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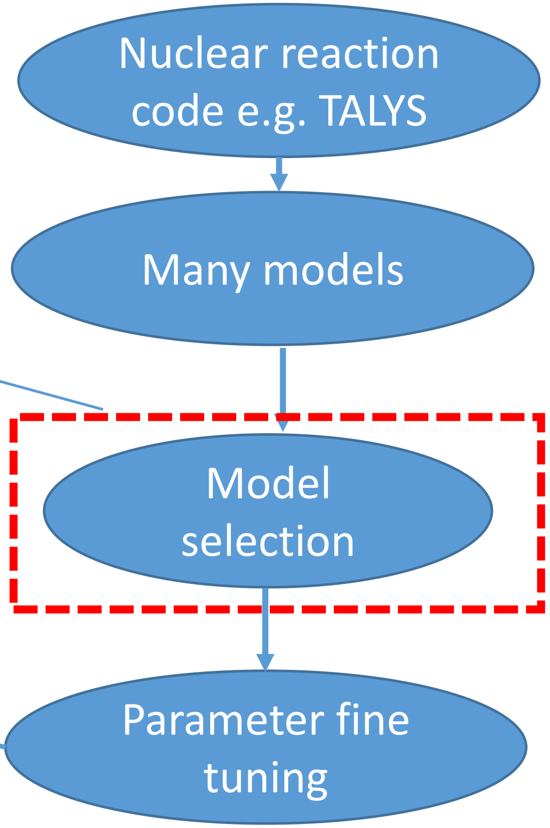
Accounting for model uncertainty in Bayesian evaluation of nuclear data

Introduction and justification

“As long as a “*near perfect model*” is not available, a pure Monte Carlo solution based on model parameters alone cannot adequately combine theoretical results and microscopic experimental data.” – **D. Rochman, A.J. Koning, E. Bauge and A.J.M. Plompen,** From flatness to steepness: Updating TALYS covariances with experimental information. Annals of Nuclear Energy, 73 7-16 (2014). https://doi.org/10.1016/j.anucene.2014.06.016

- **Current model-based nuclear data evaluations makes use of a single model vector. E.g. UMC-G/B, BMC, TMC, BFMC, iBMC, …**

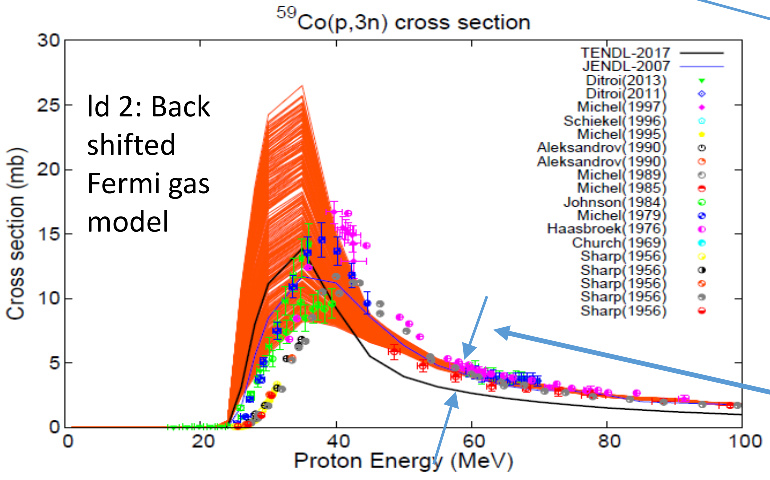
- **We are constrained by the deficiencies of the selected models**



<u>Uncertainties in nuclear data can be classified into:</u>

- Parametric uncertainties due to unknown parameter values used to define the selected models
- Measurement uncertainty due to the experimental uncertainties used in calibrating the models
- Computational uncertainties e.g. in Monte Carlo calculations

- **Model uncertainties due to the choice of the model**

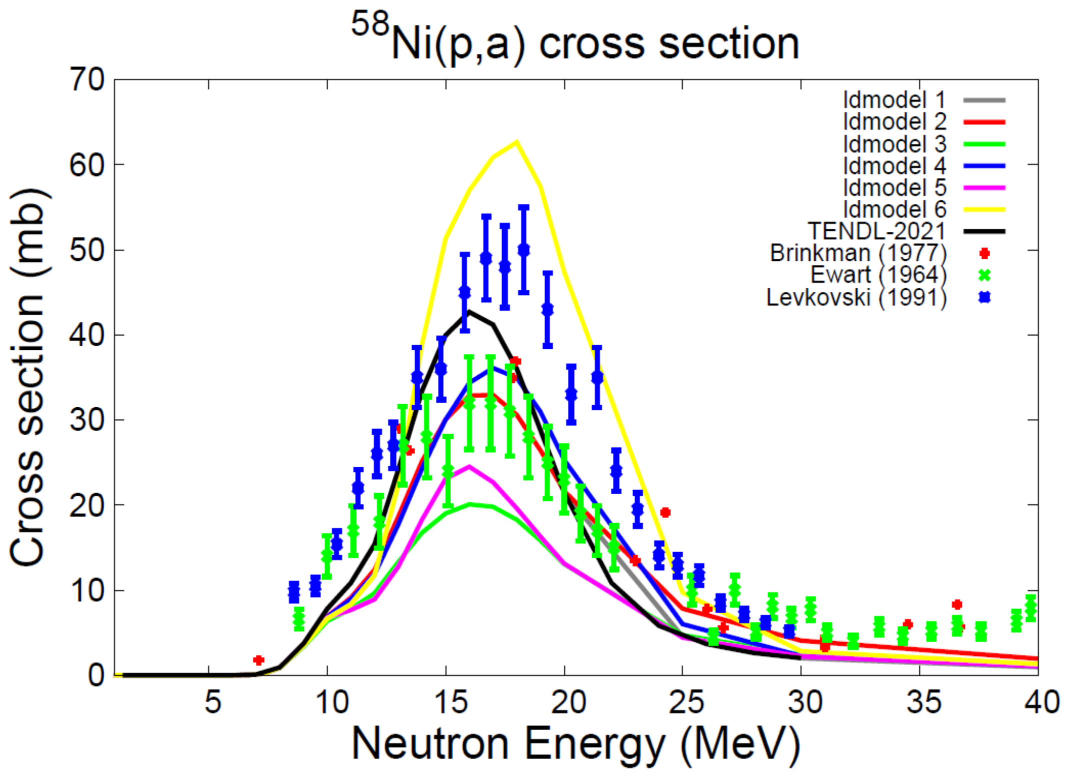


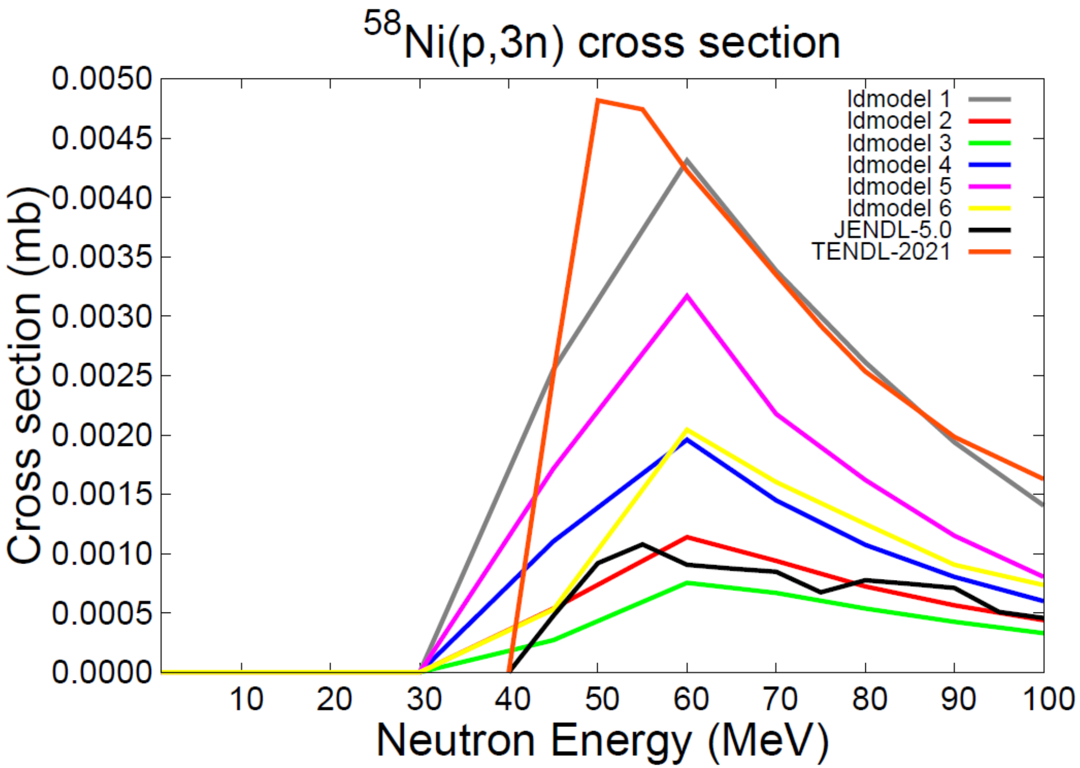
TALYS: ld 2 + other models + parameter variation

Introduction: TALYS has many models

- Each model has its own strengths.
- For example, 6 level density models implemented in TALYS

Our assumption: ‘All models are wrong, … ’
- George Box

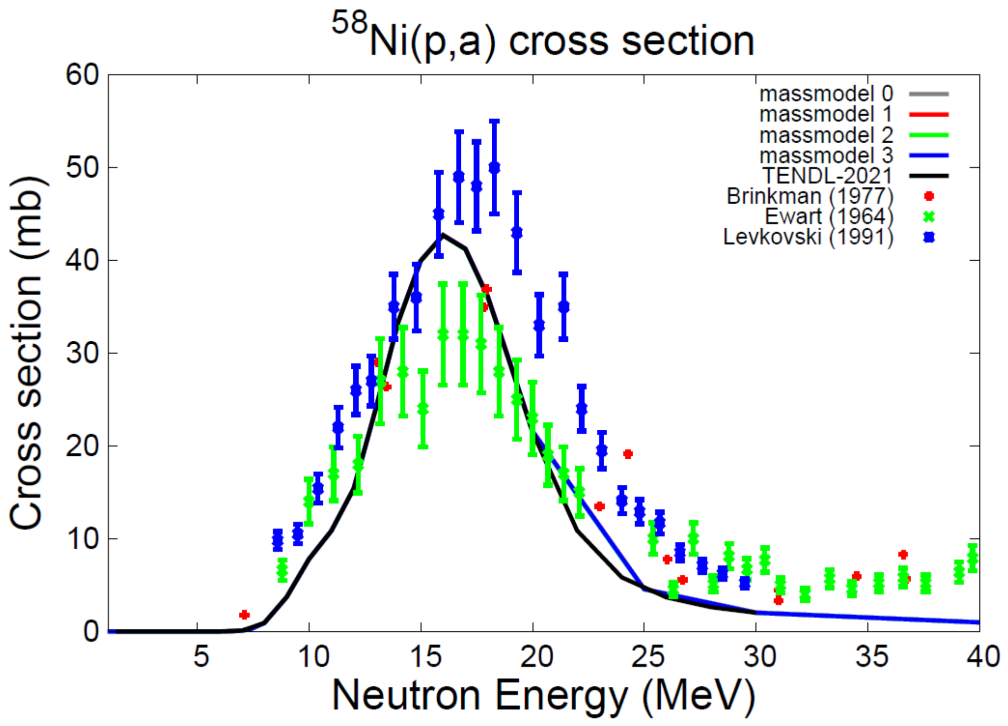


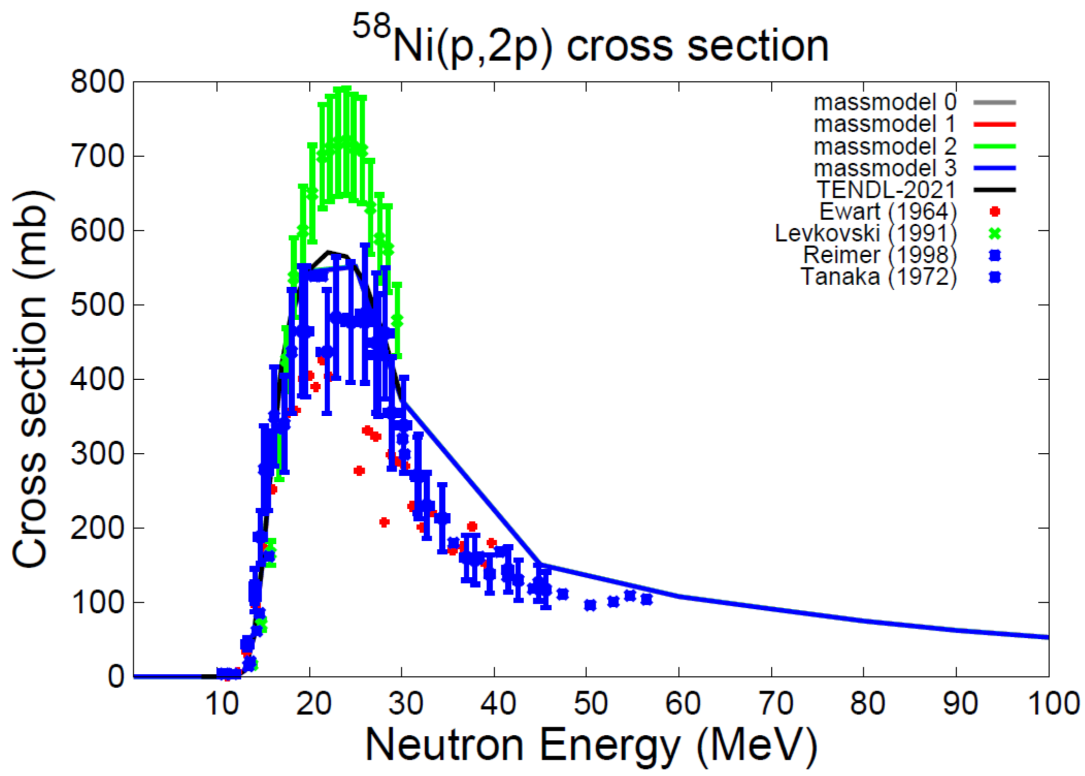


Introduction: TALYS has many models

- **The cross sections had low sensitivity to the variations of the mass models**

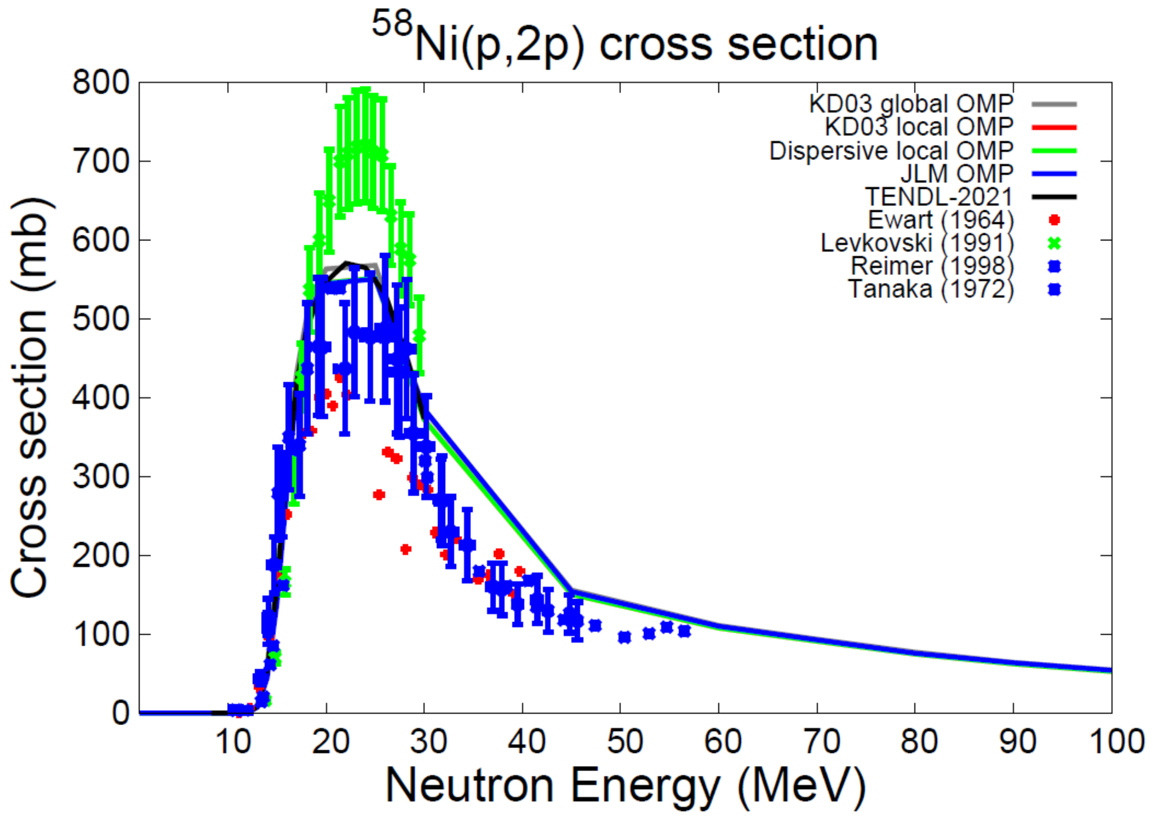
All other models were kept as the default models while the mass models were varied one-at-a-time

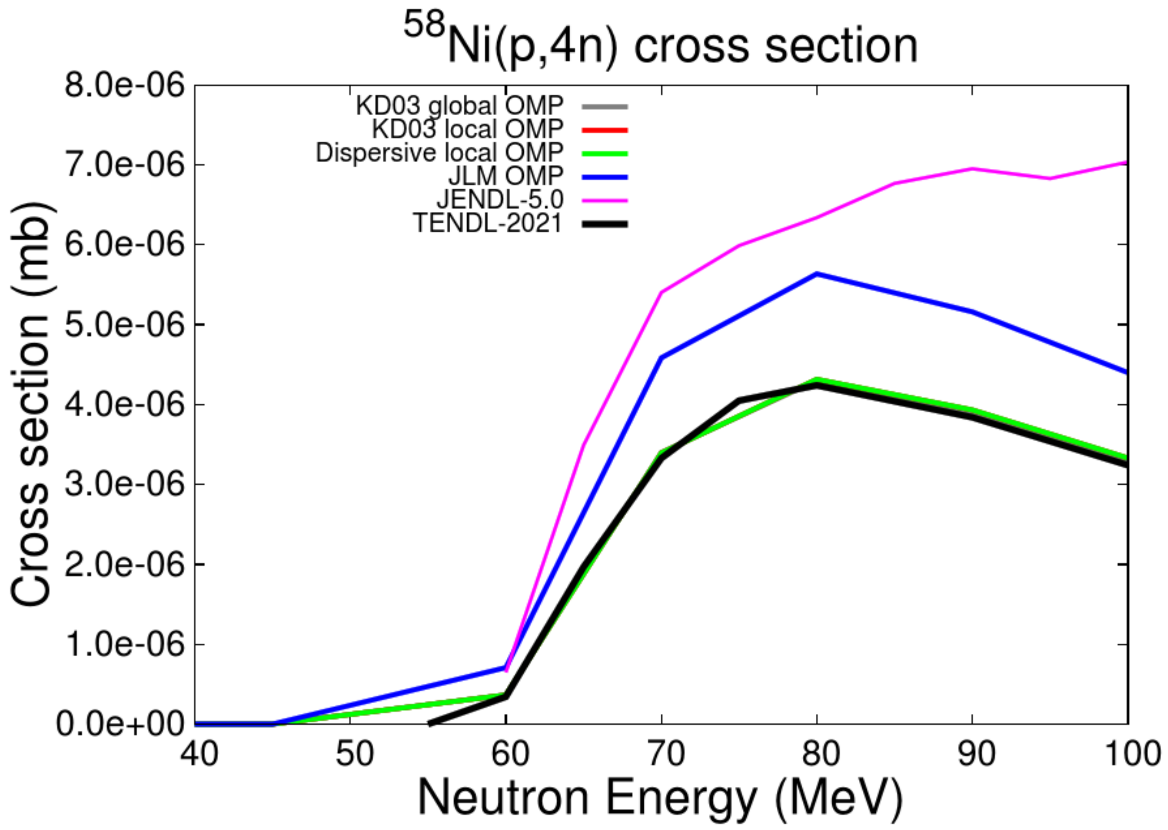




Introduction: TALYS has many models

- **The cross sections had low sensitivity to the variations of the phenomenological optical models except for the JLM model.**





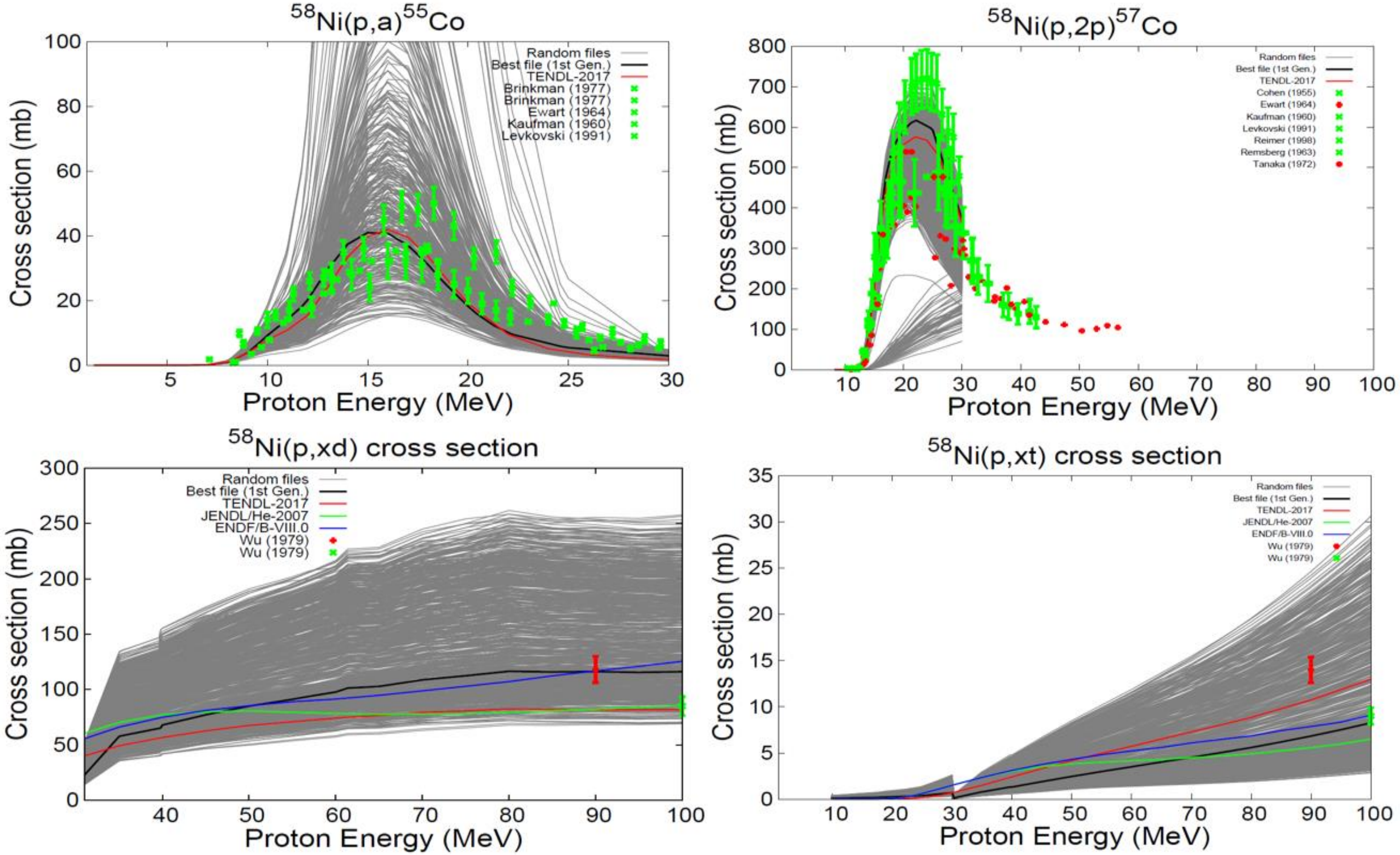
Choosing between computing models

If we assume that there is a `true' model among candidate models, we can select the best model using:

- **AIC, BIC, MLE, etc.**

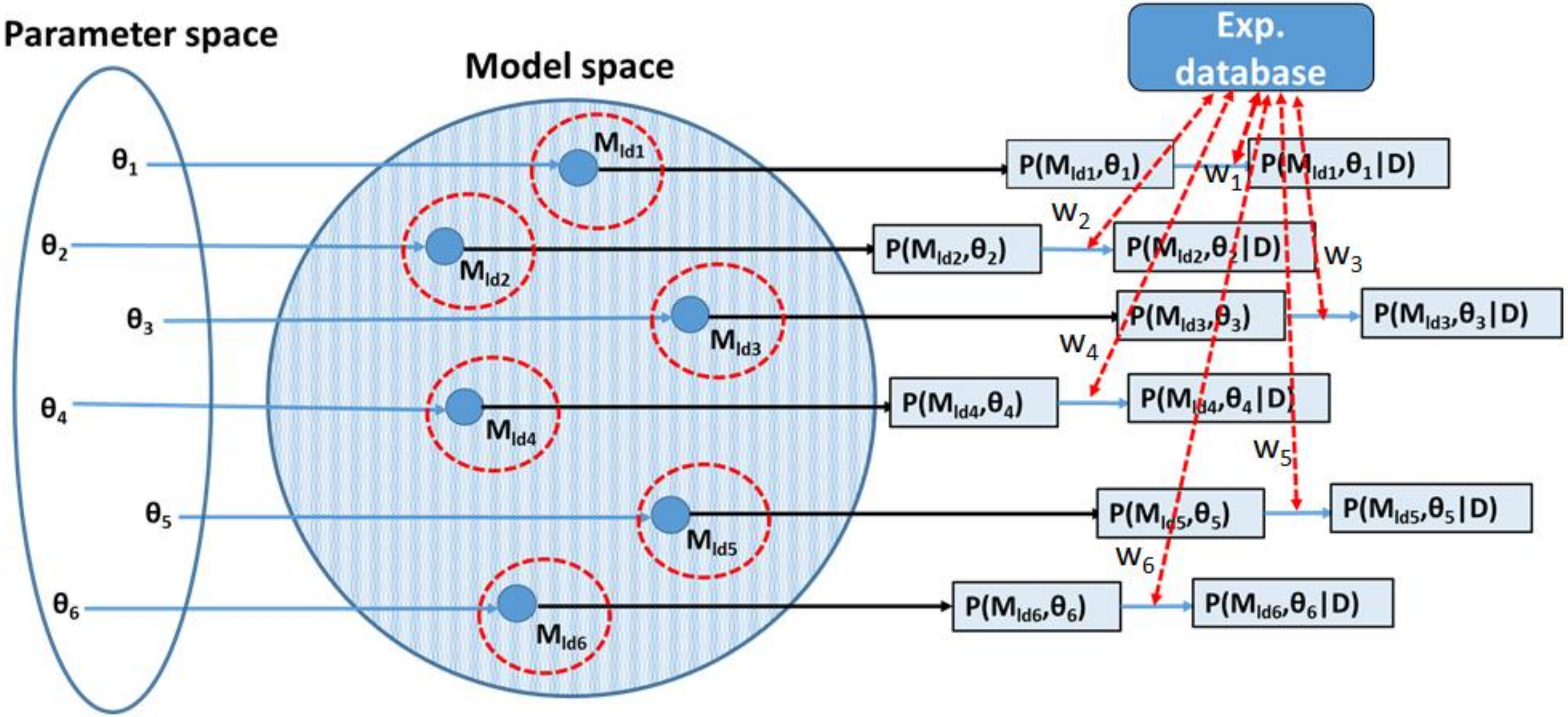
Selected model	Default
preeqmode 3: Exciton model - Numerical transition rates with optical model for collision probability	preeqmode 2: Exciton model: Numerical transition rates with energy-dependent matrix element
ldmodel 2: Back-shifted Fermi gas model	ldmodel 1: Constant temperature + Fermi gas model
widthmode 2: Hofmann-Richert-Tepel-Weidenmüller	widthmode 1: Moldauer model

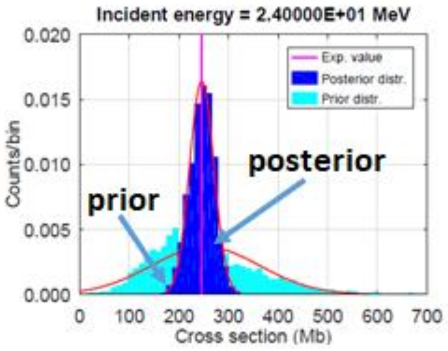
Sometimes, the selected model set can reproduce experimental data relatively well.

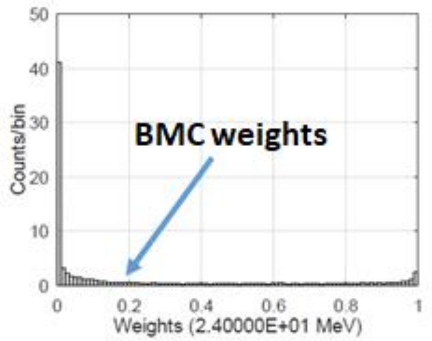


Graphical illustration of BMA: applied to level density models in TALYS

Our assumption: 'All models are wrong, … '
- George Box



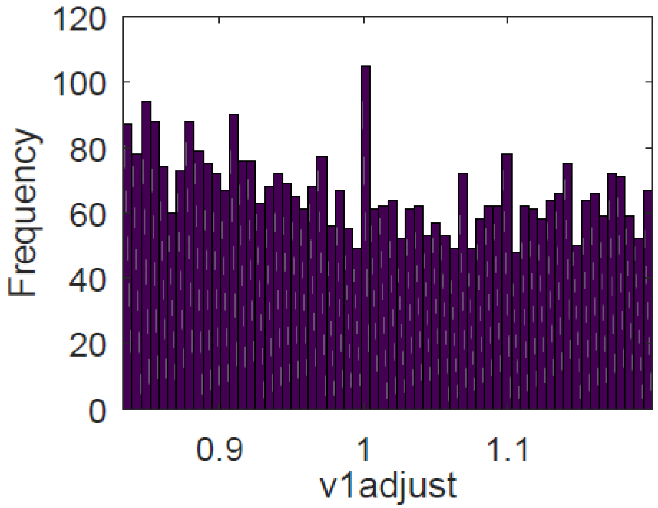


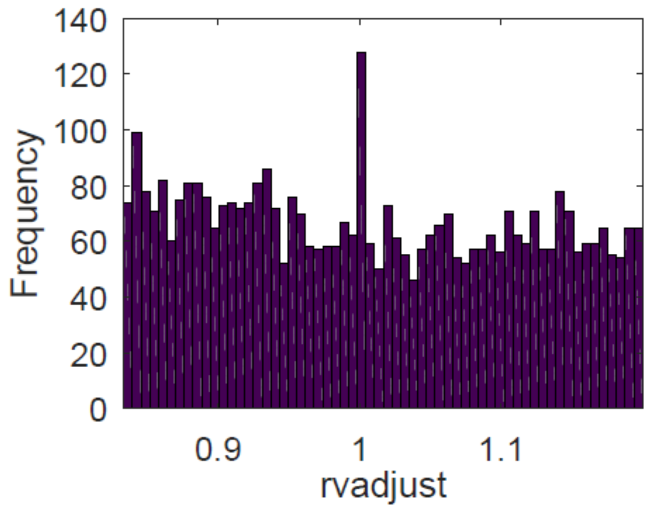


Model space, M - 6 level density (ld) models
Parameter space, θ – all TALYS parameters;

Prior distributions of parameters

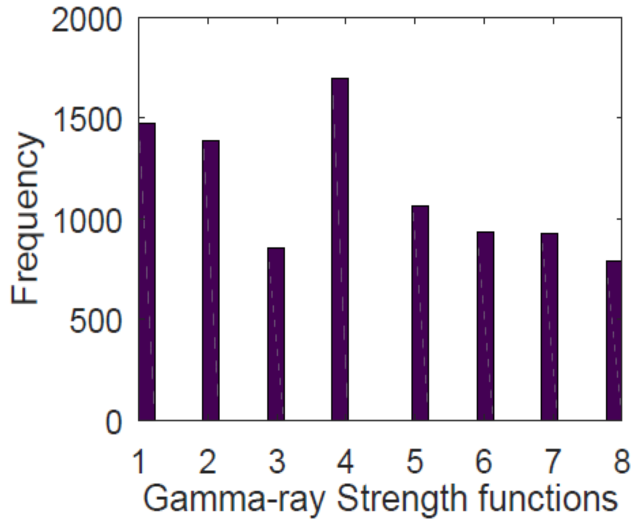
Parameter	Uncertainty [%]	Parameter	Uncertainty [%]
OMP - phenomenological			
r_V^p	2.0	a_V^p	2.0
v_1^p	2.0	v_2^p	3.0
v_3^p	3.0	v_4^p	5.0
w_1^p	10.0	w_2^p	10.0
w_3^p	10.0	w_4^p	10.0
d_1^p	10.0	d_2^p	10.0
d_3^p	10.0	r_D^p	3.0
a_D^p	2.0	r_{SO}^p	10.0
a_{SO}^p	10.0	v_{SO1}^p	5.0
v_{SO2}^p	10.0	w_{SO1}^p	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

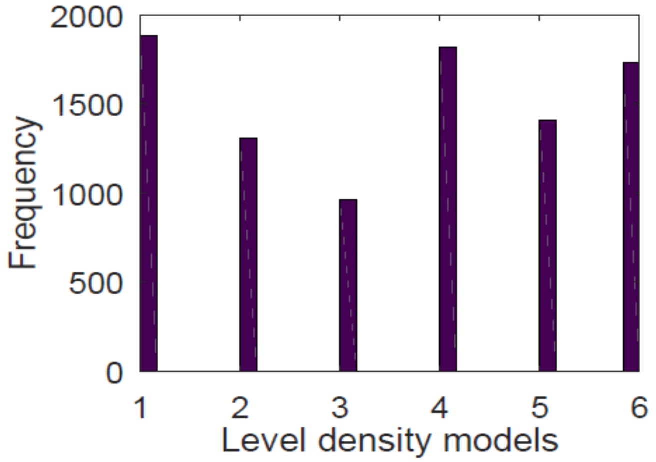




- Example: prior distributions of two optical model parameters. rvadjust – radius of the real central potential and v1adjust – is an adjustable parameter used in the computation of the depth of the real central potential.
- The parameter uncertainties were taken from TENDL and then multiplied by a factor 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

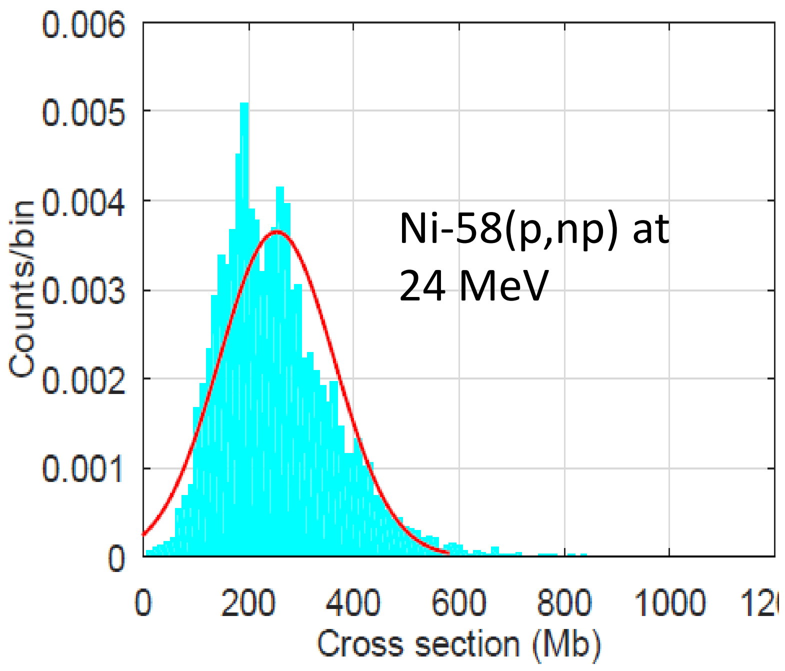
- About 100 unique model combinations generated in total

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

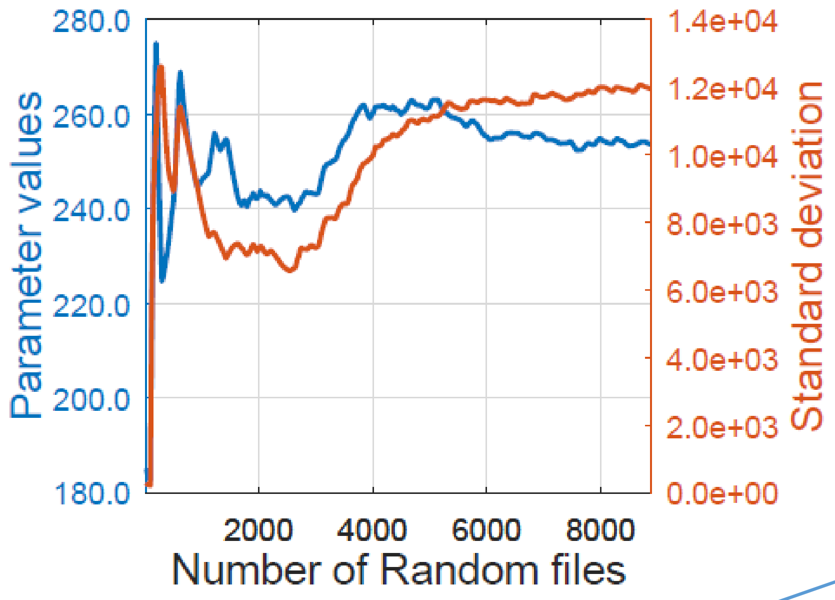
Total of 21 model types considered

Joint prior distributions of the cross sections

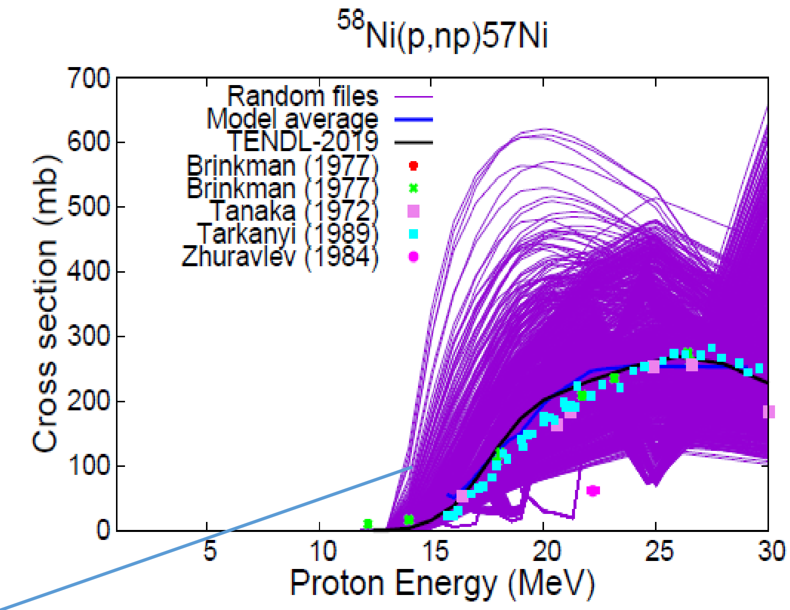
Distribution of Ni-58(p,np) cross section at 24 MeV



Convergence of random cross sections



Random cross section curves



P(M,θ,σ)

The spread in the cross section is a result of the variation of both models and their parameters

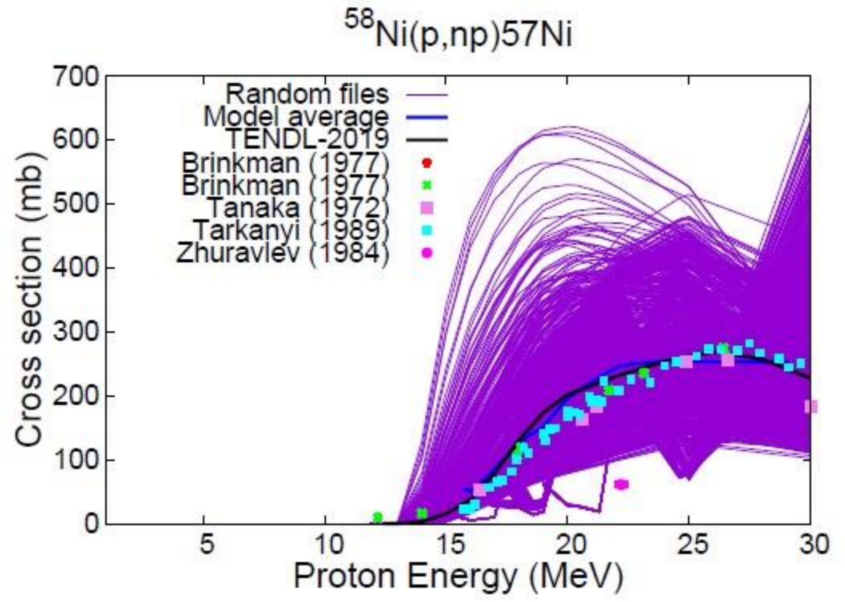
BMA without experiments

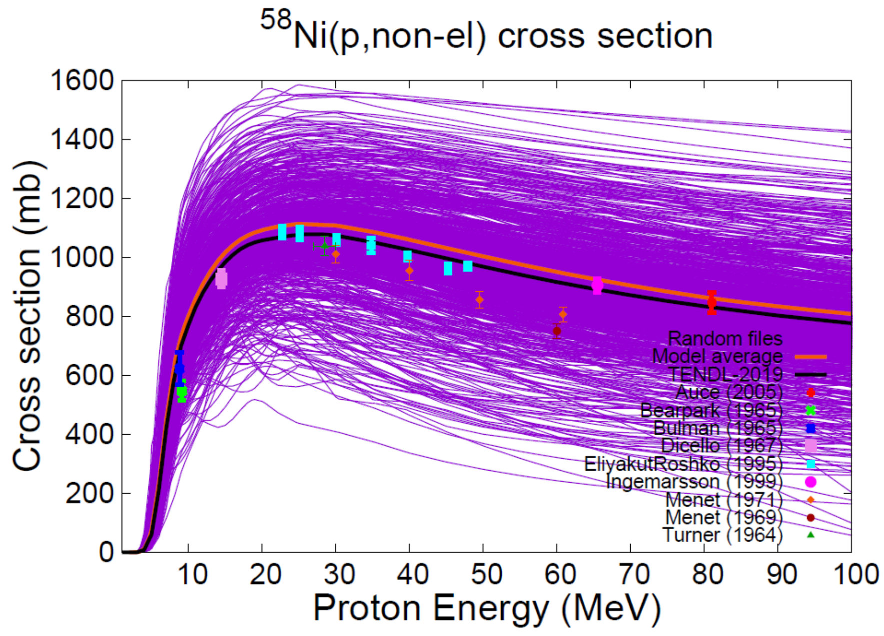
Our assumption: 'All models are wrong, … '
- George Box

A simple average over all the models for a cross section at can be given as:

$$\overline{\sigma_{cik}^{cal}} = \frac{1}{K}\sum_{k=1}^{K}\overrightarrow{\sigma_{cik}^{cal}}$$

Over 10,000 random cross section curves were produced.



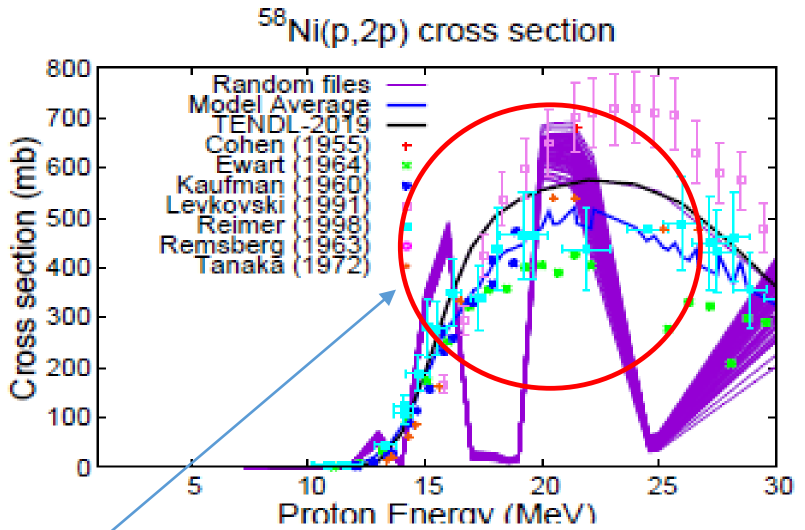


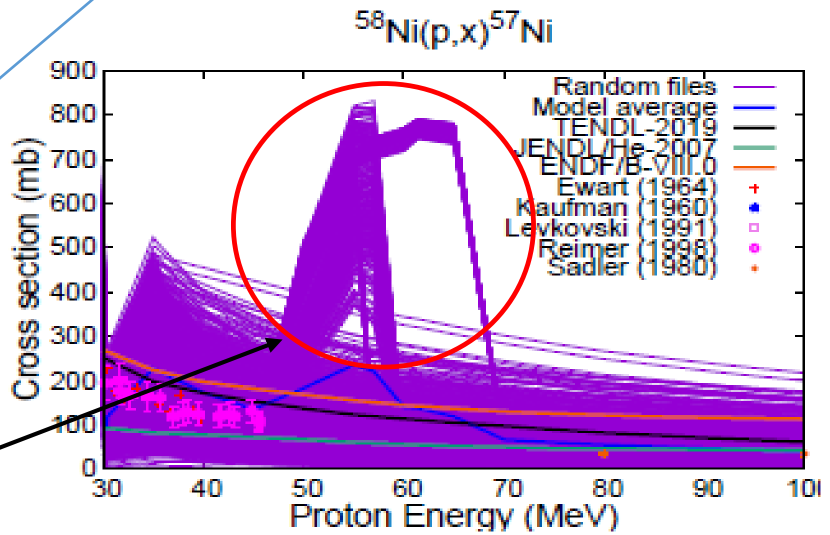
BMA without experiments - `Bad' models

Our assumption: 'All models are wrong, … '
- George Box

A simple average over all the models for a cross section at can be given as:

$$\overline{\sigma_{cik}^{cal}} = \frac{1}{K}\sum_{k=1}^{K}\overrightarrow{\sigma_{cik}^{cal}}$$





'bad models can distort a simple average over the models

- Identify and discard all 'bad' model combinations (and also from future calculations)

Bayesian Model Averaging (BMA)

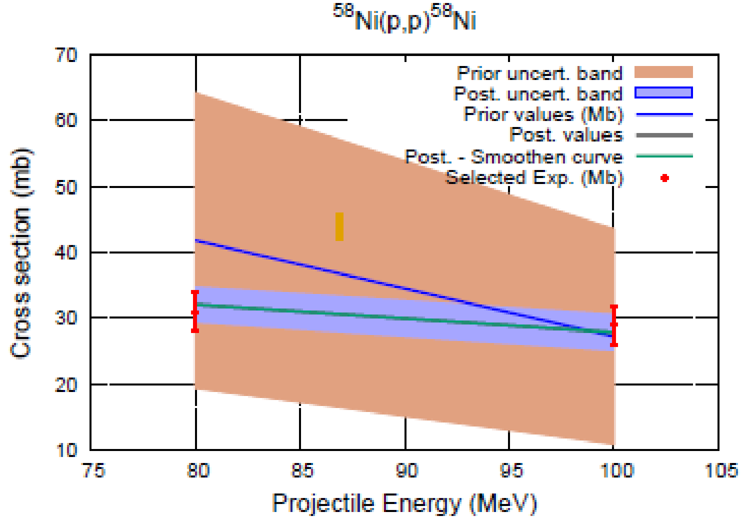
Because the updating is done locally at the energy level, kinks can be observed in the BMA posterior file which can be smoothened using spline interpolation

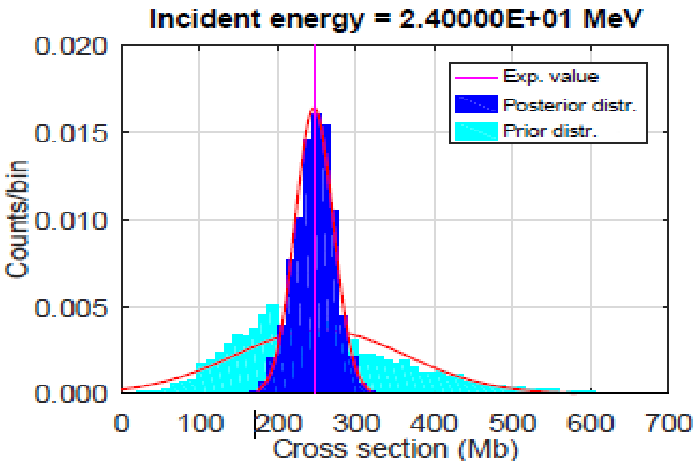
$$P\left(\overrightarrow{M_j}, \overrightarrow{\sigma_{cik}^{cal}} \middle| \overrightarrow{\sigma_{ci}^{exp}}\right) = \frac{P\left(\overrightarrow{\sigma_{ci}^{exp}} \middle| \overrightarrow{M_j}, \overrightarrow{\theta_k}, \overrightarrow{\sigma_{cik}^{cal}}\right) * P\left(\overrightarrow{M_j}, \overrightarrow{\theta_k}, \overrightarrow{\sigma_{cik}^{cal}}\right)}{P\left(\overrightarrow{\sigma_{E_i}^{exp}}\right)}$$

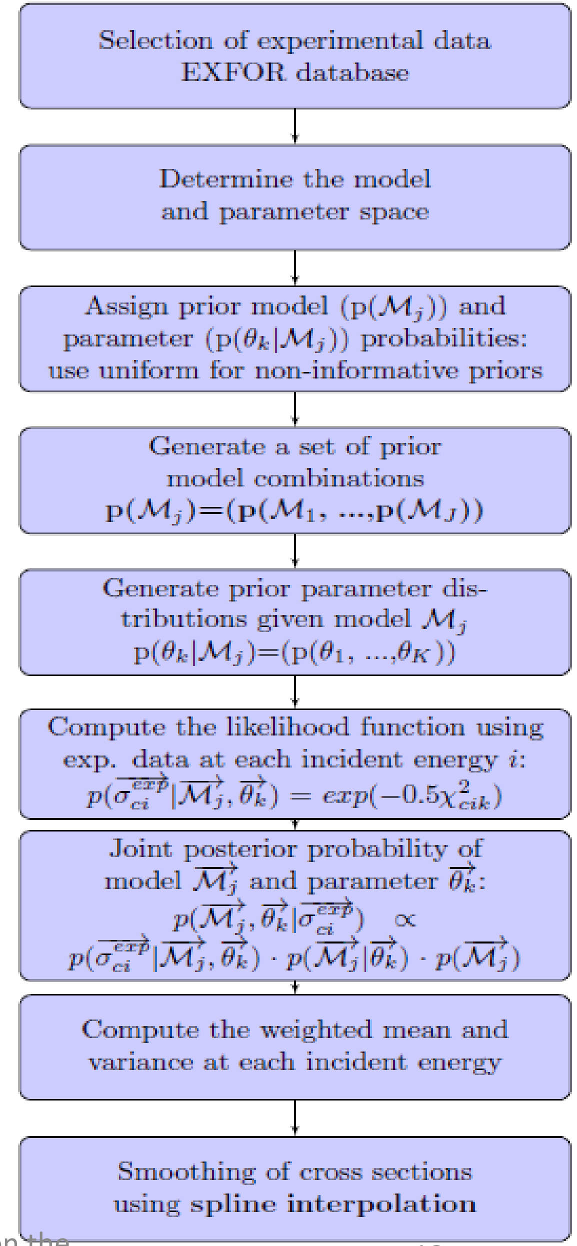
$$\propto P\left(\overrightarrow{\sigma_{cik}^{exp}} \middle| \overrightarrow{M_j}, \overrightarrow{\theta_k}, \overrightarrow{\sigma_{cik}^{cal}}\right) * P\left(\overrightarrow{M_j}, \overrightarrow{\theta_k}, \overrightarrow{\sigma_{cik}^{cal}}\right)$$

Likelihood function:

$$P\left(\overrightarrow{\sigma_{cik}^{exp}} \middle| \overrightarrow{M_j}, \overrightarrow{\theta_k} \overrightarrow{\sigma_{cik}^{cal}}\right) = exp\left(-\frac{\chi_{cik}^2}{2}\right)$$







Bayesian Model Averaging (BMA)

Because the updating is done locally at the energy level, kinks can be observed in the BMA posterior file which can be smoothened using spline interpolation

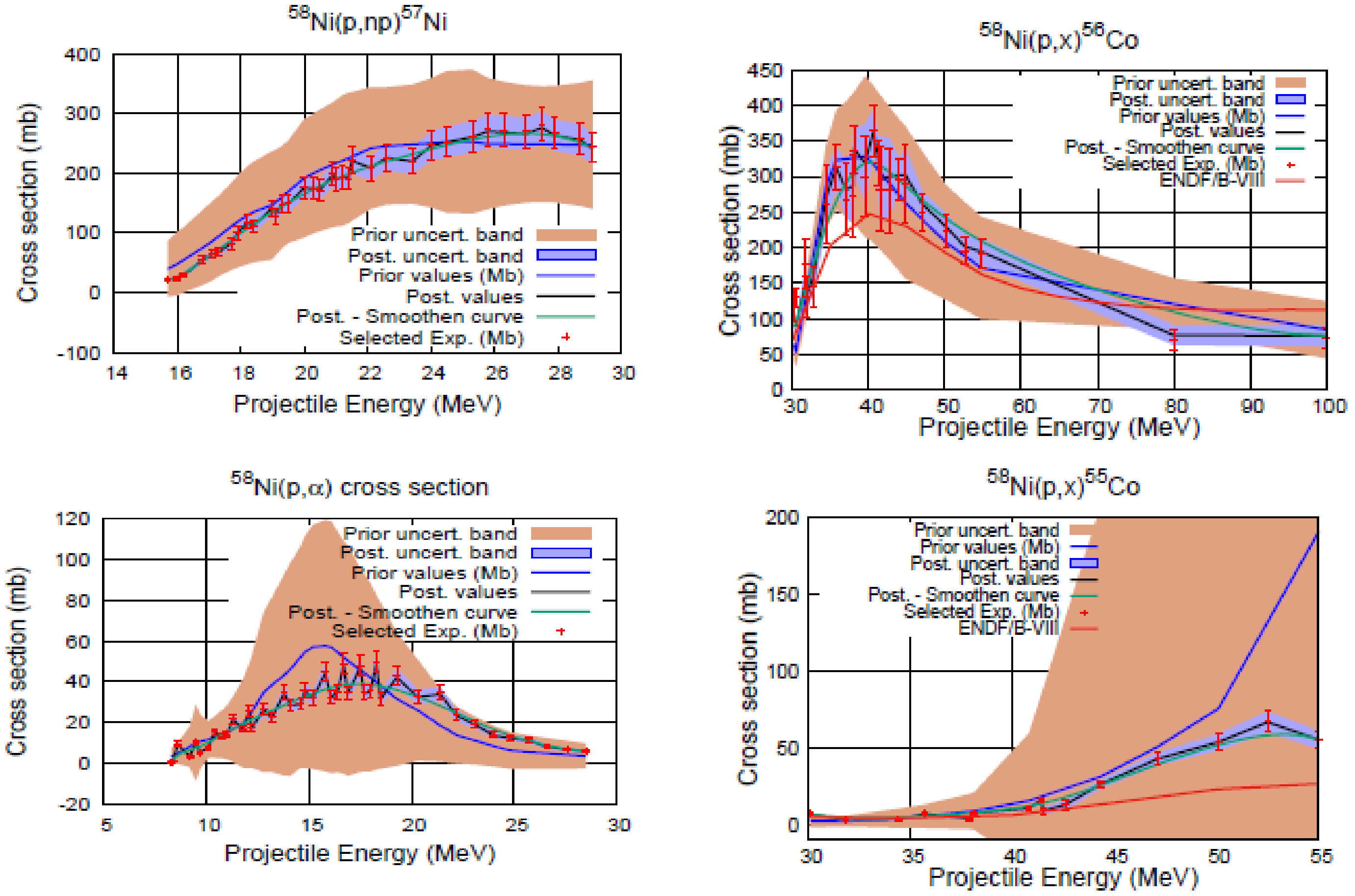
$$P\left(\overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}} \middle| \overrightarrow{\sigma^{exp}_{E_i}}\right) = \frac{P\left(\overrightarrow{\sigma^{exp}_{E_i}} \middle| \overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}}\right) * P\left(\overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}}\right)}{P\left(\overrightarrow{\sigma^{exp}_{E_i}}\right)}$$

$$\propto P\left(\overrightarrow{\sigma^{exp}_{E_i}} \middle| \overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}}\right) * P\left(\overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}}\right)$$

Likelihood function:

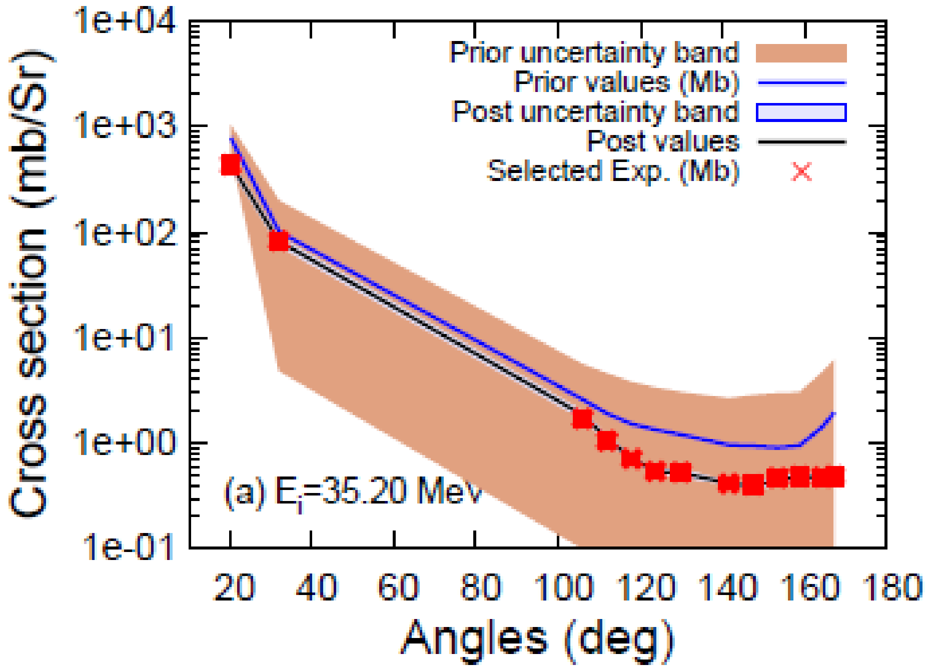
$$P\left(\overrightarrow{\sigma^{exp}_{E_i}} \middle| \overrightarrow{M_j}, \overrightarrow{\sigma^{cal}_{E_i}}\right) = exp\left(-\frac{\chi^2_{E_i}}{2}\right)$$

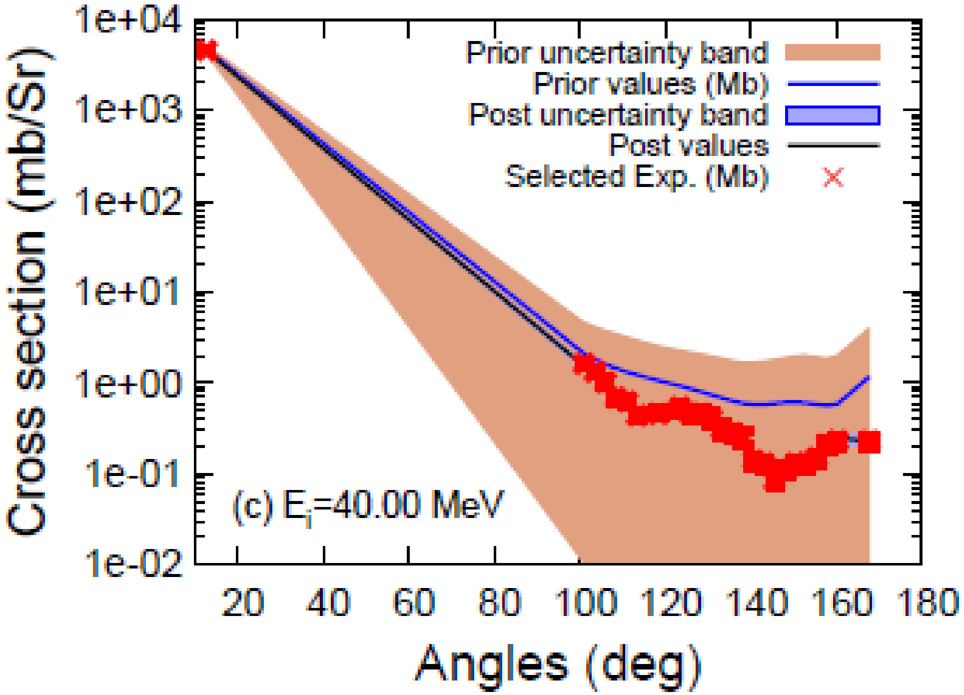
Selection of experiments is very important here



BMA with experiments

- **Elastic angular distributions**





- **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:**

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

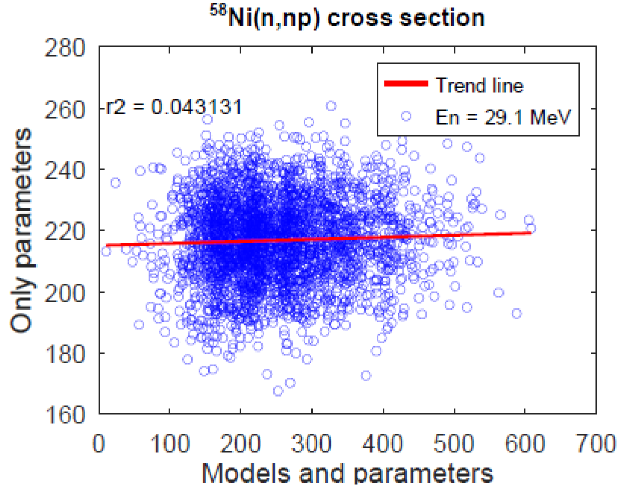
Total variance

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

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:**

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

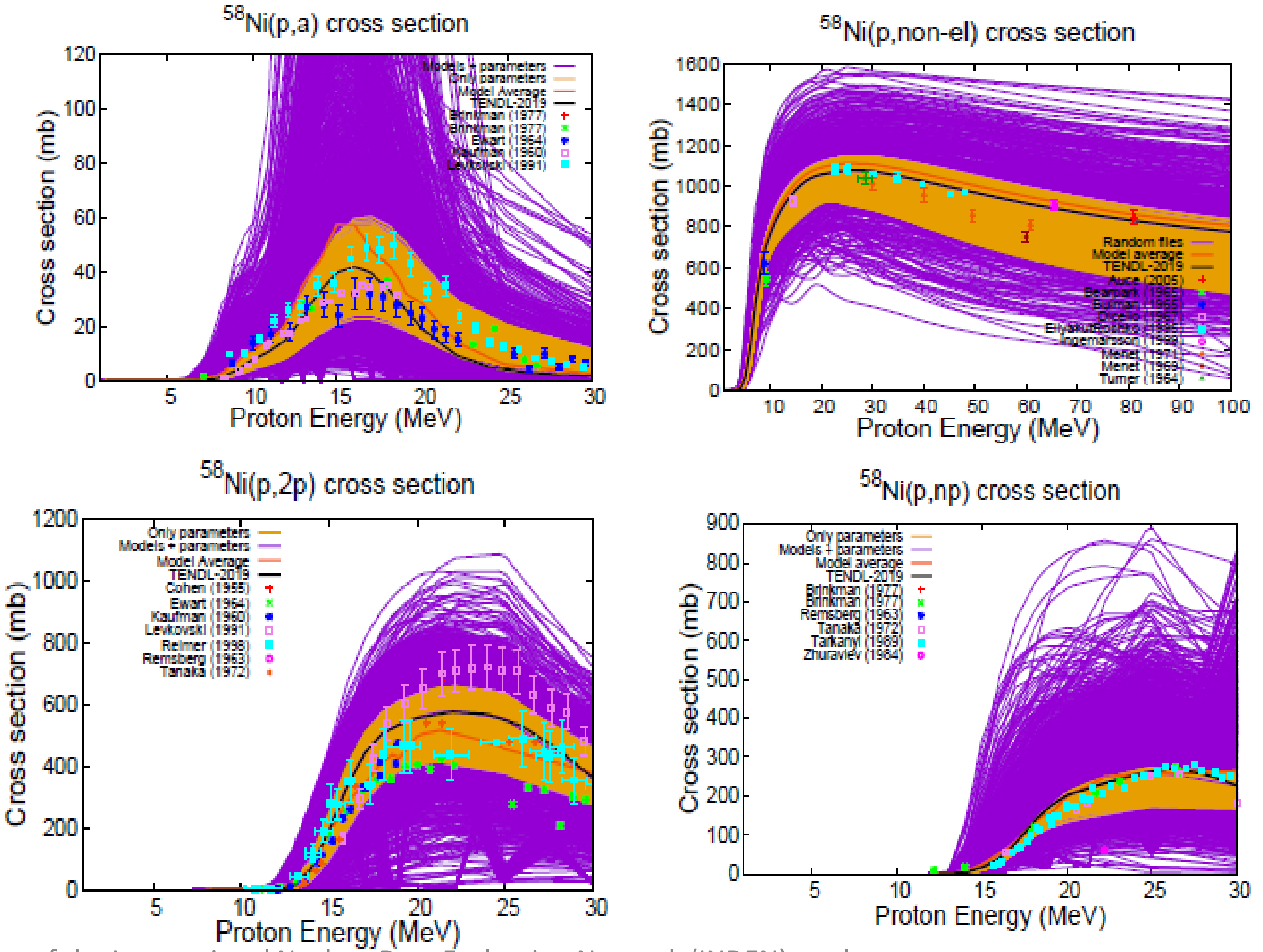
V_{tot}^{ci}: Total variance

V_{mod}^{ci}: Model variance at energy i

V_{par}^{ci}: Parameter variance

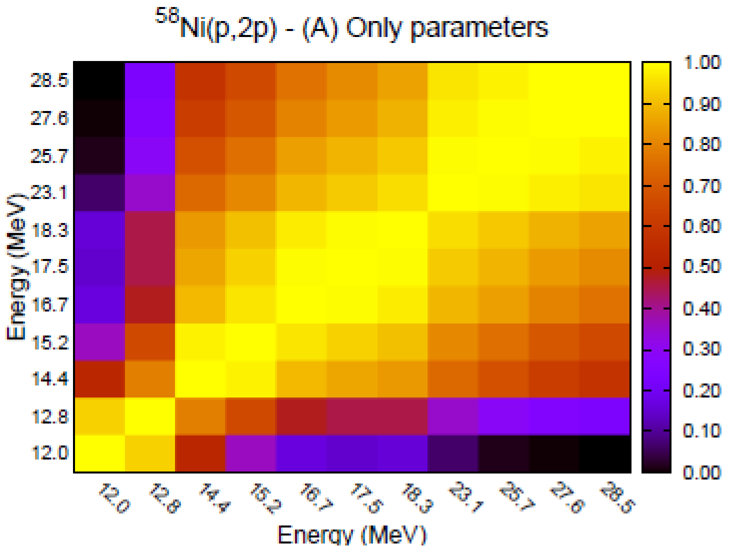
$$U_{mod}^{ci} = \sqrt{V_{tot}^{ci} - V_{par}^{ci}}$$

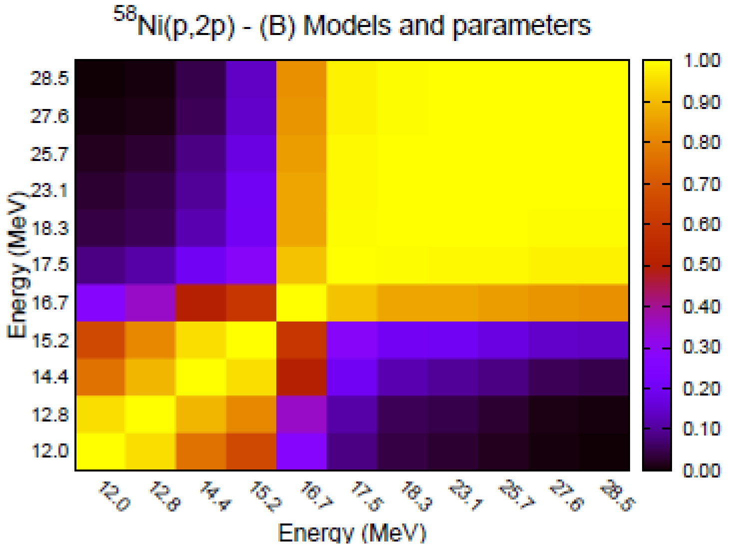
U_{mod}^{ci}: Model uncertainty



Prior and posterior correlations

- **Both prior and posterior correlations can be obtained**





Conclusion

- **Bayesian Model Averaging (BMA) together with smooth functions can produce fits in good agreement with experimental data**

- **An entire evaluation can be produced including prior and posterior covariances and correlations**

- **For channels and energy ranges where data is not available, we simply average over the models**

- 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.
- Next: Explore the use of energy dependent weights in BMA of nuclear data

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