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Belgian Nuclear Research Centre

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Enhancing Nuclear Data predictions through Bayesian Model Averaging

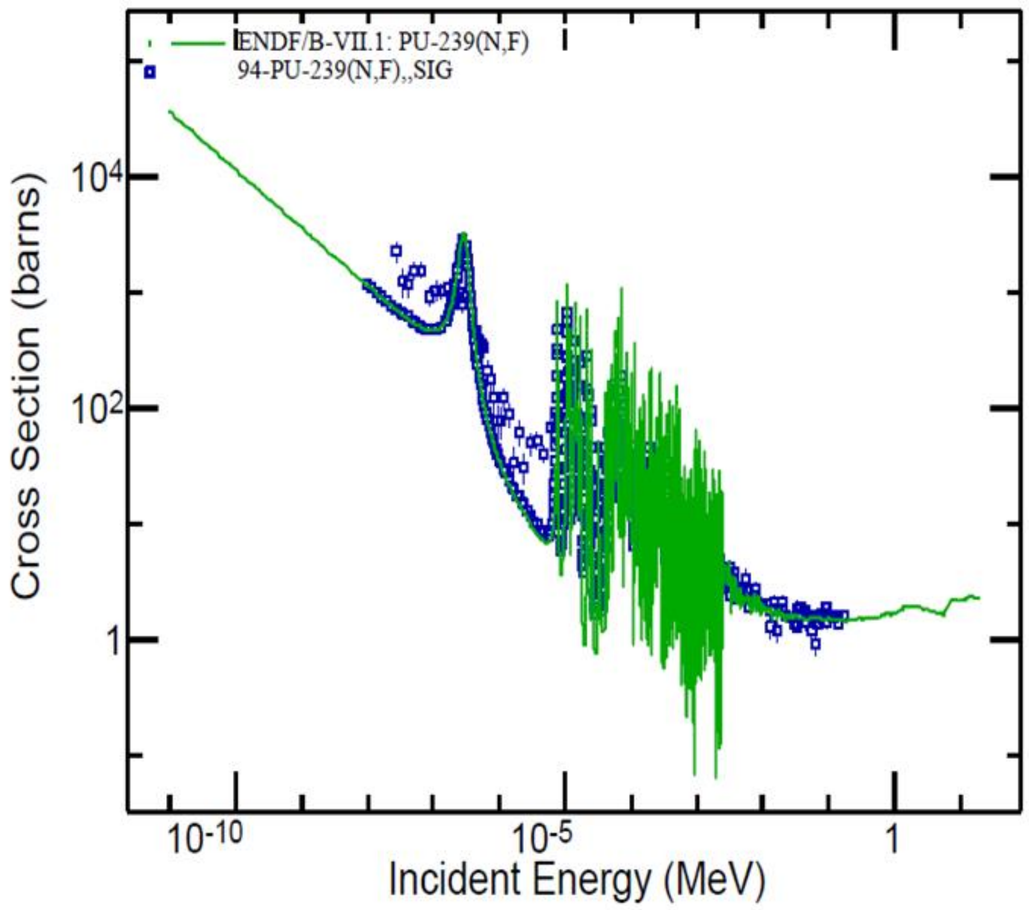
Consultancy Meeting of the International Nuclear Data Evaluation Network (INDEN)
on the Evaluated Data of Structural Materials 2024

Introduction

- Nuclear data evaluation involves predicting, for e.g., neutron cross section at an energy, E.

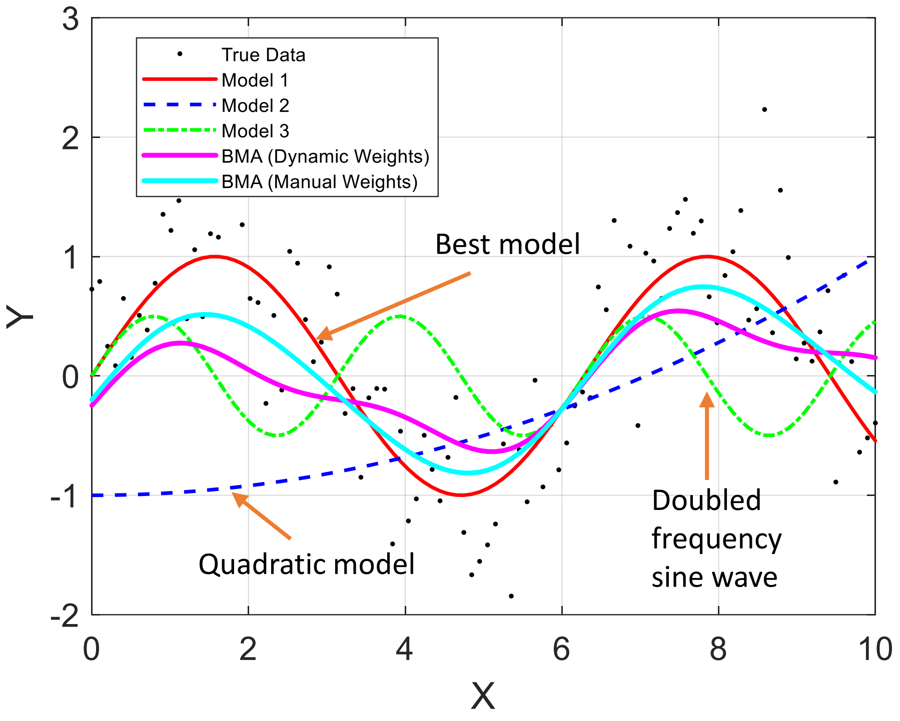
- **Let's assume we have three models:**

- **Model 1:** A theoretical model that works well at lower energies but is less accurate at high energies.
- **Model 2:** A model that performs well at high energies but is less reliable at lower energies.
- **Model 3:** A hybrid model that combines elements of both, but with higher uncertainty.



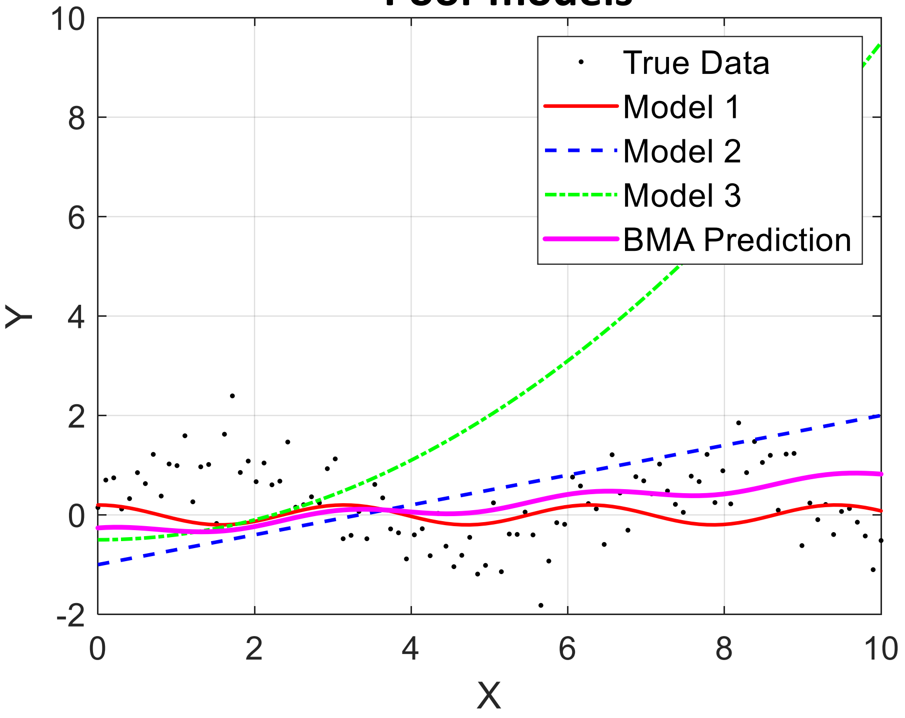
Using Global weights

- **Using global weights for models is akin to model selection.**
- **No experiment uncertainties**



Good models

Poor models



- Let's assume the following weights for each model:

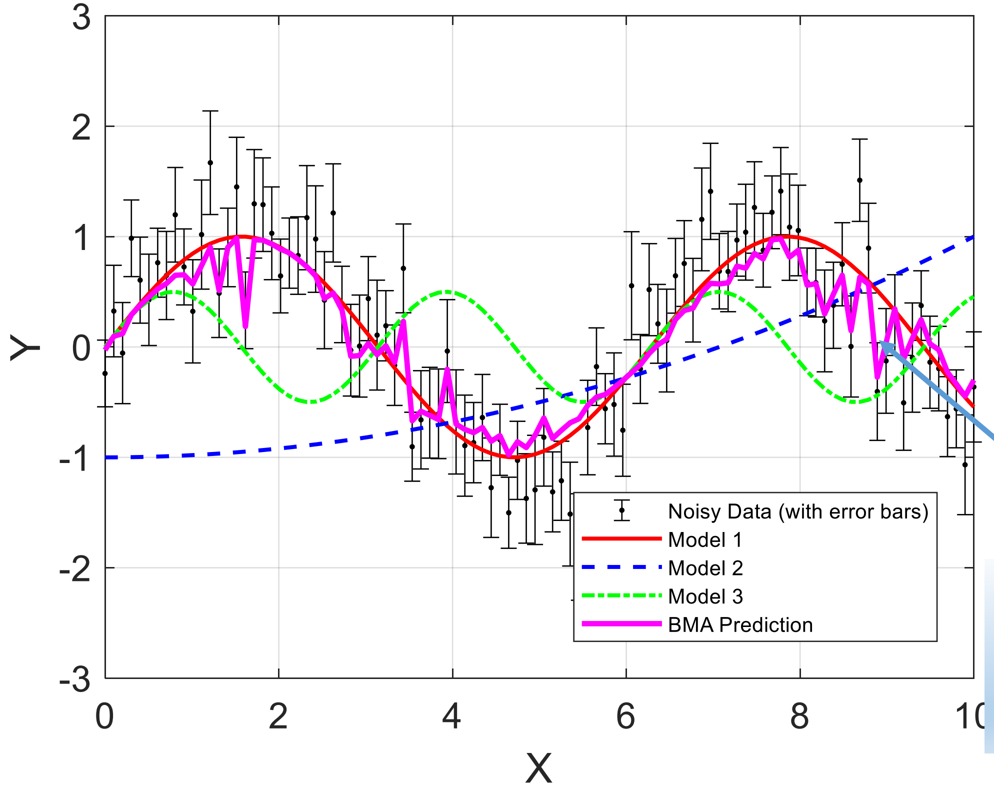
- **Model 1: 0.5;**
- **Model 2: 0.3;**
- **Model 3: 0.2**
- **weighted average:**

$$\sigma_{avg} = 0.5\sigma_1 + 0.3\sigma_2 + 0.2\sigma_3$$

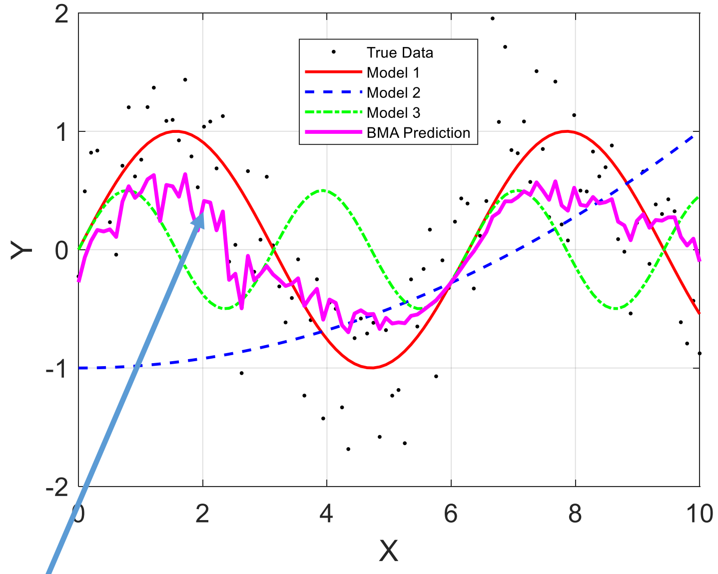
Data used here is synthetic data

Applying local weights

- Introduce experimental uncertainties
- local weights (weights as a function of x)



With experimental uncertainties

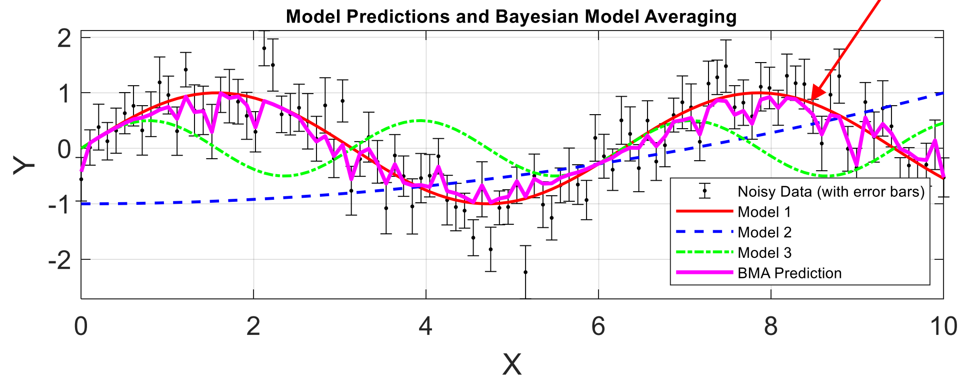


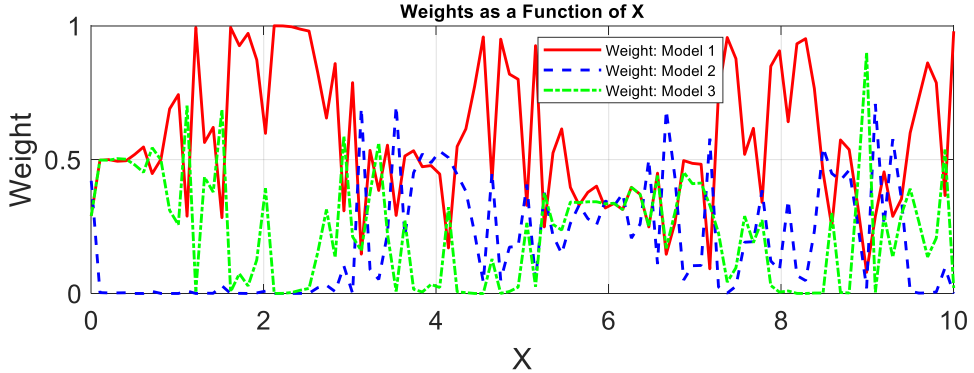
Without experimental uncertainties

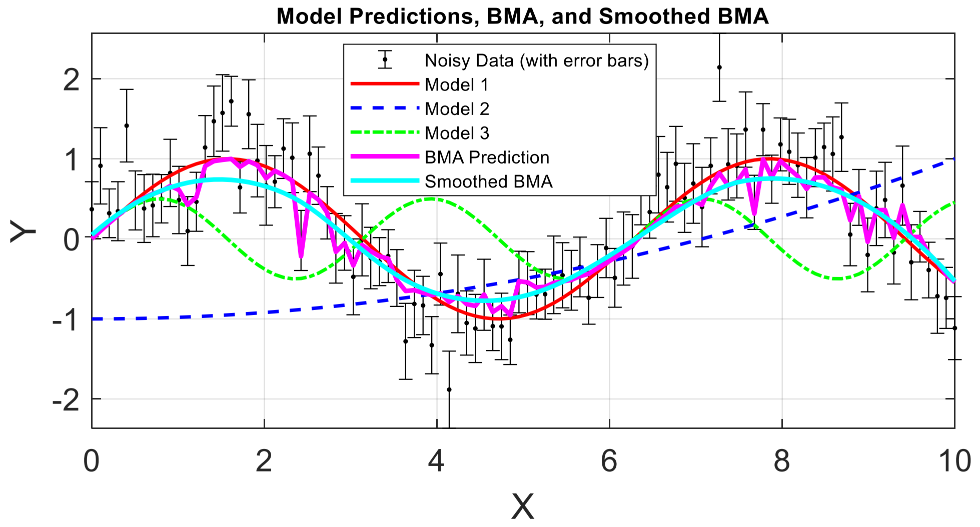
Kinks can be observed in the BMA plot

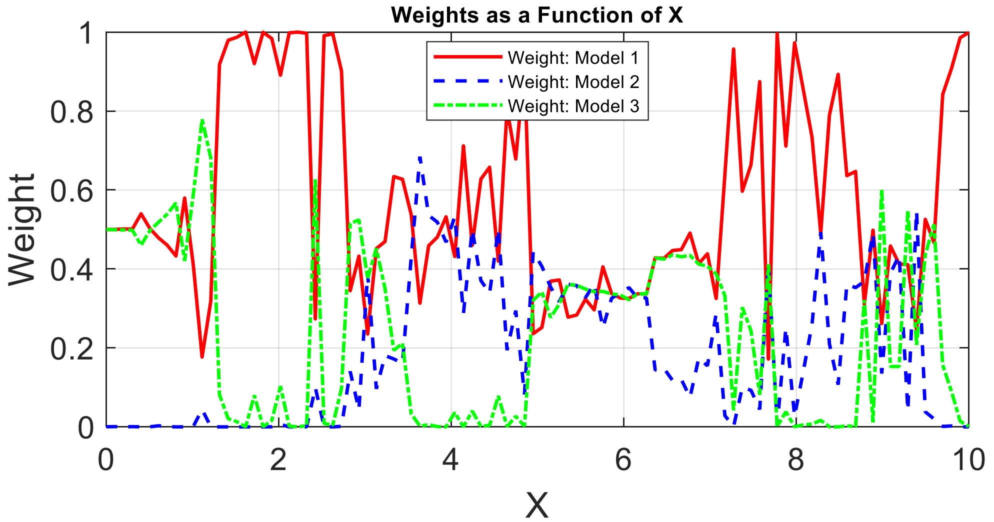
- Weights based on the likelihood function

Smoothened curve





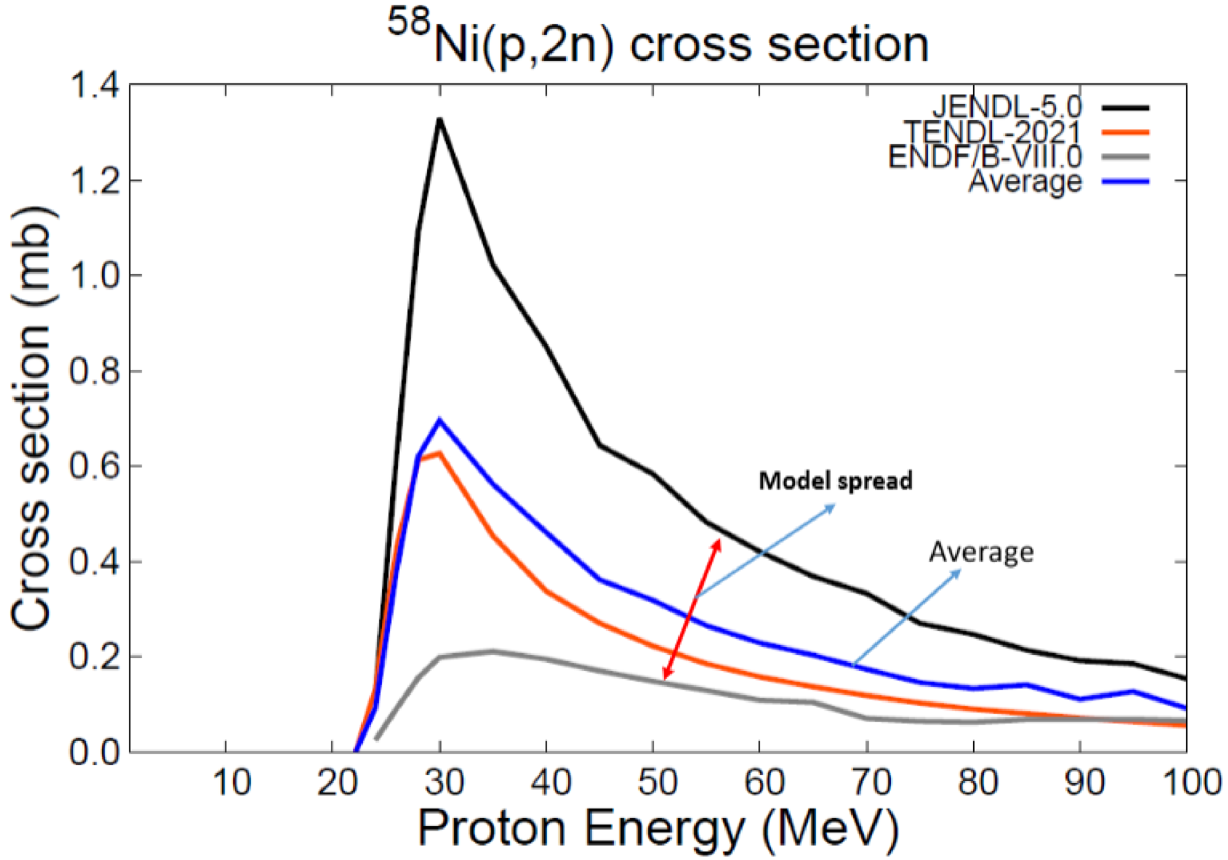




Averaging using equal weights

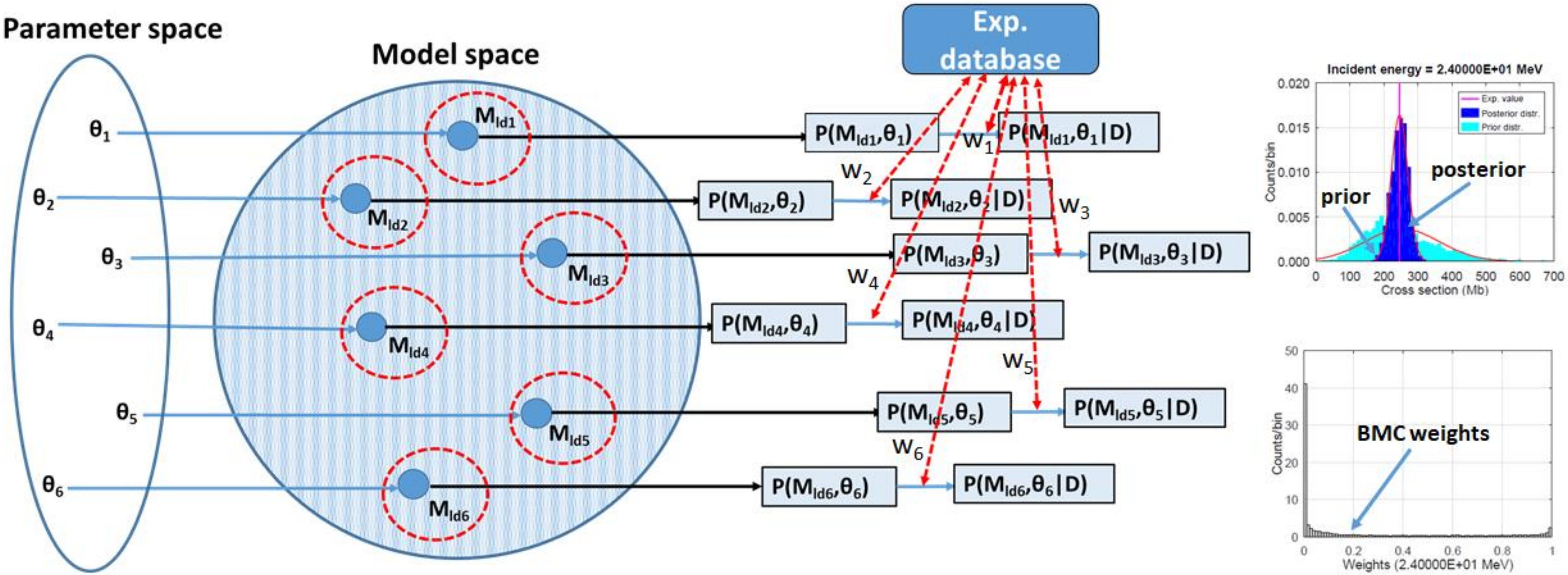
- We can assume that the evaluations from ENDF/B-VIII.0; TENDL-2021 and JENDL-5.0 are individual models.
- We assume again that all have equal weights, we can take an arithmetic average over the considered energy region.

We can build an entire nuclear data library based on the already existing nuclear data library.



No experimental data are not available, we can average over the libraries OR over models.

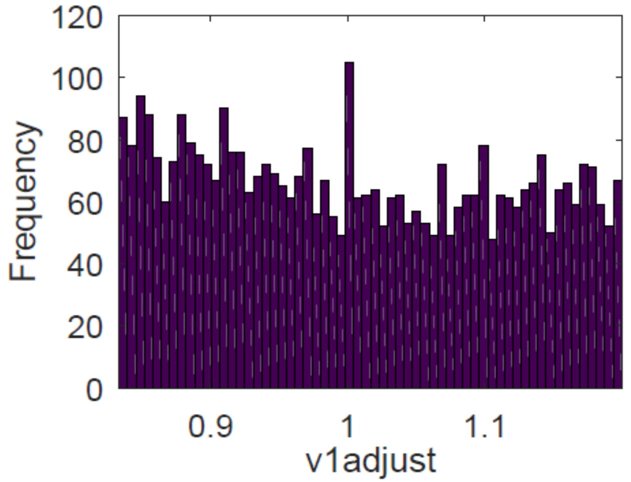
Graphical illustration of BMA: applied to level density models in TALYS

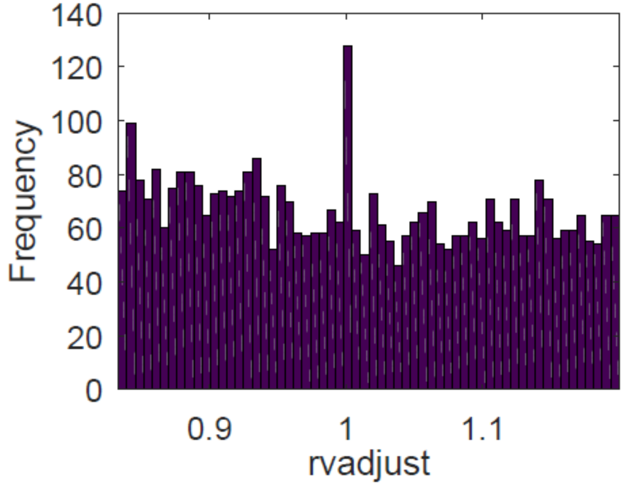


Model space, M - 6 level density (ld) models
Parameter space, θ – all TALYS parameters;

Prior distributions of parameters

Parameter	Uncertainty [%]	Parameter	Uncertainty [%]
OMP - phenomenological			
r_V^p	2.0	a_V^p	2.0
v_1^p	2.0	v_2^p	3.0
v_3^p	3.0	v_4^p	5.0
w_1^p	10.0	w_2^p	10.0
w_3^p	10.0	w_4^p	10.0
d_1^p	10.0	d_2^p	10.0
d_3^p	10.0	r_D^p	3.0
a_D^p	2.0	r_{SO}^p	10.0
a_{SO}^p	10.0	v_{SO1}^p	5.0
v_{SO2}^p	10.0	w_{SO1}^p	20.0
w_{SO2}^p	20.0	r_c^p	10.0
OMP - Semi-microscopic optical model (JLM)			
λ_V	5	$\lambda_V 1$	5
λ_W	5	$\lambda_W 1$	5
level density parameters			
a	11.25-0.03125.A	σ^2	30.0
E_0	20.0	T	10.0
k_{rot}	80.0	R_σ	30.0
Pre-equilibrium			
R_γ	50.0	M^2	30.0
g_π	11.25-0.03125.A	g_ν	11.25-0.03125.A
C_{break}	80.0	C_{knock}	80.0
C_{strip}	80.0	E_{surf}	20.0
$R_{\nu\nu}$	30.0	$R_{\pi\nu}$	30.0
$R_{\pi\pi}$	30.0	$R_{\nu\pi}$	30.0
Gamma ray strength function			
Γ_γ	5.0	$\sigma_{E\ell}$	20
$\Gamma_{E\ell}$	20	$E_{E\ell}$	10

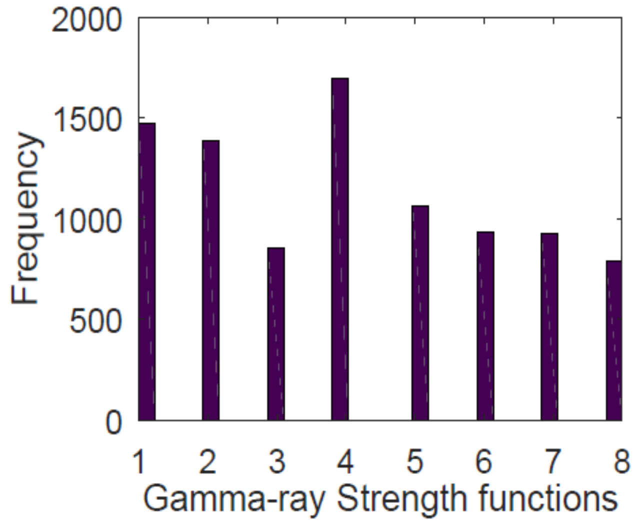


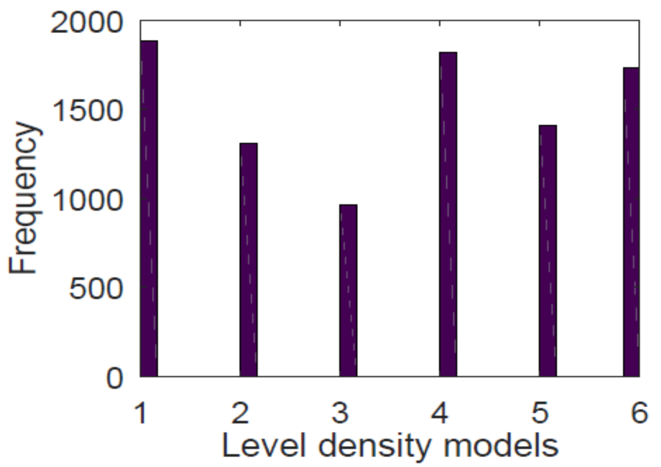


- Example: prior distributions of two optical model parameters. rvadjust – radius of the real central potential and v1adjust – is an adjustable parameter used in the computation of the depth of the real central potential.

- The parameter uncertainties were taken from TENDL and then multiplied by a factor of 5.

Prior distributions of models





- Example: prior distributions for 8 gamma ray strength functions and 6 level density models

- Uniform prior
- Each model is assigned a unique identifier before sampling

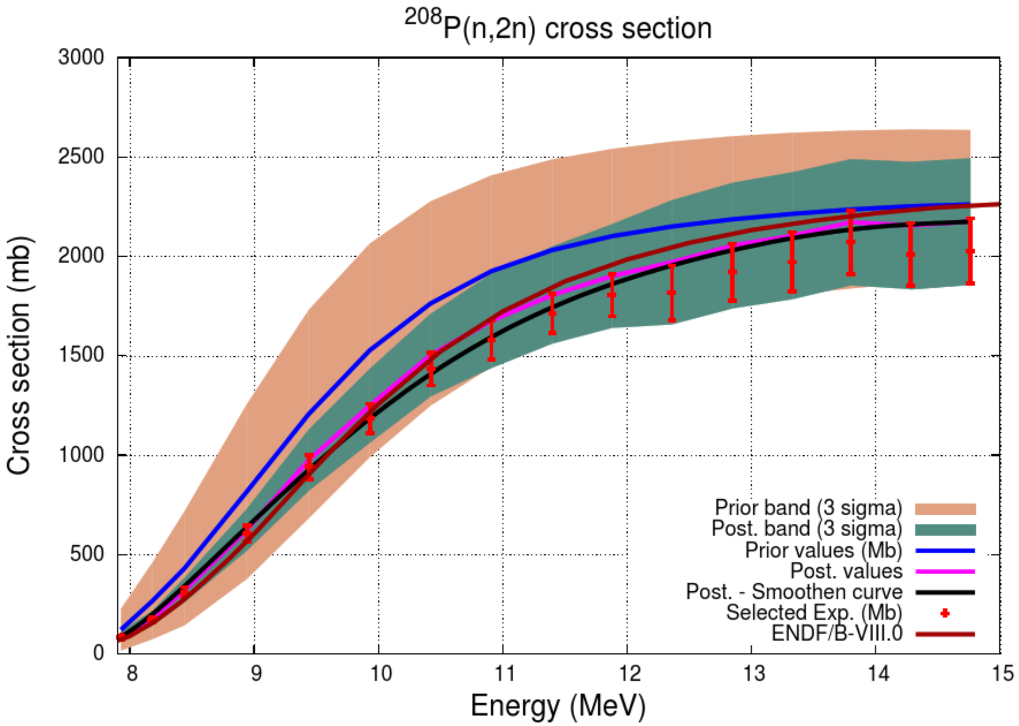
- About 100 unique model combinations generated in total

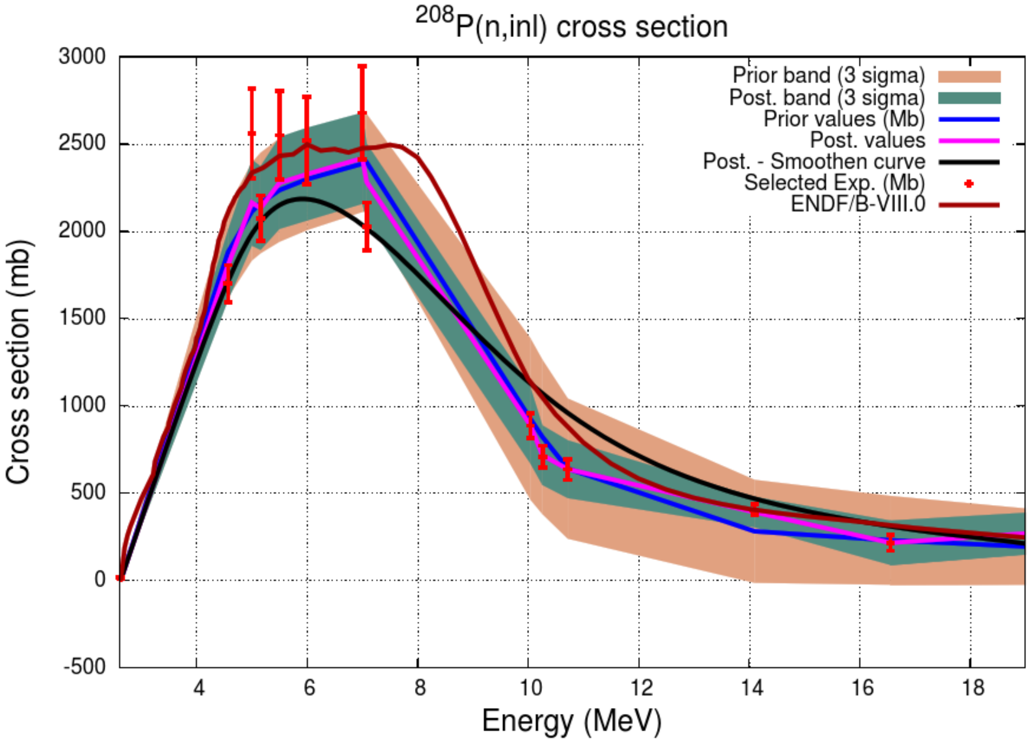
TALYS keywords	Number of models	Model Name
preeqmode	4	Pre-equilibrium (PE)
ldmodel	6	Level density models
ctmglobal	1	Constant Temperature
massmodel	4	Mass model
widthmode	4	Width fluctuation
spincutmodel	2	Spin cut-off parameter
gshell	1	Shell effects
statepot	1	Excited state in Optical Model
spherical	1	Spherical Optical Model
radialmodel	2	Radial matter densities
shellmodel	2	Liquid drop expression
kvibmodel	2	Vibrational enhancement
preeqspin	3	Spin distribution (PE)
preeqsurface	1	Surface corrections (PE)
preeqcomplex	1	Kalbach model (pickup)
twocomponent	1	Component exciton model
pairmodel	2	Pairing correction (PE)
expmass	1	Experimental masses
strength	8	Gamma-strength function
strengthM1	2	M1 gamma-ray strength function
jlmmode	4	JLM optical model

Total of 21 model types considered

BMA applied to n+Pb208 in the fast region

Comparing with ENDF/B-VIII.0

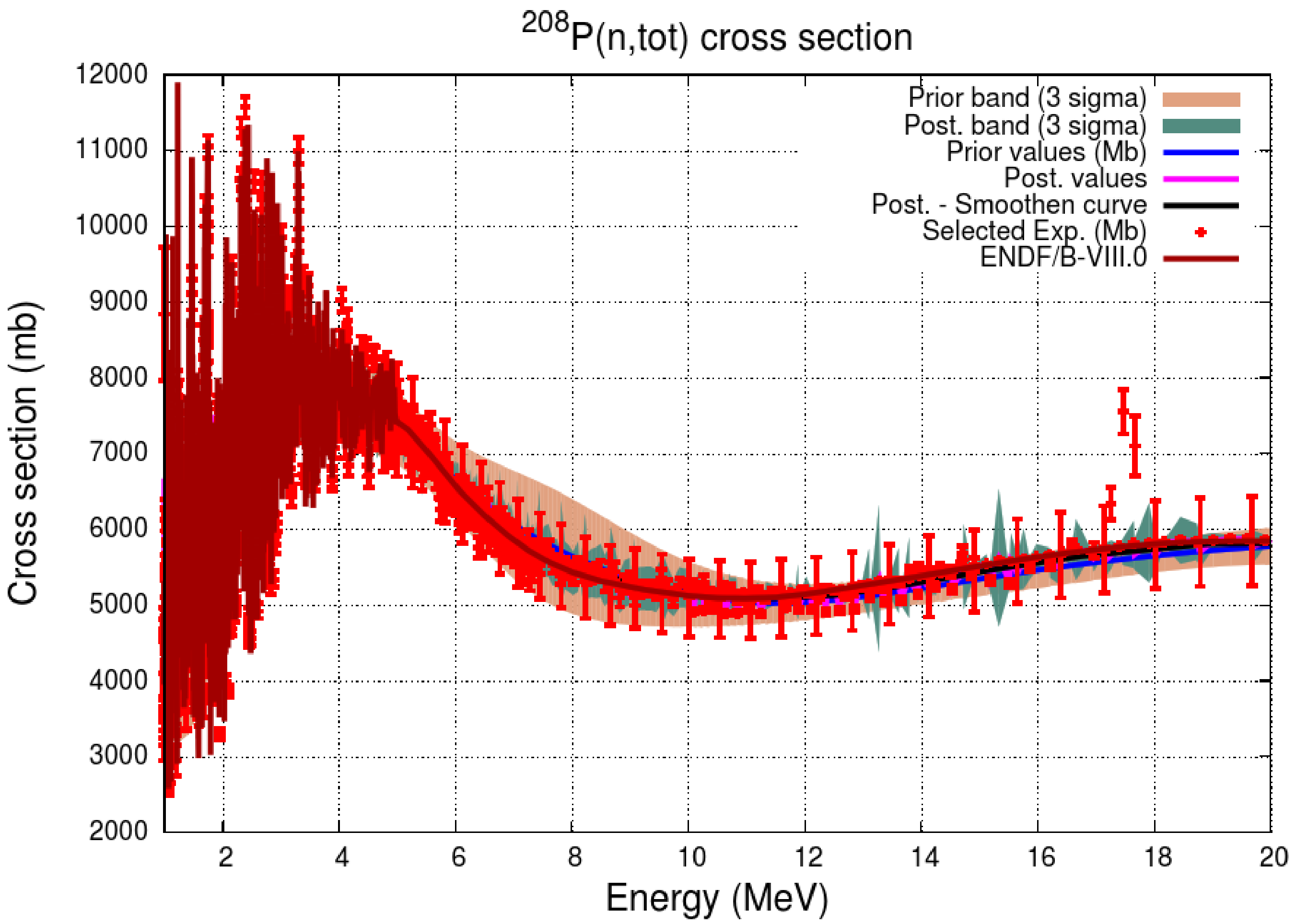




5000 random ENDF files produced.

Comparing with ENDF/B-VIII.0

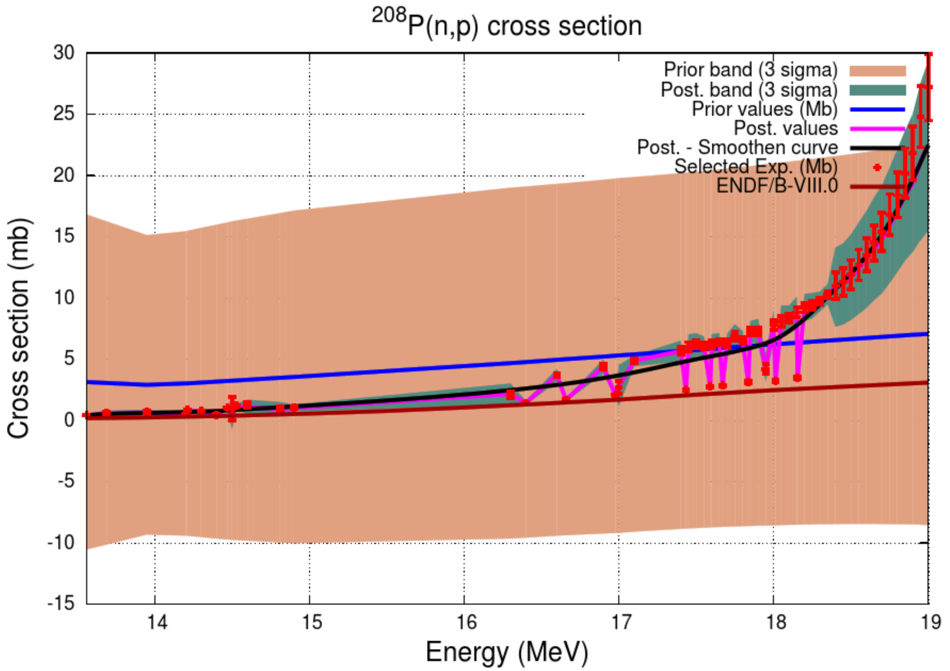
- Generally, the uncertainties for the neutron induced cross sections were narrow.

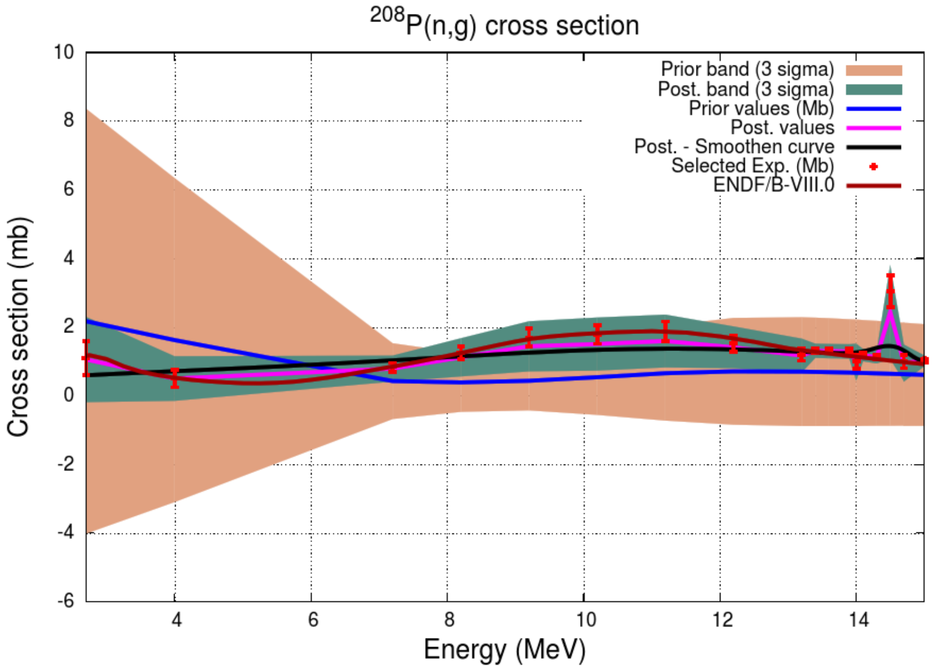


5000 random ENDF files produced.

BMA applied to n+Pb208 in the fast region

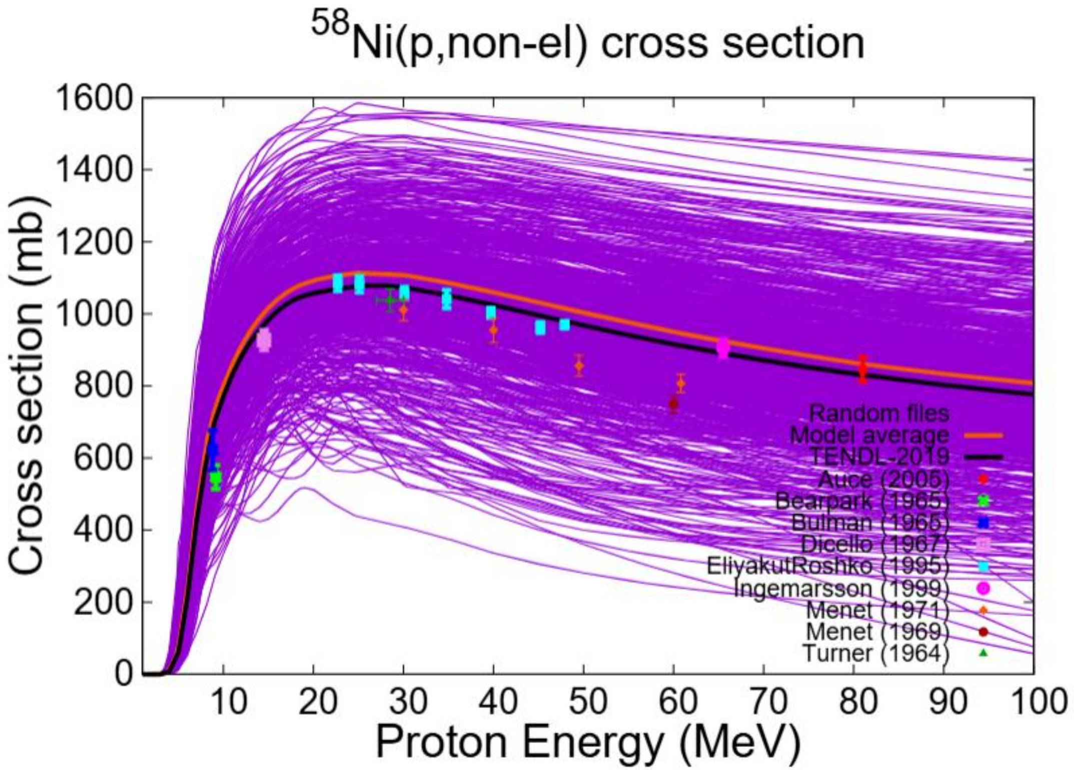
Comparing with ENDF/B-VIII.0



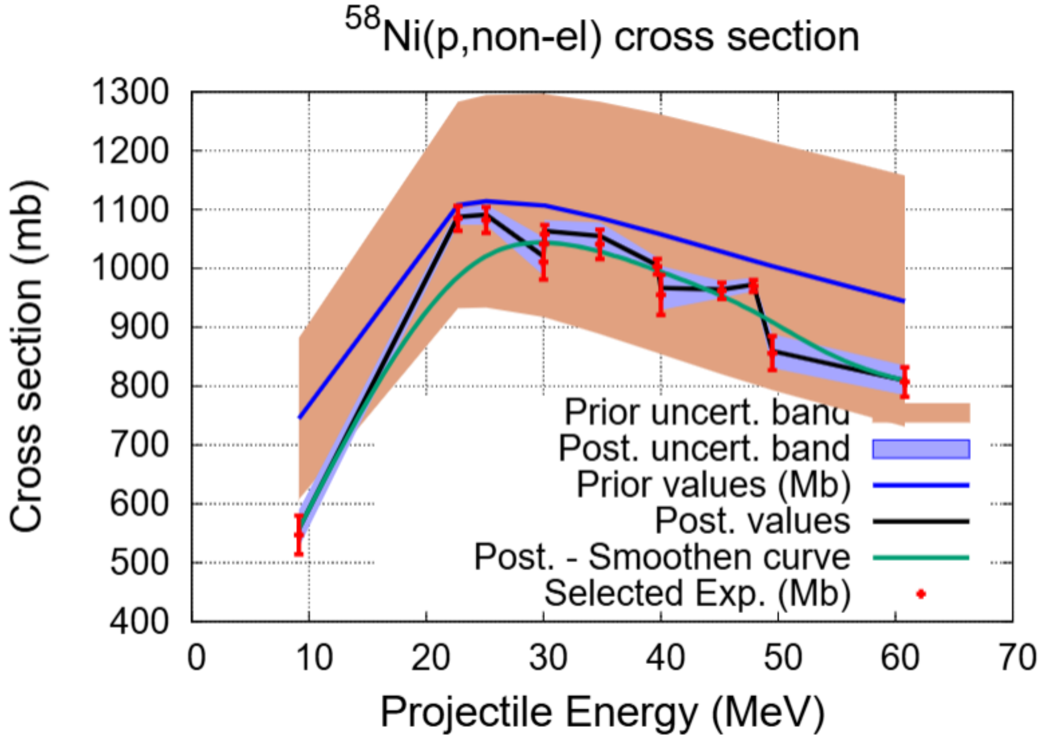


5000 random ENDF files produced.

BMA applied to p+Ni58 in the fast region



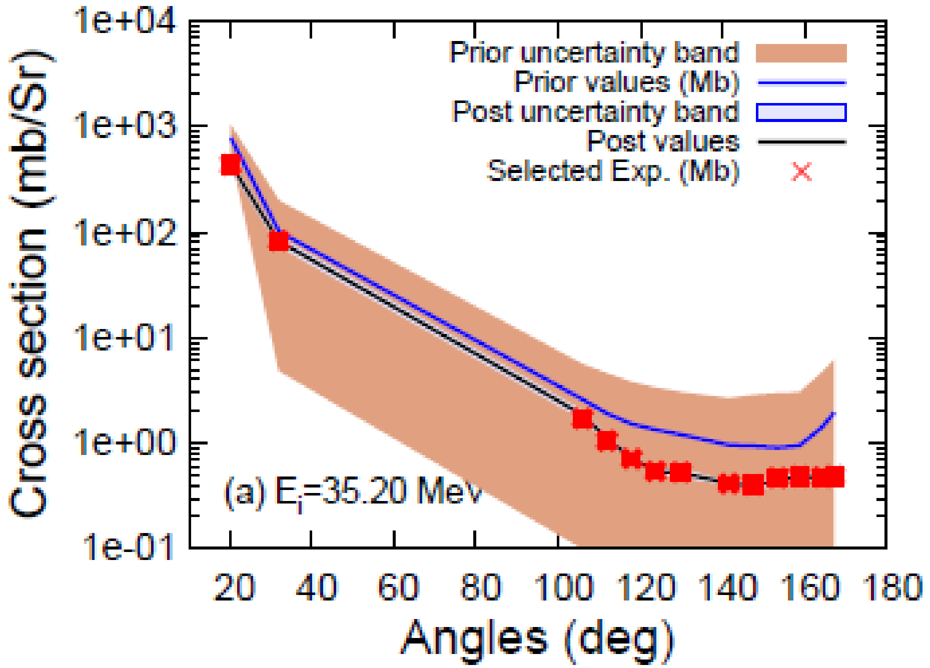
9000 random ENDF files produced.

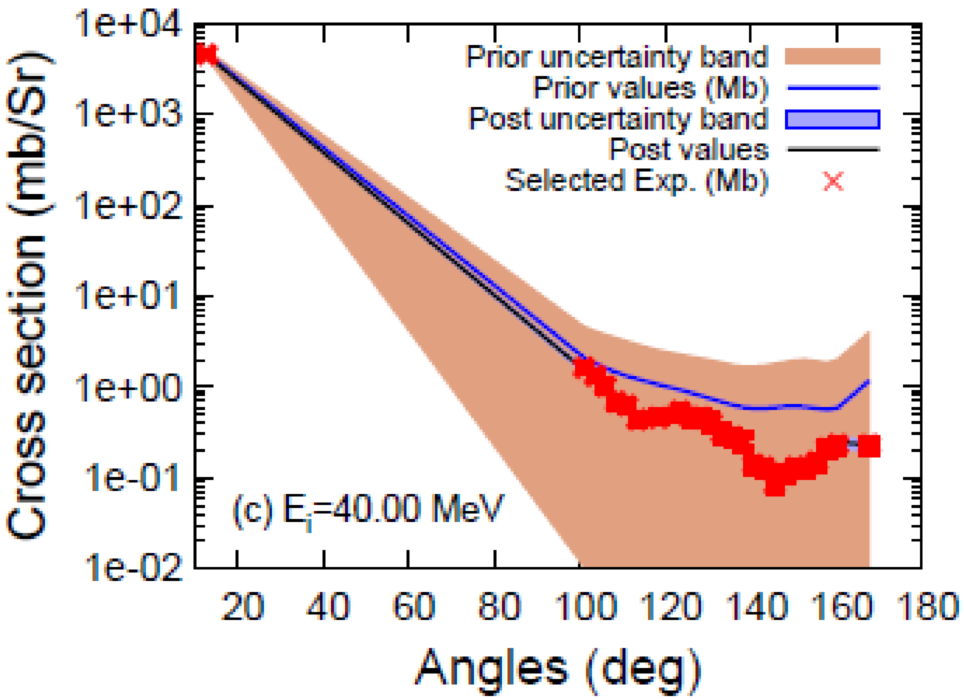


Uncertainty = +/- 1 sigma

BMA with experiments

- **Elastic angular distributions (p+Ni58)**





- **A smooth function was applied to smoothen the posterior mean curve**

Extracting model and parameter uncertainties

- **Assuming no correlations between the different model vectors and the parameters,**
  - **➔ the total variance at energy *i* for channel *c* can be given (similar to the TMC method) as:**

$$V_{tot}^{ci} = V_{mod}^{ci} + V_{par}^{ci}$$

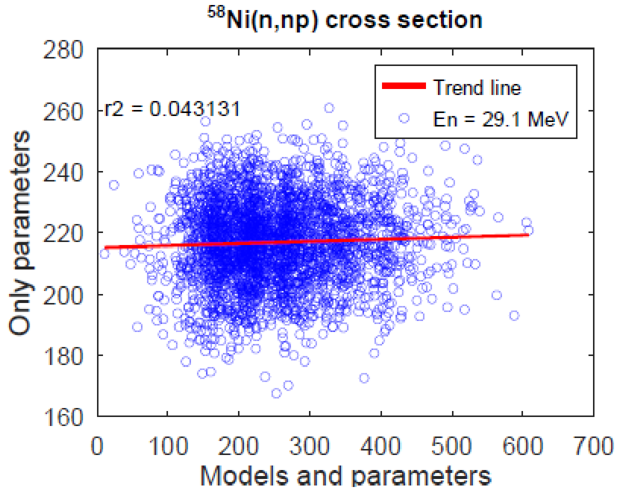
Total variance

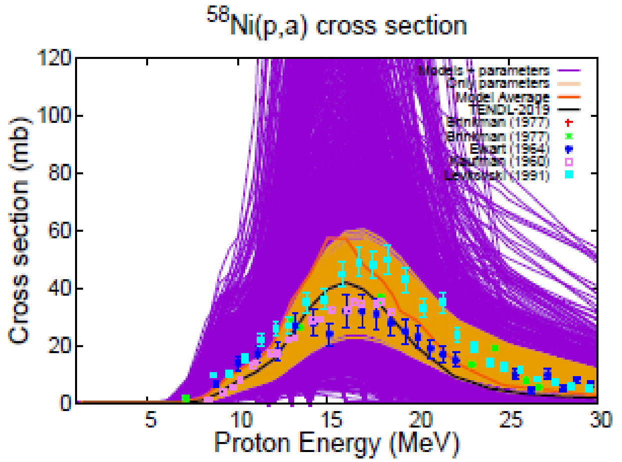
Model variance at energy i

Parameter variance

$$U_{mod}^{ci} = \sqrt{V_{tot}^{ci} - V_{par}^{ci}}$$

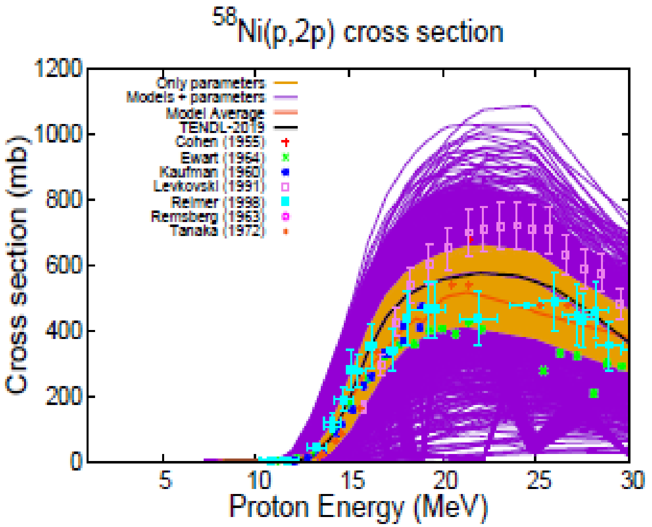
Model uncertainty





Model and parameter uncertainties for ^{58}Ni(p,np)

Incident energy (MeV)	Total uncertainty (1σ)	Model uncertainty (1σ)	Parameter uncertainty (1σ)
15.7	46.5	46.44	2.5
16.0	52.9	52.84	2.9
16.2	54.4	54.27	3.0
16.8	62.5	62.35	3.7
17.1	66.1	66.00	4.1
17.3	66.9	66.81	4.3
17.7	72.0	71.86	4.8
17.9	76.0	75.87	5.1
18.2	80.9	80.72	5.5
18.4	83.9	83.73	5.9
19.0	90.3	90.05	7.0
19.1	87.9	87.57	7.2
19.3	85.1	84.76	7.7
19.5	85.4	85.01	8.3
20.0	98.7	98.18	9.9



Conclusion

- Bayesian Model Averaging (BMA) together with smooth functions can produce fits in good agreement with experimental data for both neutron and proton induced reactions
- **An entire evaluation can be produced including prior and posterior covariances and correlations**
- An entire nuclear data library can be produced from averaging over all the existing nuclear data libraries.
- As spin-off, model uncertainties at each incident energy can be extracted.
- This can be extended to criticality systems in a Total-Total Monte Carlo way
- Downside of the method is that it is computationally expensive and also, experimental data used must be chosen carefully.
- Explore the use of energy dependent parameters in BMA of nuclear data

Acknowledgment

- Many thanks to D. Rochman, G. Schnabel, and A.J. Koning for many discussions on this topic.

- Ref. [1]. Alhassan, E., Rochman, D., Schnabel, G., & Koning, A. J. (2024). Bayesian Model Averaging (BMA) for nuclear data evaluation. NUCL SCI TECH 35, 205 (2024). https://doi.org/10.1007/s41365-024-01543-w

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