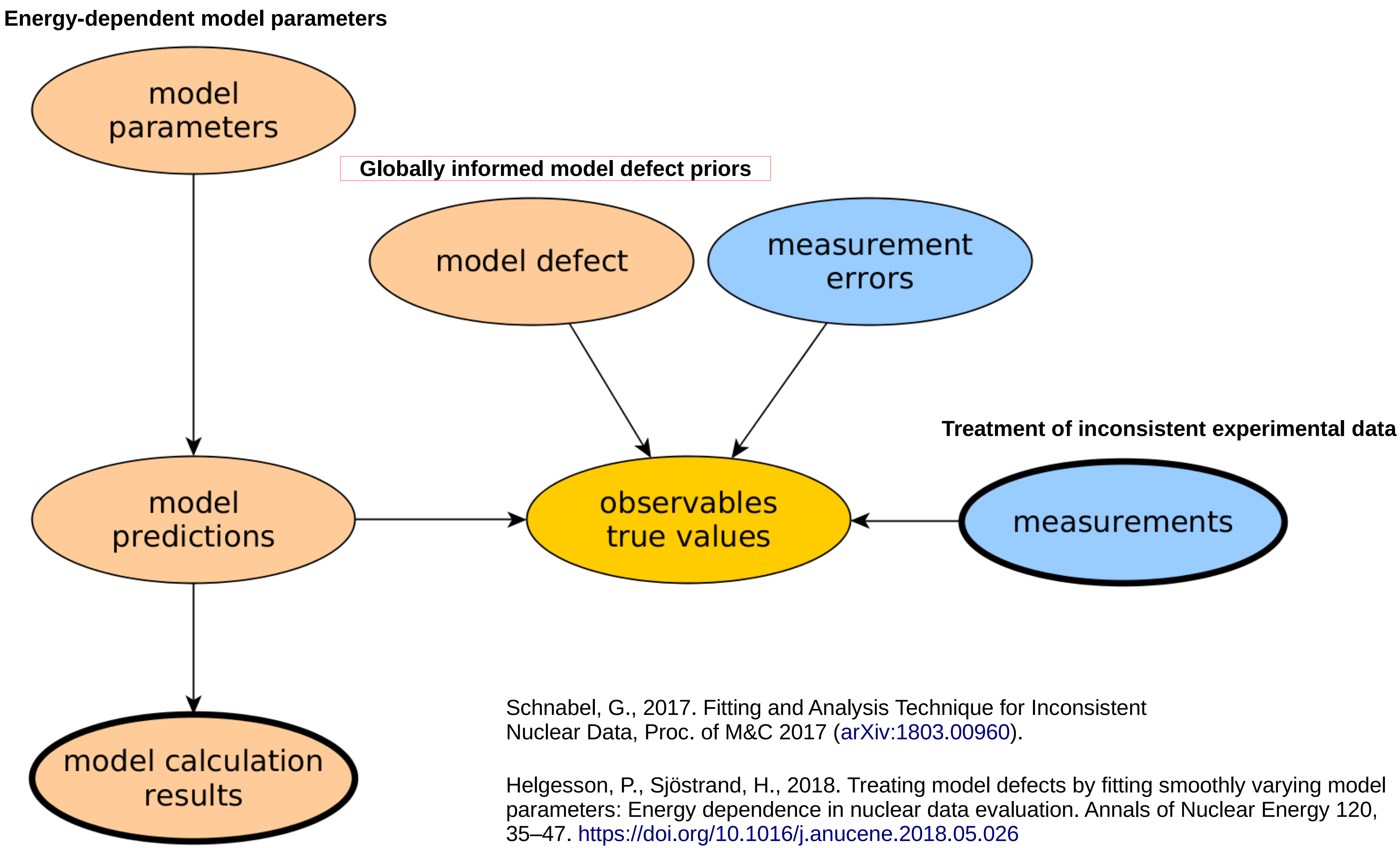
Comparison of correlations



Global fit standard TALYS
Local fit energy-dependent parameters augmented with GPs

Globally informed defect priors



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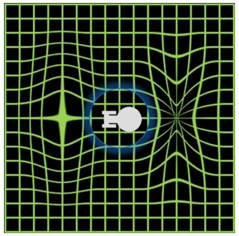
$$k(E, E') = \delta^2 \exp\left(-\frac{1}{2}\frac{(E-E')^2}{\lambda^2}\right)$$

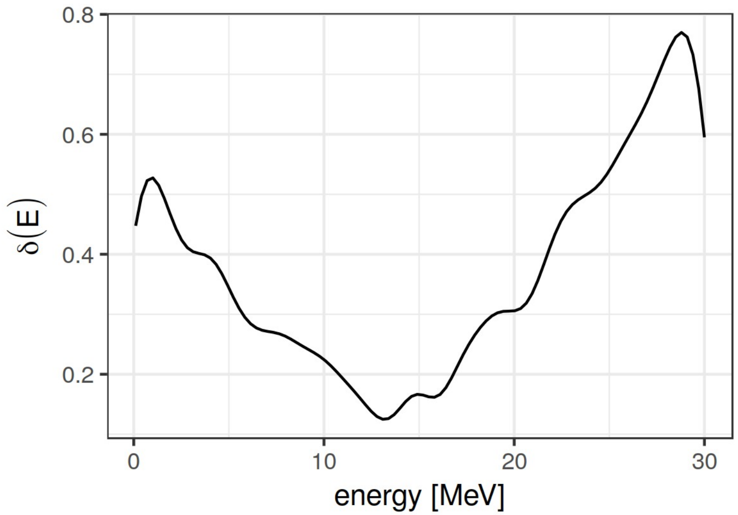
Dynamic time warping GP

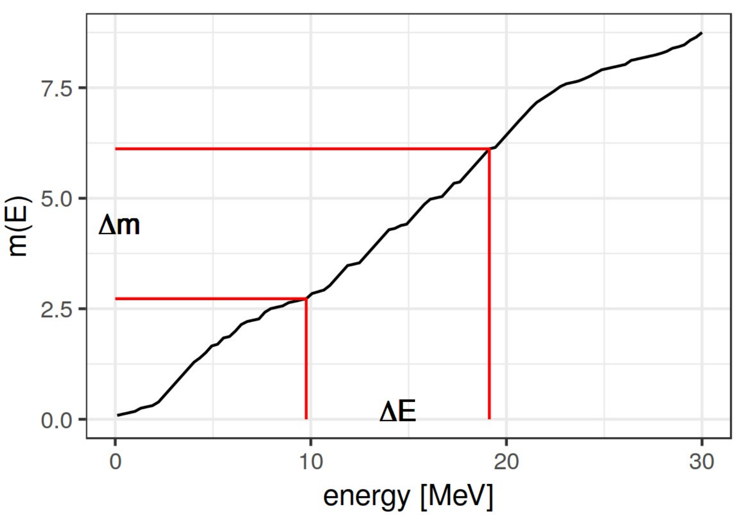
$$k(E, E') = \delta(E)\delta(E') \exp\left(-\frac{1}{2}\Big(m(E) - m(E')\Big)^2\right)$$

$$\delta(E) = \sum_{i=1}^{99} \left(\frac{E_{i+1} - E}{E_{i+1} - E_i}\mathbf{y_i} + \frac{E - E_i}{E_{i+1} - E_i}\mathbf{y_{i+1}}\right) \mathcal{I}_{(E_i \le E < E_{i+1})}(E)$$

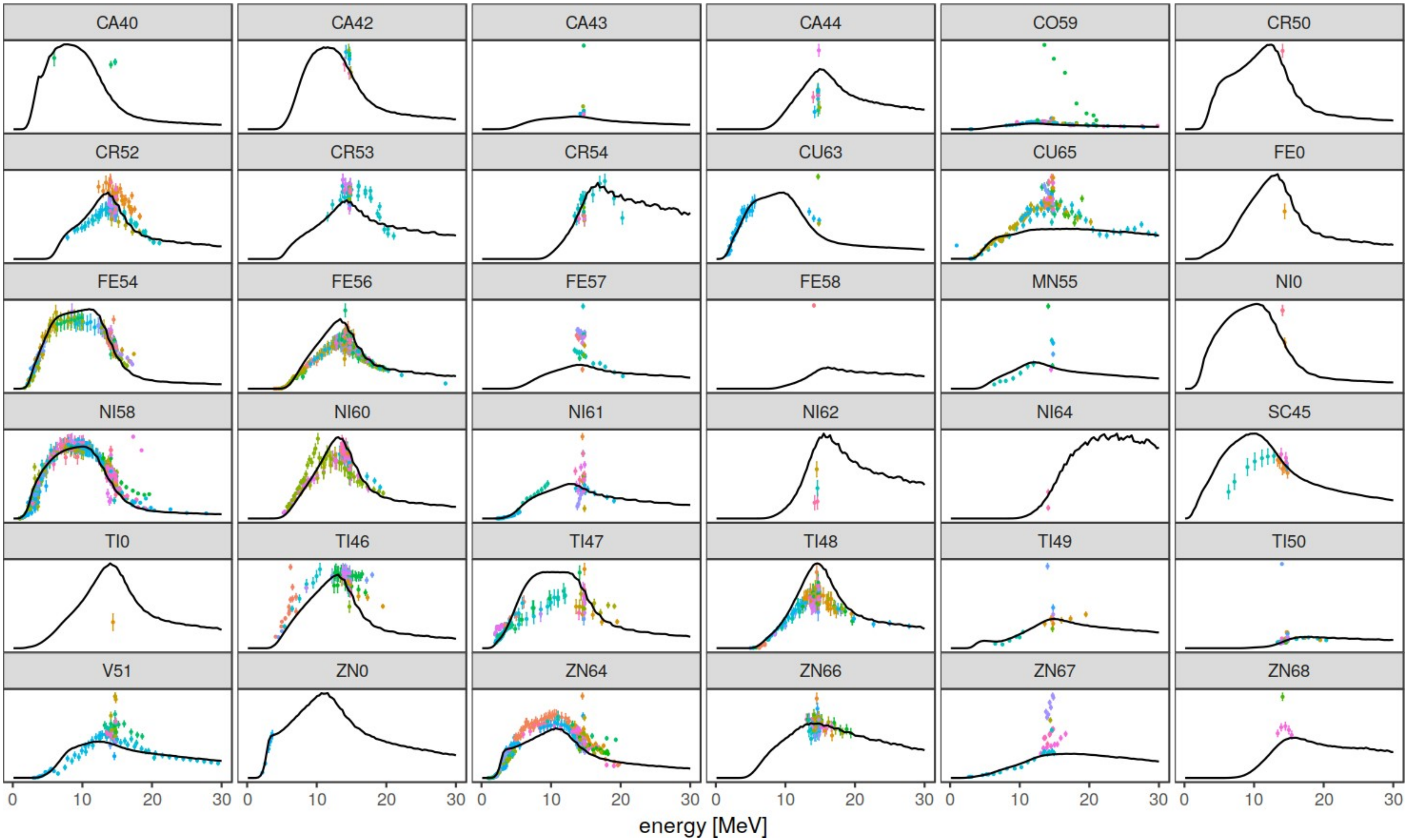
$$m(E) = \sum_{i=1}^{99} \left(\frac{E_{i+1} - E}{E_{i+1} - E_i}\mathbf{z_i} + \frac{E - E_i}{E_{i+1} - E_i}\mathbf{z_{i+1}}\right) \mathcal{I}_{(E_i \le E < E_{i+1})}(E)$$



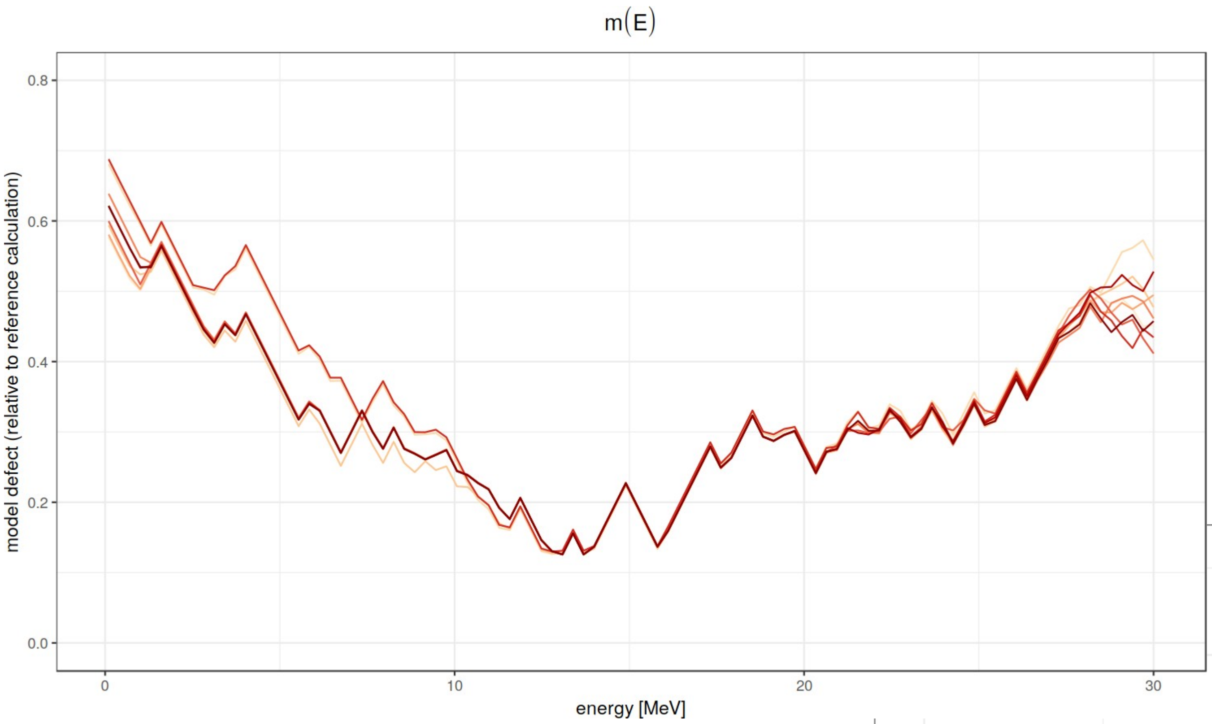




Global prior construction (n,p) reactions as examples

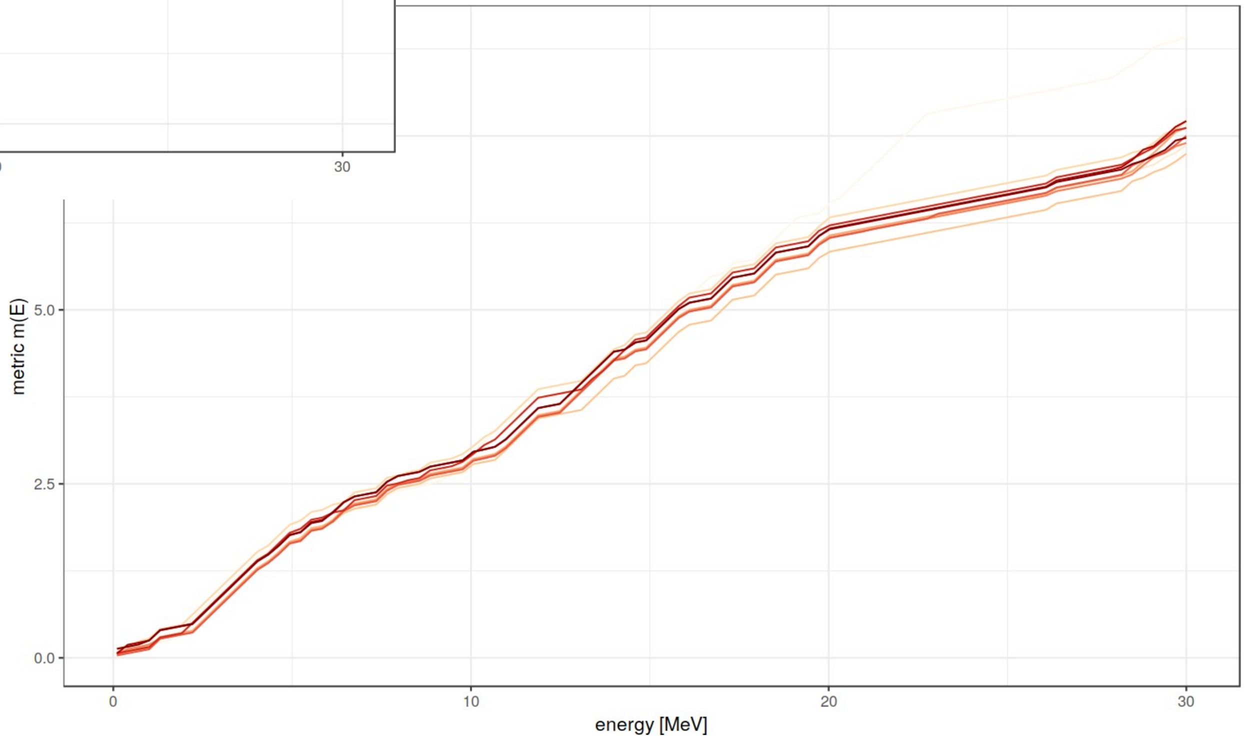


Resulting defect prior



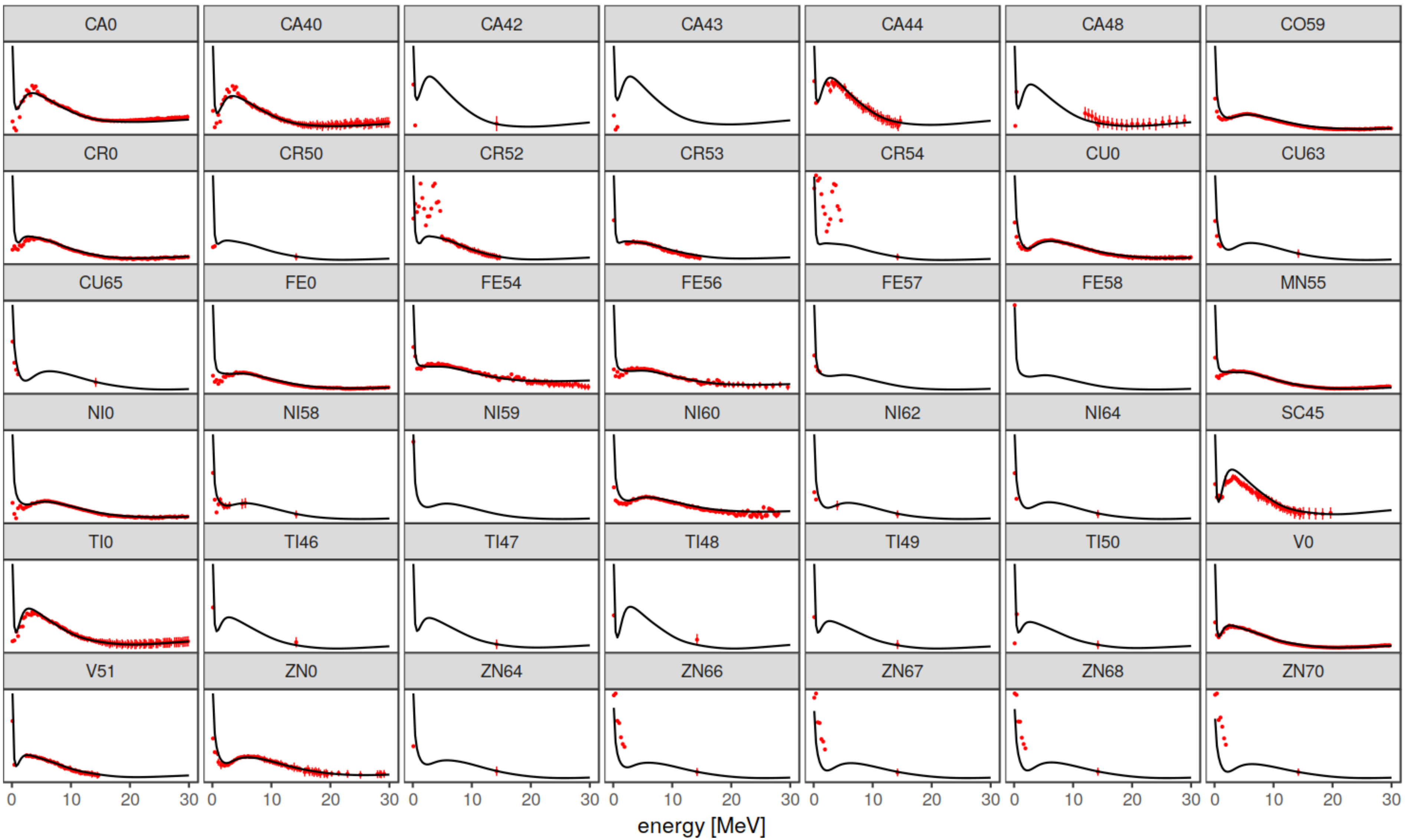
Link to animation [MP4]

Link to animation [GIF]

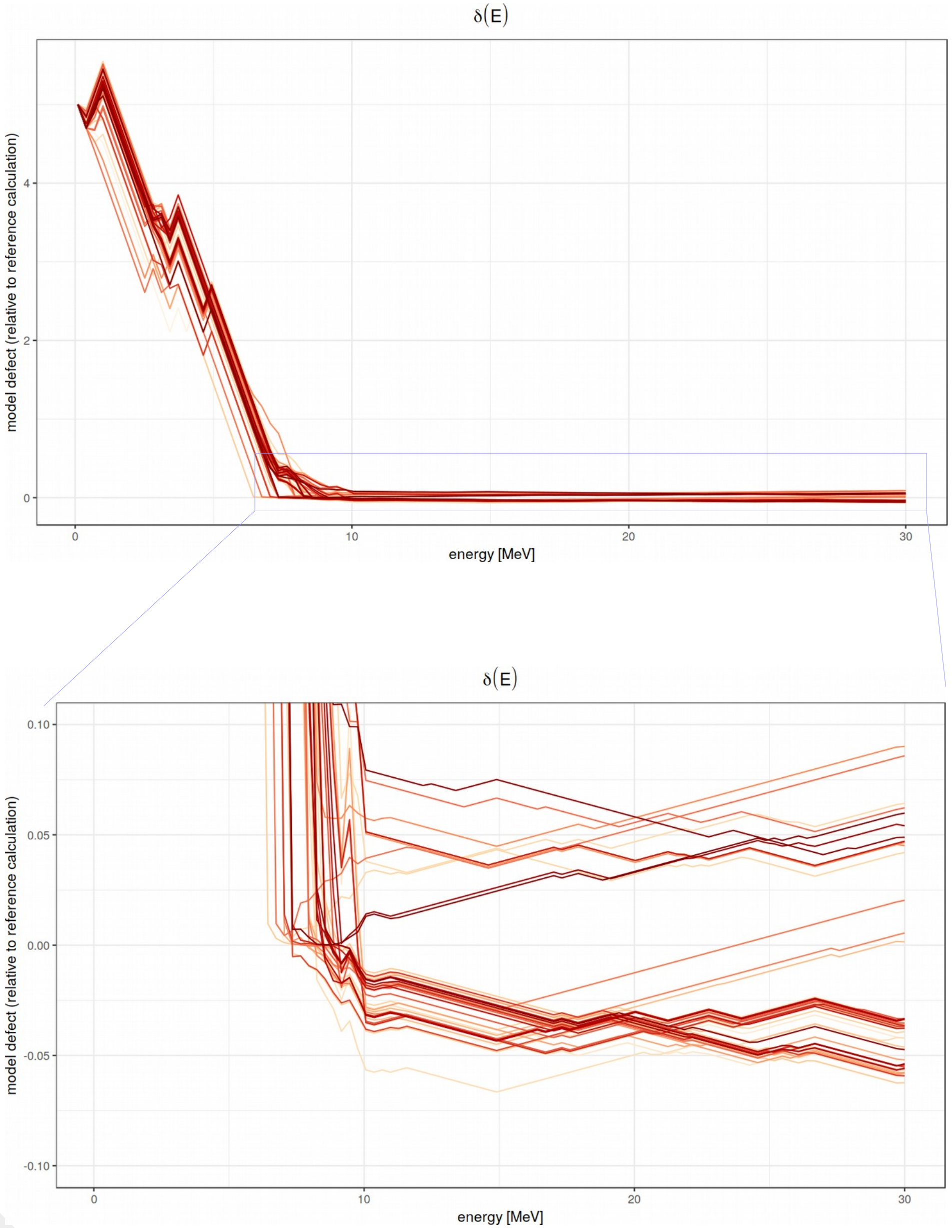


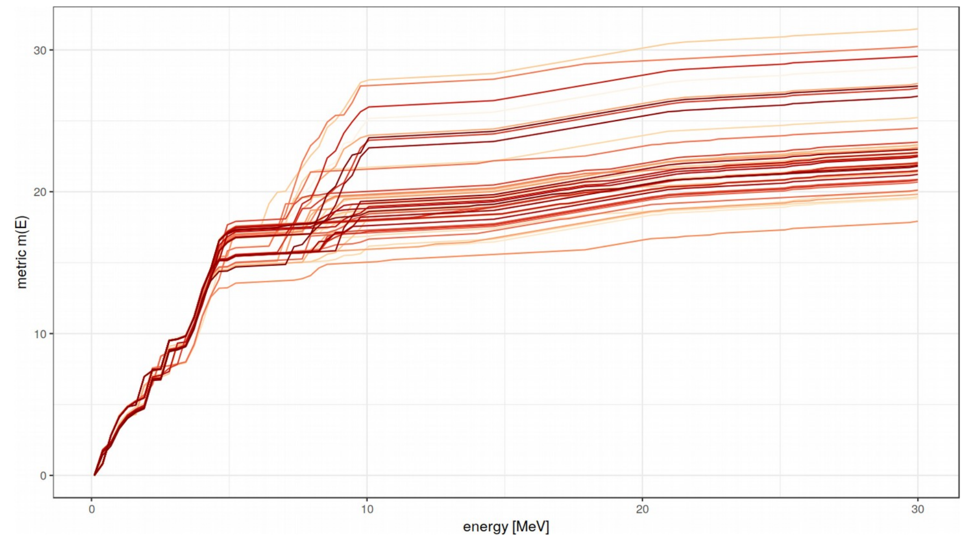
Remark
Reasonable constraints are important for a successful optimization (e.g., lower bound for length-scale, upper bound for maximal local difference of amplitude, etc.)

Global defect (n,tot)



Marlike maxim with (n,tot) data



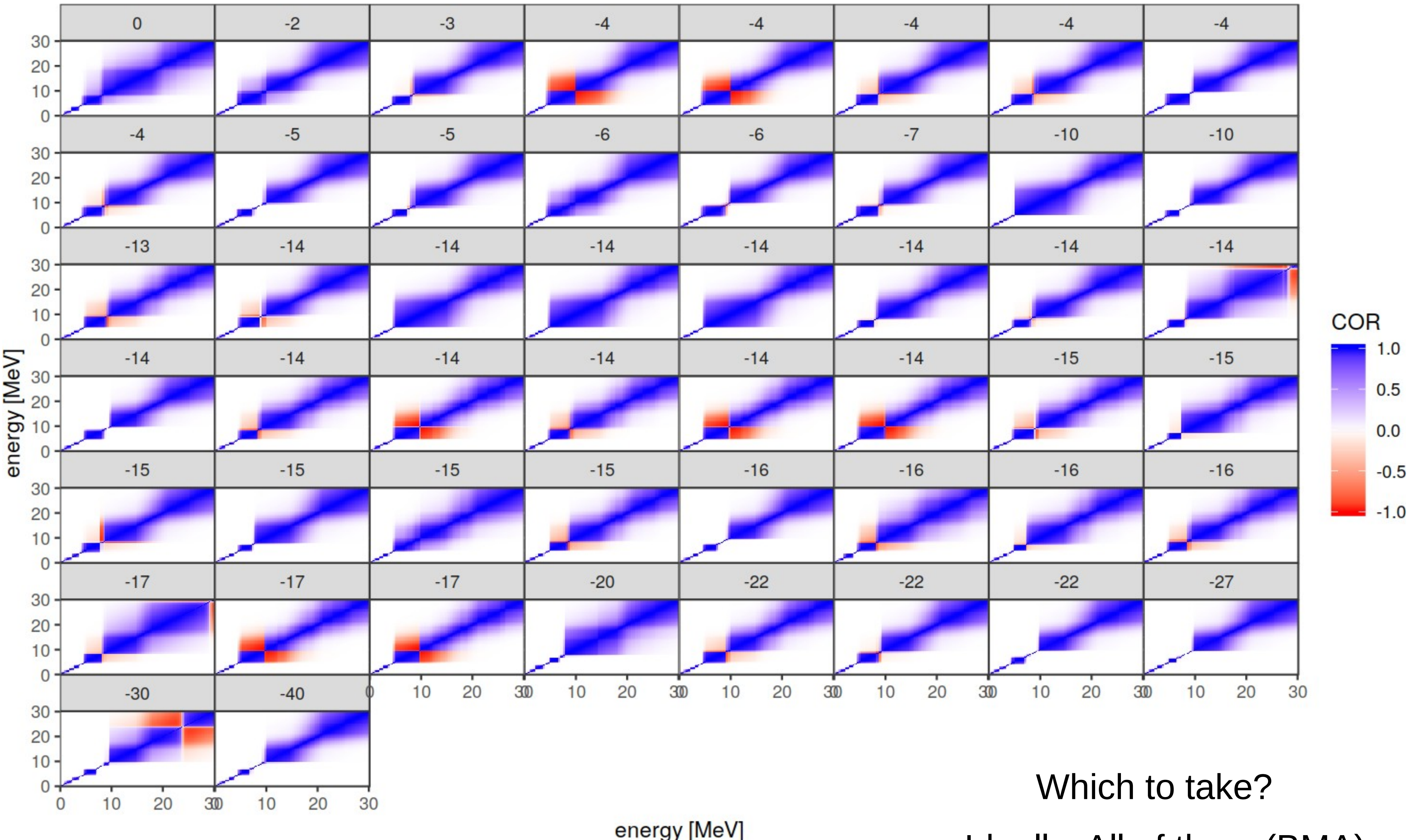


Remark
Optimization was guided by allowing more flexibility at lower than at higher energies.

Link to animation [GIF]

Link to animation [MP4]

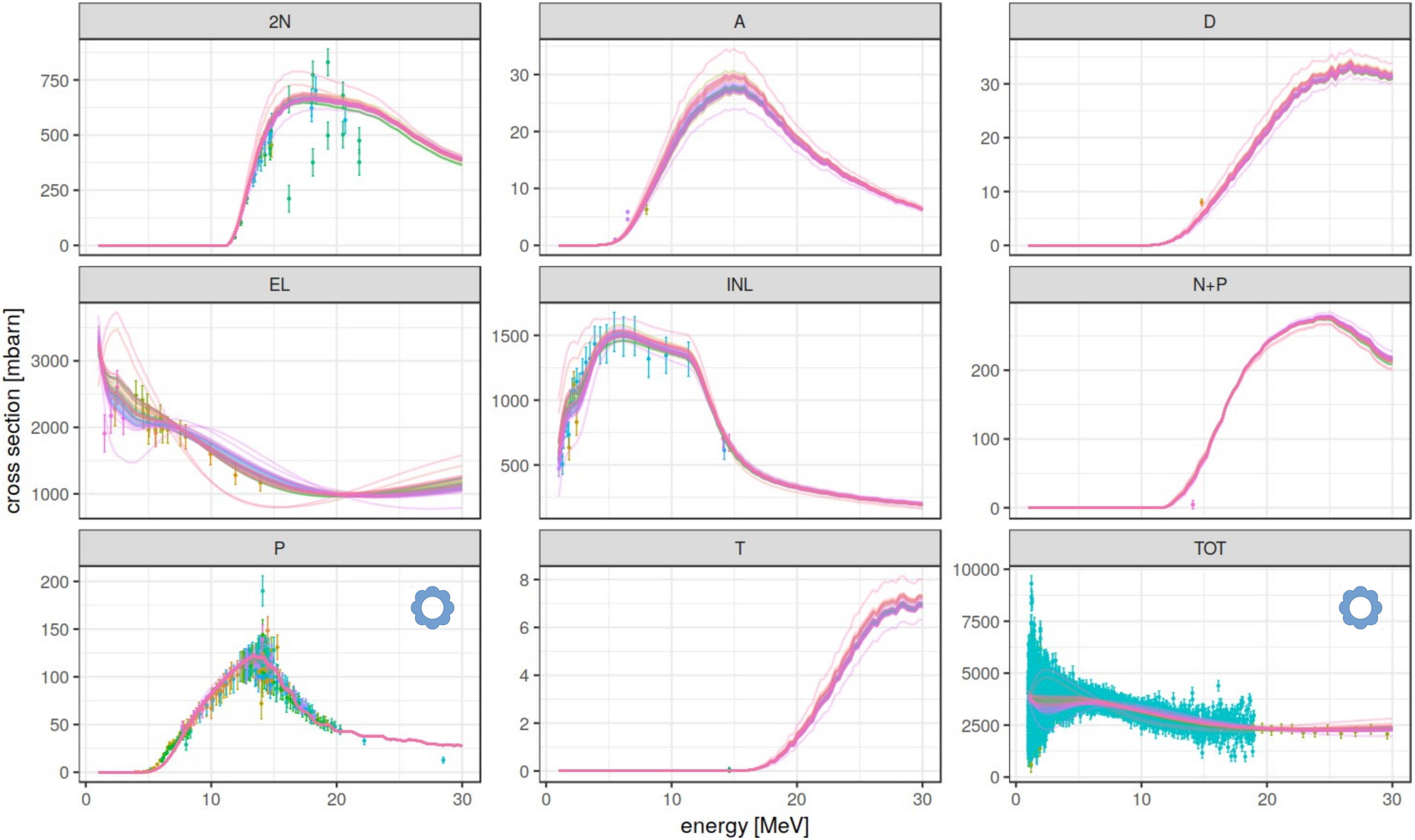
Correlation matrices of defect (n,tot)



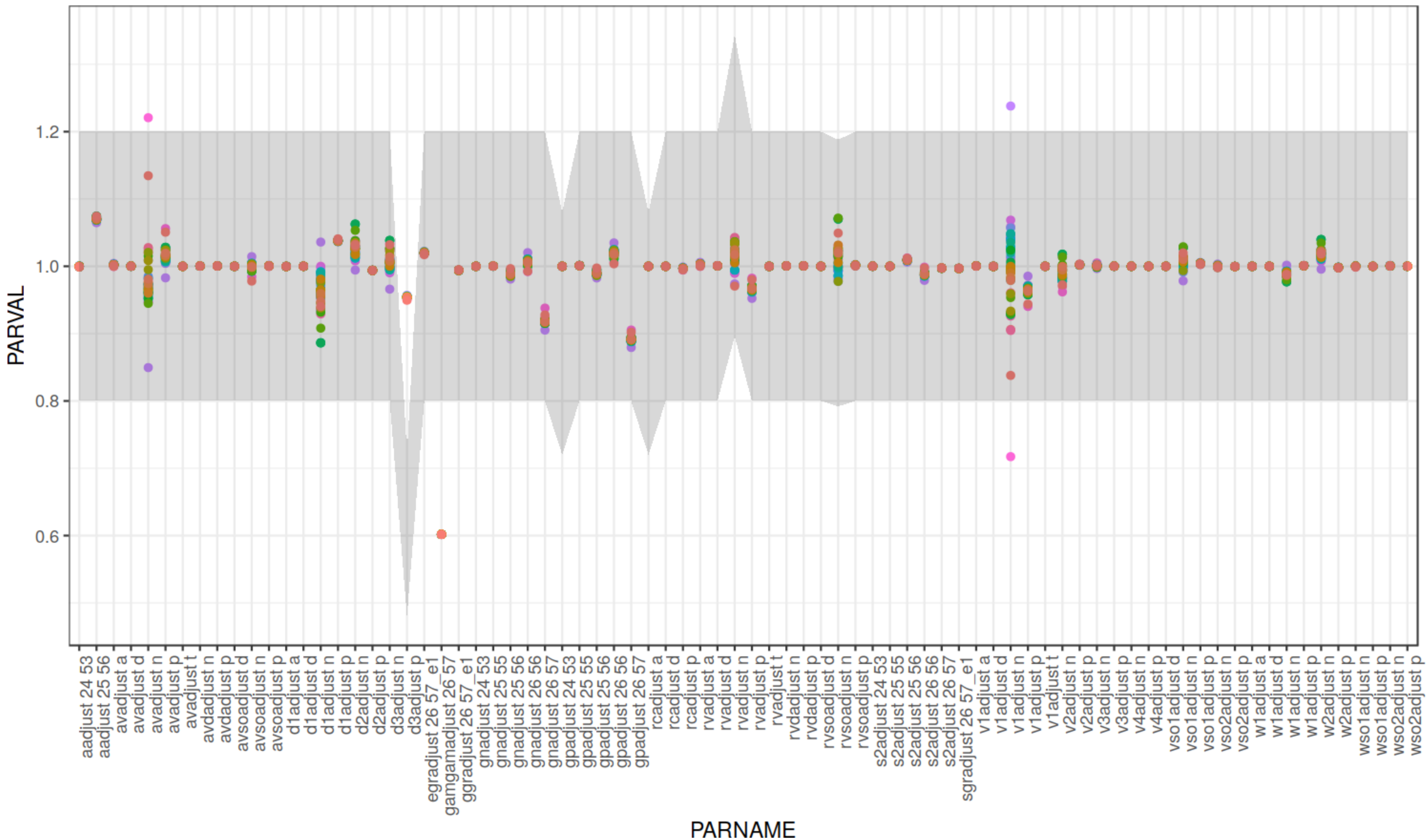
Which to take?

Ideally: All of them (BMA)

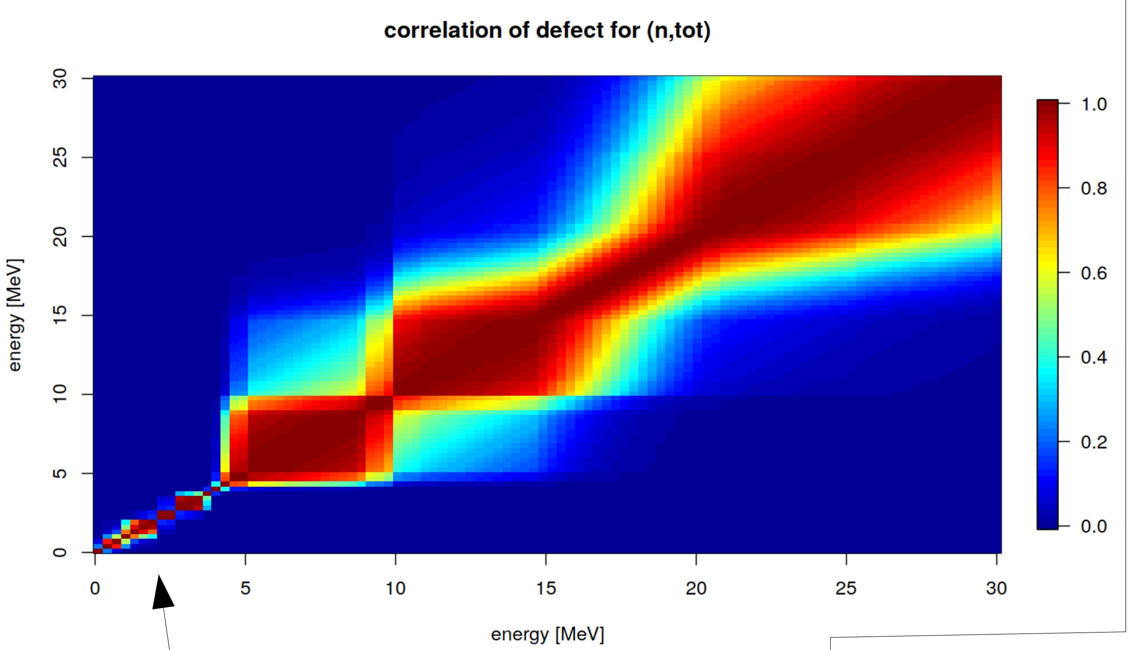
Poor man's BMA [again ^{56}Fe update (n,p) and (n,tot)]

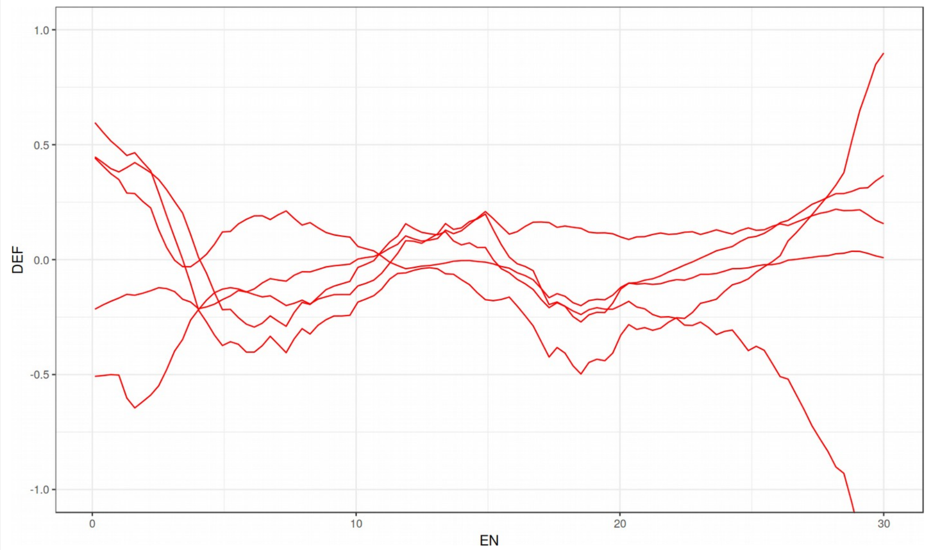


Poor man's BMA
[again ^{56}Fe update (n,p) and (n,tot)]

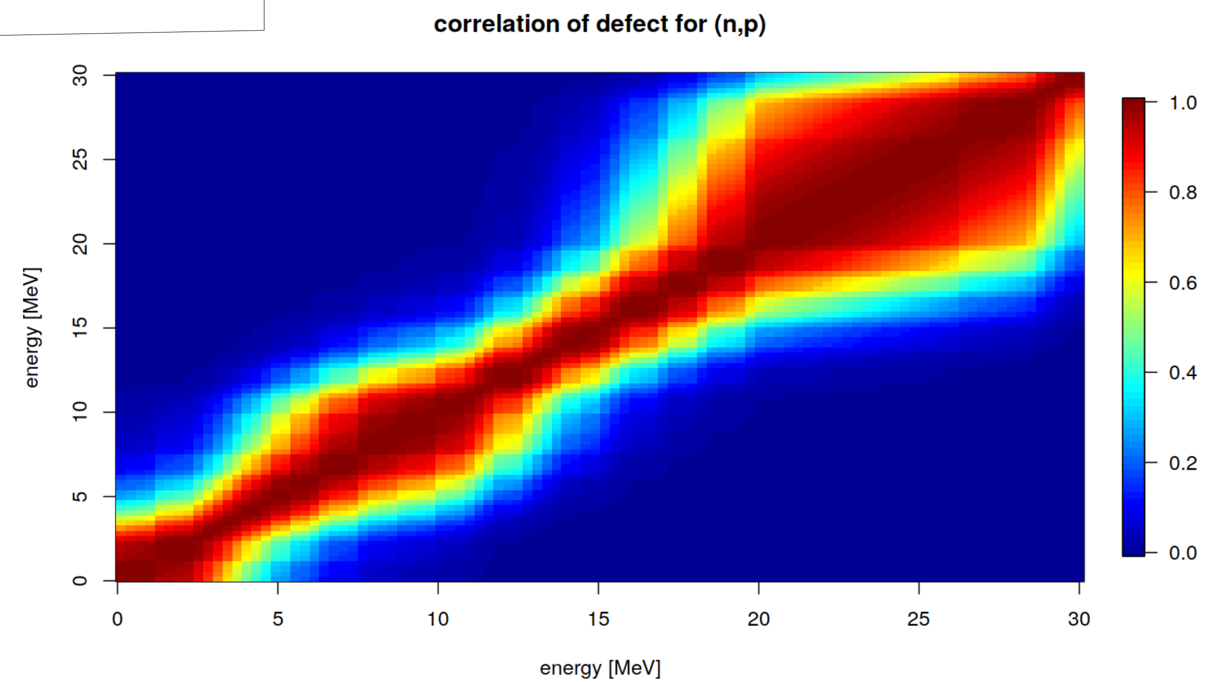


Correlation structure





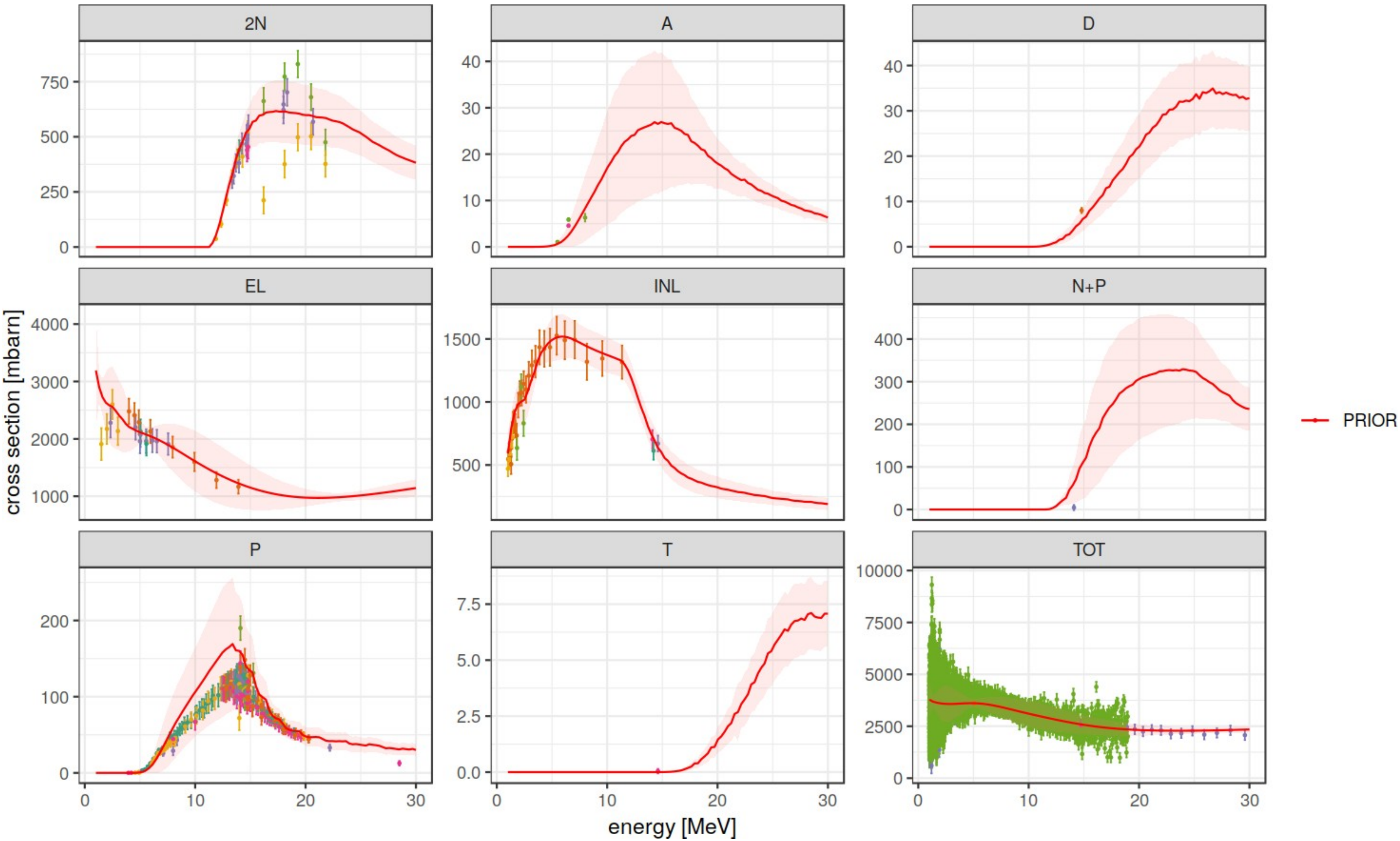
resonance region



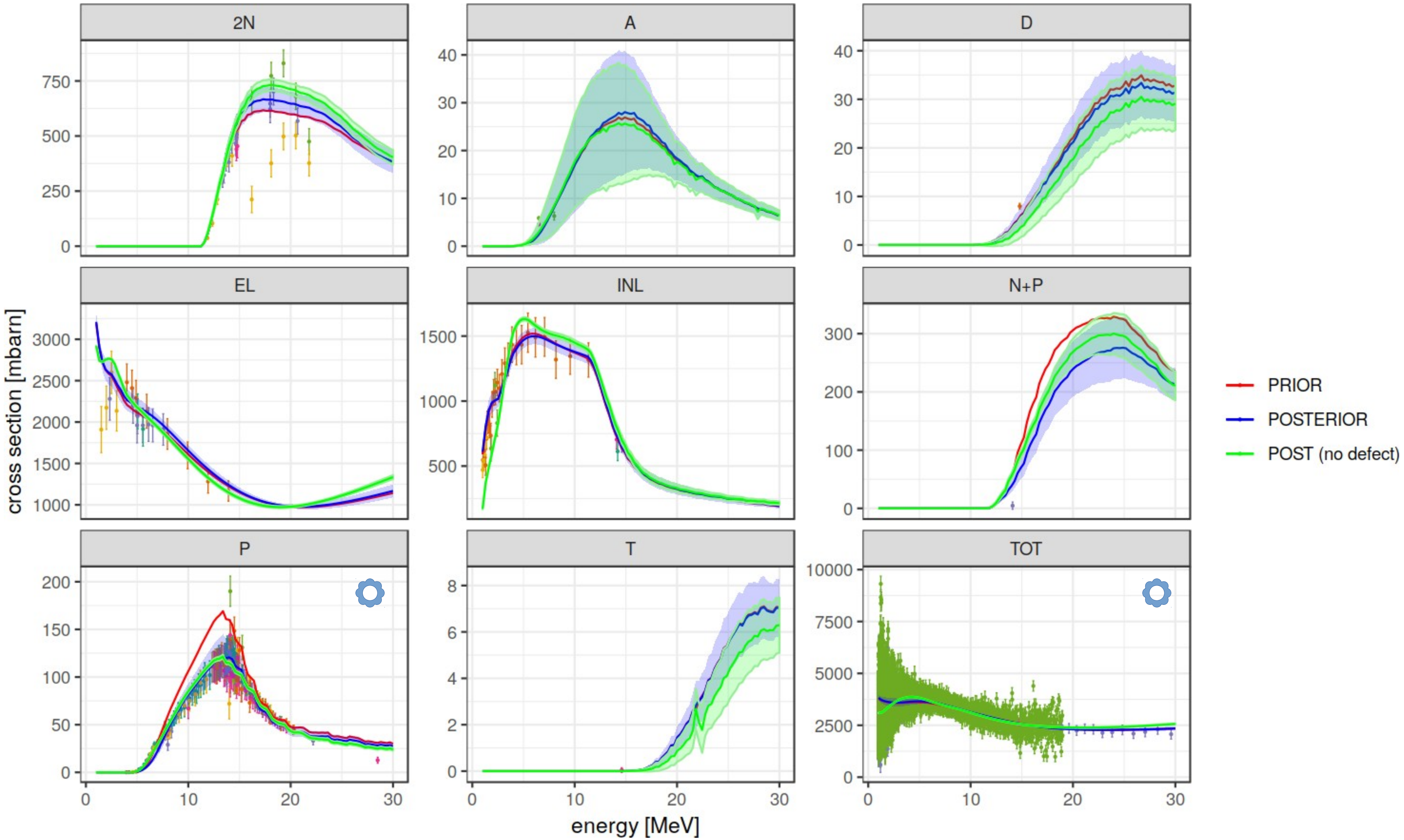
Link to animation [GIF]

Link to animation [MP4]

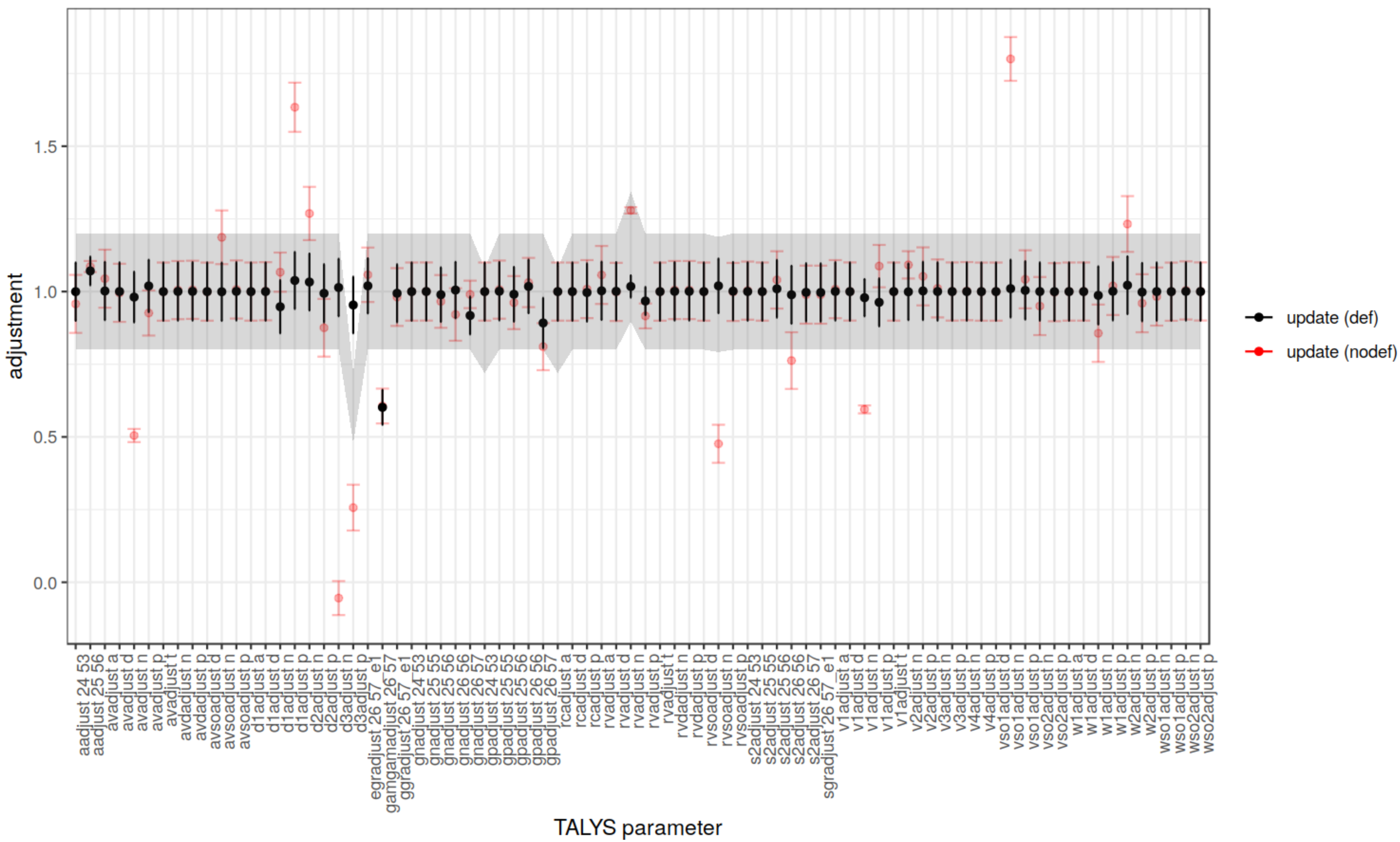
^{56}Fe differential cross sections (n, ...)



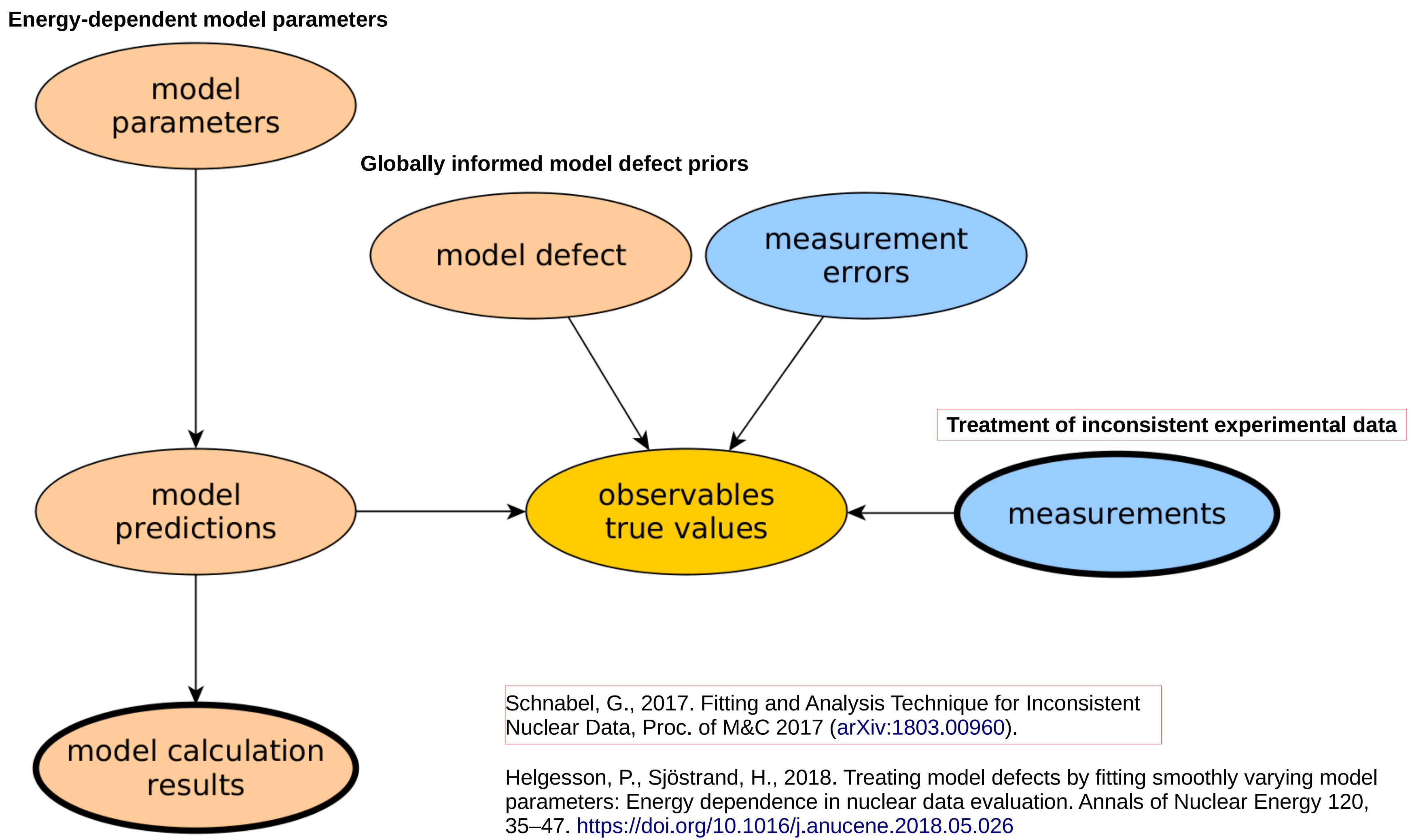
Comparison update (def/nodef)



Consistent parameters



Treatment of inconsistent data



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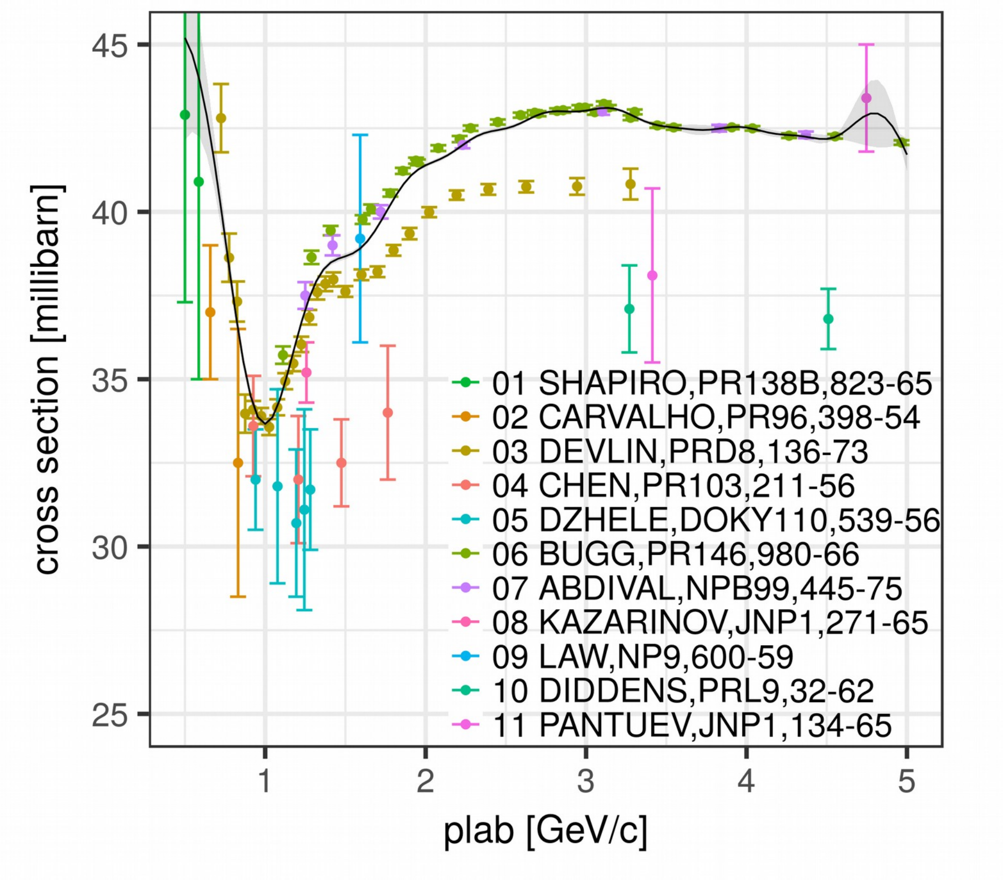
Inconsistent data = trouble

Proton-Neutron total cross



Fit of

$$\sigma_{\text{fit}}(E) = \frac{\sum_{i=1}^{M} y_i \mathcal{N}\left(E \mid x_i, \lambda^2\right)}{\sum_{j=1}^{M} \mathcal{N}\left(E \mid x_j, \lambda^2\right)}$$

to the neutron-proton total cross section using just statistical uncertainties B_{stat}

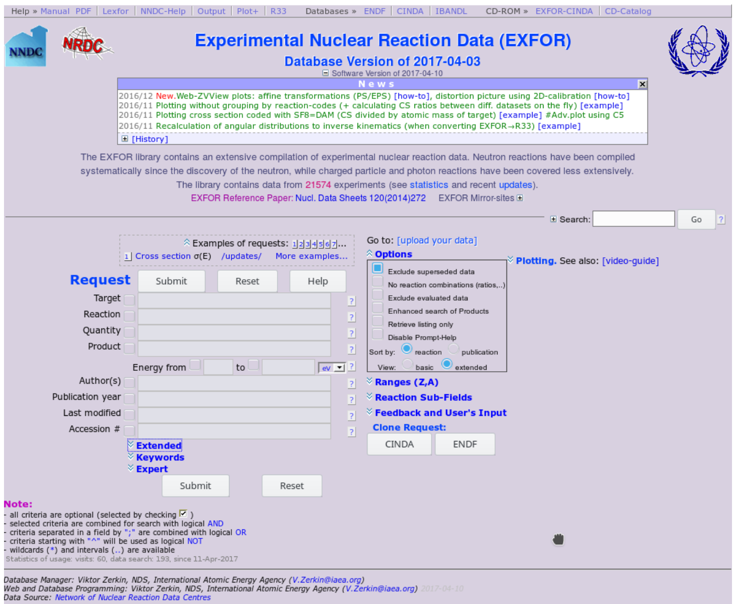
Problems

Final fit underestimates uncertainty

Associated $\chi^2/N \approx 16$ too large

Without visual inspection we do not know why

Large amount of data

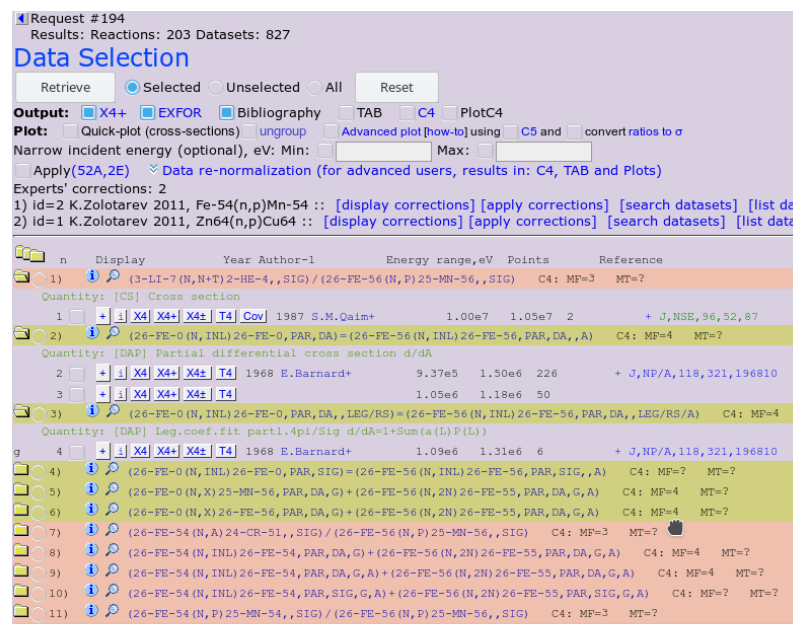


Database as of: 2017-04-

Number of ENTRY	21574	experimental works
Number of SUBENT	150976	data tables
Number of Datasets	167857	data tables of reactions
Number of Datapoints	**14739297**	total number of data points

Example: **EXFOR Database**

- Around **15 million data points**
- No covariance matrices for many measurements
- Direct fitting of models/functions not reasonable



Empirical Bayesian approach

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}_1 & & \\ & \mathbf{B}_2 & \\ & & \ddots \end{bmatrix} \qquad \vec{\sigma}_{\text{exp}} = \begin{pmatrix} \vec{\sigma}_{\text{exp},1} \\ \vec{\sigma}_{\text{exp},2} \\ \vdots \end{pmatrix}$$

Suggestion of a reasonable parametrization *(others are possible!)*

Additional normalization error (e.g. sample thickness, calibration, ...)

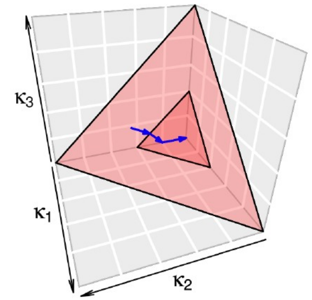
$$\tilde{\mathbf{B}}_i = \mathbf{B}_i + {\kappa_i}^2 \vec{\sigma}_{\text{exp},i} \vec{\sigma}^T_{\text{exp},i}$$

$$\pi_1(\vec{p}_{\text{true}}, \vec{\kappa} \,|\, \vec{\sigma}_{\text{exp}}, \vec{p}_0, \mathbf{A}_0) \propto \ell(\vec{\sigma}_{\text{exp}} \,|\, \vec{p}_{\text{true}}, \tilde{\mathbf{B}}(\vec{\kappa})) \times \pi_0(\vec{p}_{\text{true}} \,|\, \vec{p}_0, \mathbf{A}_0)$$

$$\times \pi_0(\vec{\kappa})$$

Criteria for choice of prior

- Simple parametrization
- “Uninformative”
- Favor sparse solutions



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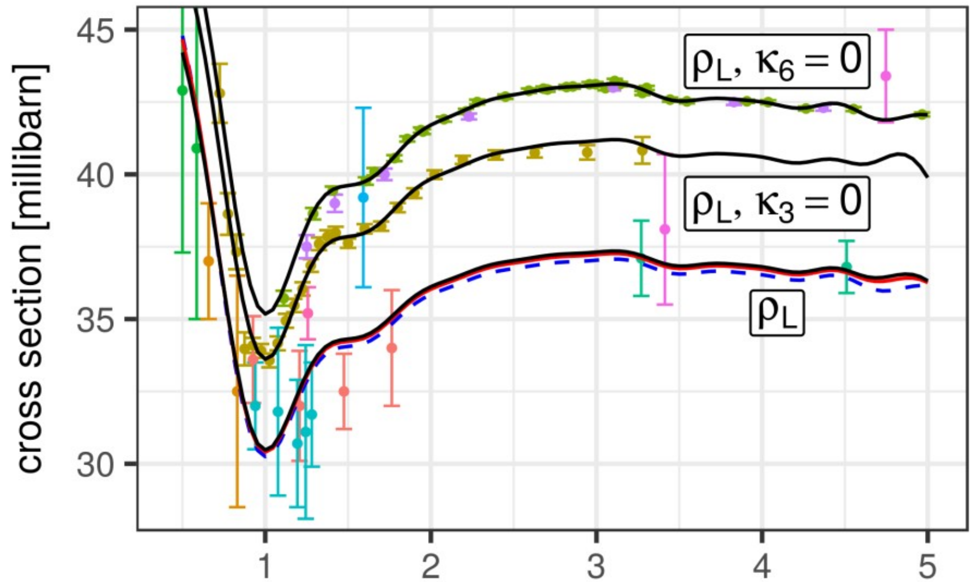
Schematic application



$$\tilde{\mathbf{B}}_i = \mathbf{B}_i + {\color{red}\kappa_i}^2 \vec{\sigma}_{\mathrm{exp},i} \vec{\sigma}^T_{\mathrm{exp},i}$$

	δ	ℓ	κ_1	κ_2	κ_3	κ_4	κ_5	κ_6	κ_7	κ_8	κ_9	κ_{10}	κ_{11}	χ^2/N
GLS	—	—	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	16.13
ρ_U	—	—	**.00**	.04	.10	**.00**	**.00**	.14	.13	.06	.10	**.00**	.13	0.73
ρ_N	.11	—	**.00**	.03	.07	**.00**	**.00**	.10	.09	.04	.05	**.00**	.09	0.79
ρ_L	.13	1.0×10^0	**.00**	**.00**	.07	**.00**	**.00**	.09	.09	.03	**.00**	**.00**	.08	0.82
ρ_L	.13	1.8×10^{-3}	**.00**	.09	**[.00]**	.07	.07	.03	.03	.01	**.00**	.07	**.00**	0.98
ρ_L	.13	1.2×10^{-5}	**.00**	.12	.03	.10	.10	**[.00]**	**.00**	.06	**.00**	.10	**.00**	1.07
ρ_L	.17	—	**.00**	**.00**	.07	**.00**	**.00**	.10	.09	.04	**.00**	**.00**	.09	0.81

TABLE I. Posterior maxima $\boldsymbol{\kappa}$ based on the prior distributions specified in eqs. (50) to (52). For the pdfs ρ_N and ρ_L, results based on different values of δ are presented. Square brackets denote that the respective κ_i was fixed at zero. The index i refers to the experiment data set, see fig. 2. The value χ^2/N is the result of eq. (19) divided by the number of data points. Relative likelihoods ℓ are stated for the case ρ_L with $\delta = 0.13$.

Recent: Integral adjustment

- We add an extra uncertainty to each experiment.

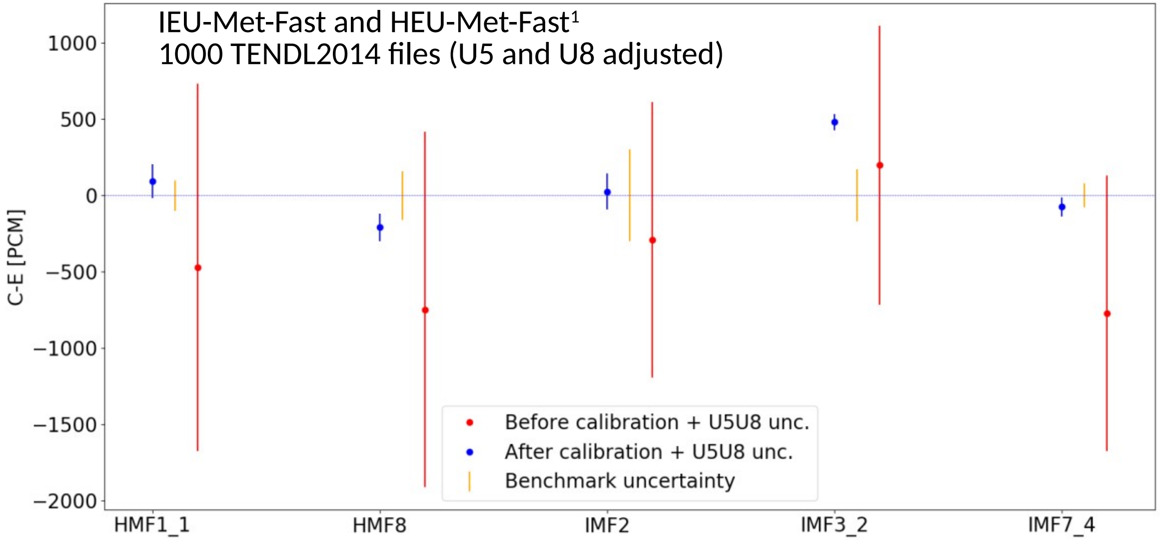
$$\sigma_{B,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{\substack{\text{overall p} \\ \text{where } p \neq J}} \sigma_{ND,p}^2$$

$$\sigma_{B,l,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{extra,l}^2 + \sigma_{extra,common}^2$$

- σ_{extra} found by maxzimizing L:

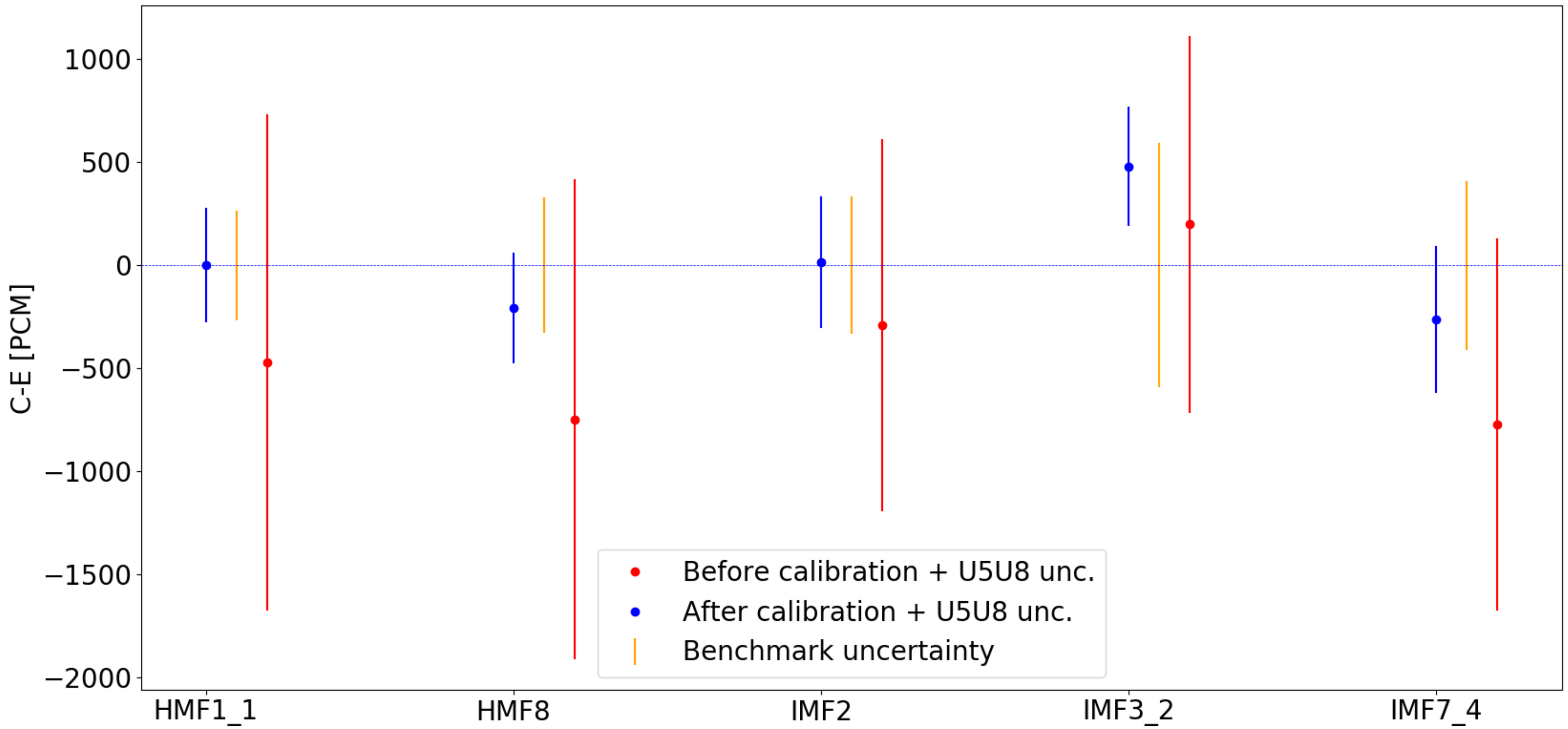
$$L = \frac{1}{\sqrt{(2\pi)^N |\mathrm{cov}_{\mathrm{stat,exp,extra}}|}} \sum_i e^{\left(\frac{-\chi_i^2}{2}\right)}$$

Sjöstrand, H., Schnabel, G., Helgesson P., Monte Carlo integral adjustment of nuclear data libraries – experimental covariances and inconsistent data, WONDER 2018



[1]Curtesy of Steven Van Der Marck

Some results



Benchmark uncertainties [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Fully correlated
No ML: Reported uncertainties	100	160	300	170	80	0
Uptated uncertainties	153	204	300	580	390	0
With correlation	267	329	333	591	409	257

Outlook

- Perform an evaluation of ^{56}Fe with GPs on parameter side[1]
- Interface recent methodological developments with TALYS/TENDL
- Continue development of methodology for integral adjustment

1) UU contribution to Eurofusion2018
VR contribution to PPPT nuclear data development: Evaluation of neutron cross section data in the fast energy range