Bayesian model selection and averaging in TENDL-based evaluation of nuclear data

SCK CEN
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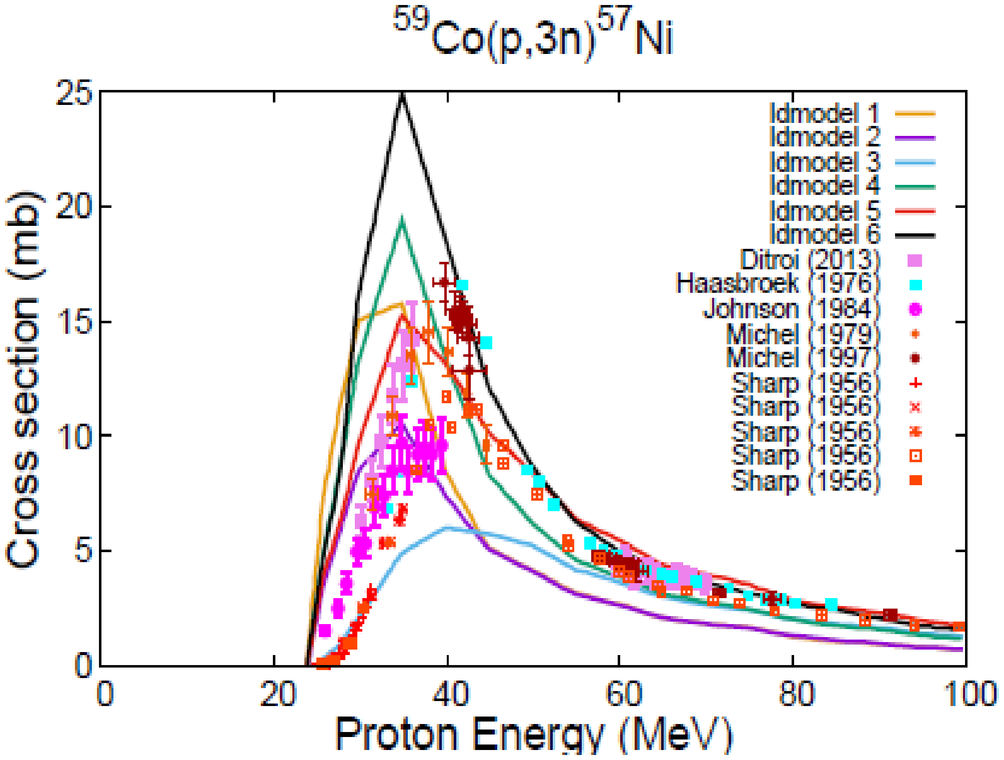
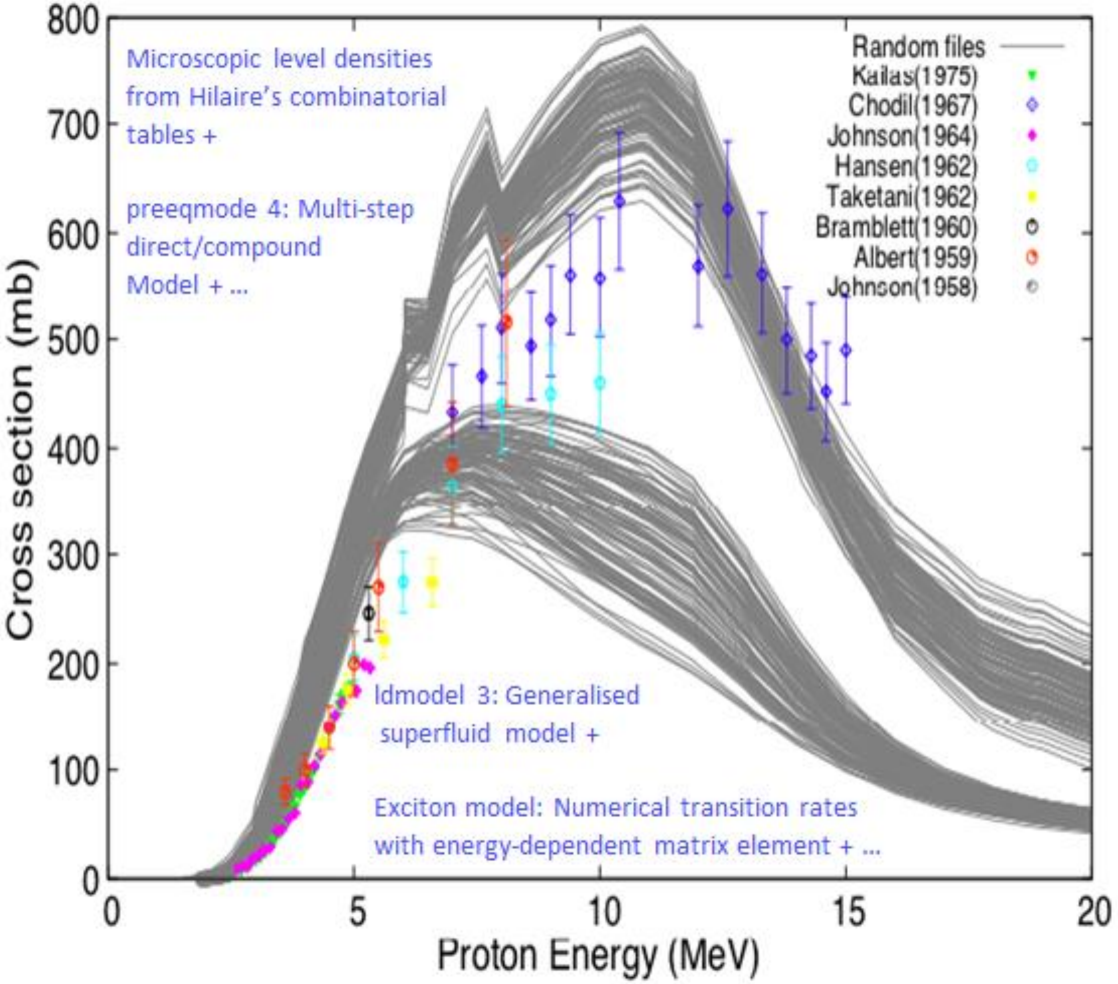
Introduction: TALYS has many models

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



Problem: How can a user choose/select which model to use OR make use of all models?

^{59}Co(p,n) cross section



Choosing between competing models (1)

Running assumption: 'one of the models contains the true distribution

Lets consider L computing models, M_j, where = 1,2, …, L;

Let $P\left(\overrightarrow{M_j}, \overrightarrow{\sigma_{E_i}^{cal}}\right)$ → **prior distribution of model** M_j

$P\left(\overrightarrow{\sigma_{E_i}^{exp}} \middle| \overrightarrow{M_j}, \overrightarrow{\sigma_{E_i}^{cal}}\right)$ → likelihood function

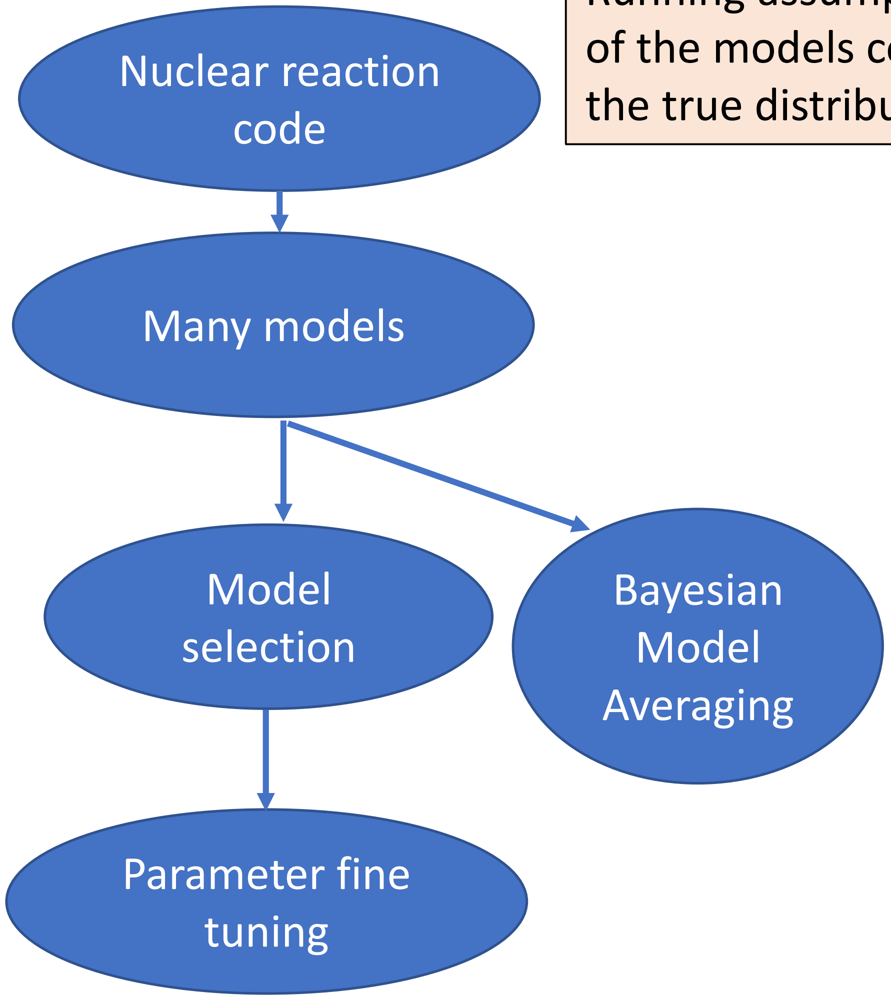
$\overrightarrow{\sigma_{E_i}^{exp}}$ → differential experimental data

We can assign Bayesian Monte Carlo (BMC) weights as:

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

Backward Forward Monte Carlo (BFMC) weights:

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



Choosing between competing models (2)

Running assumption: ‘one of the models contains the true distribution

Akaike Information Criterion (AIC):

$$AIC(M) = 2\log-likelihood_{\max}(M) - 2\dim(M)$$

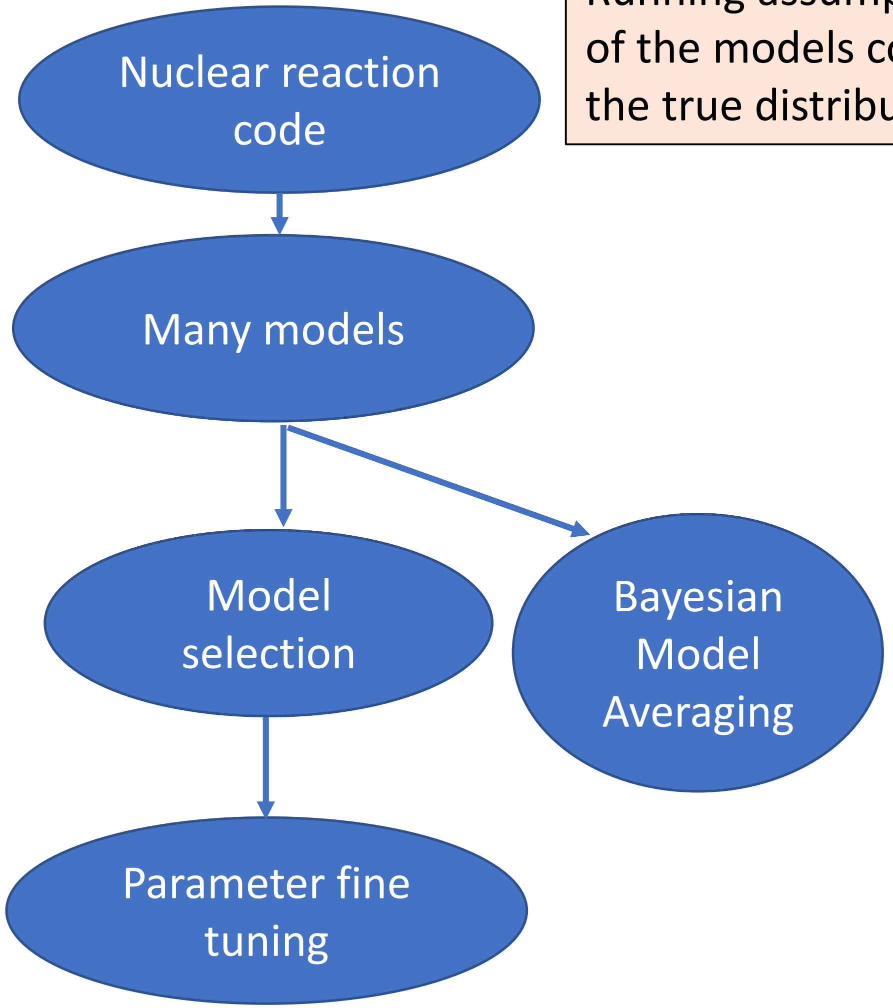
Bayesian Information Criterion (BIC):

$$BIC(M) = 2\log-likelihood_{\max}(M) - (\log n)\dim(M)$$

Where: dim(M) is the number of parameters estimated in the model (M), and with n the sample size of the data.

Given two model, M_i and M_j, the Bayes factor:

$$B_{ij} \frac{L(\overrightarrow{\sigma_E} \mid M_{i,p})}{L(\overrightarrow{\sigma_E} \mid M_{j,p})}$$

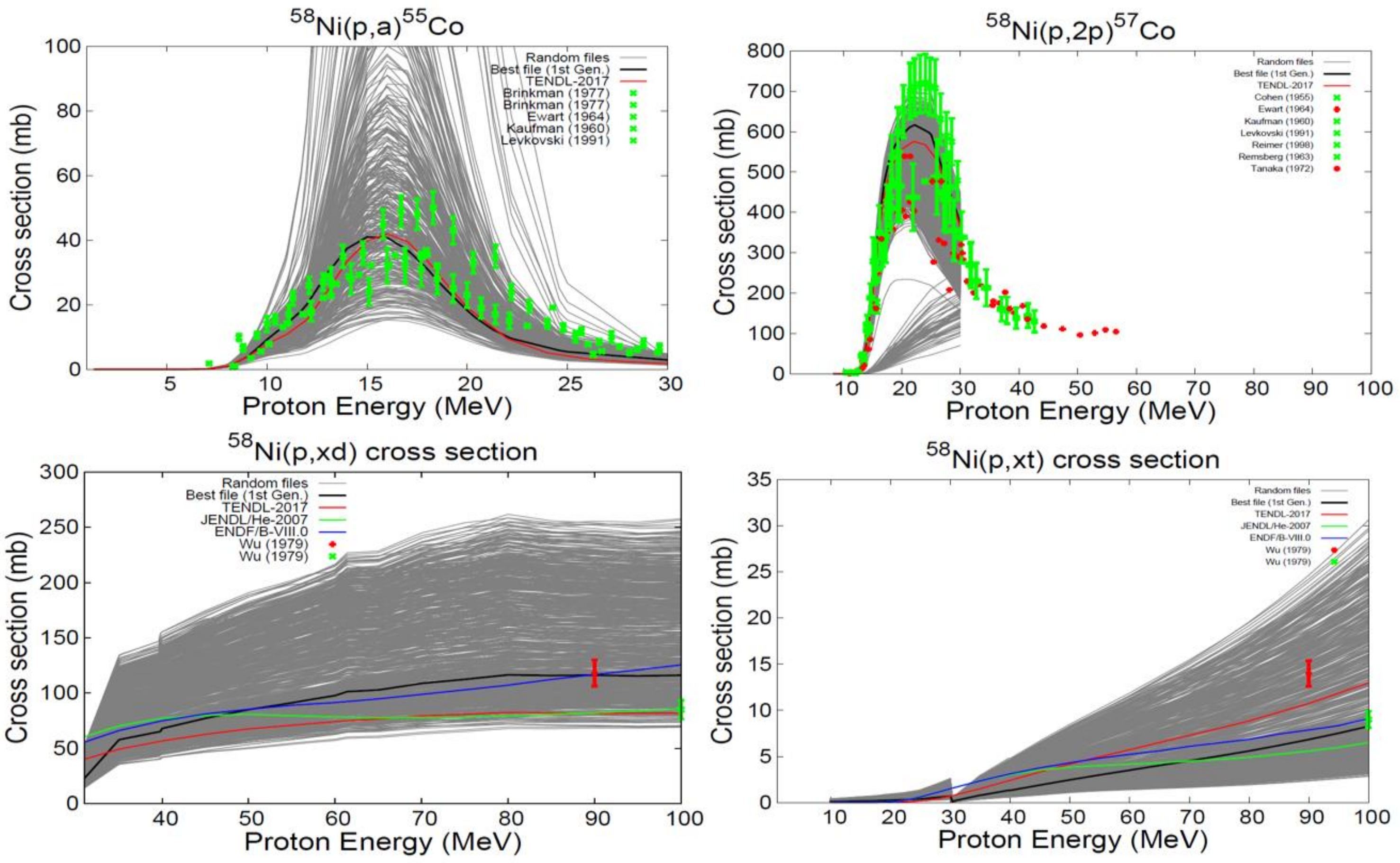


Choosing between computing models (3)

In the example here; all the different selection methods converged to the MLE value.

- **Note: the length of the parameter vector was assumed to be the same for all model sets.**

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



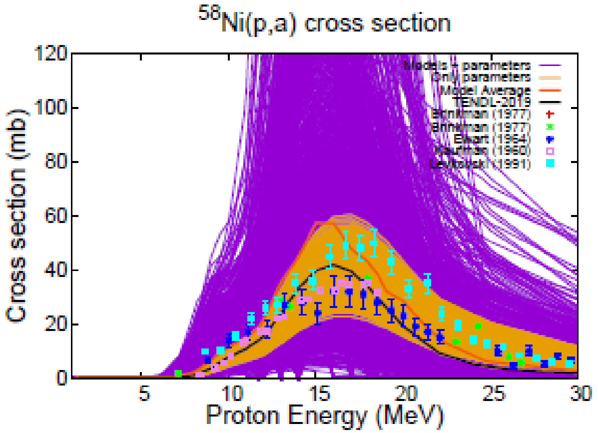
Simple Model Averaging

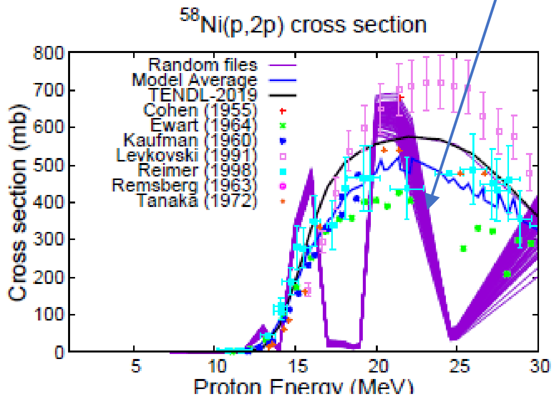
Our assumption: 'All models are wrong, … '
- George Box

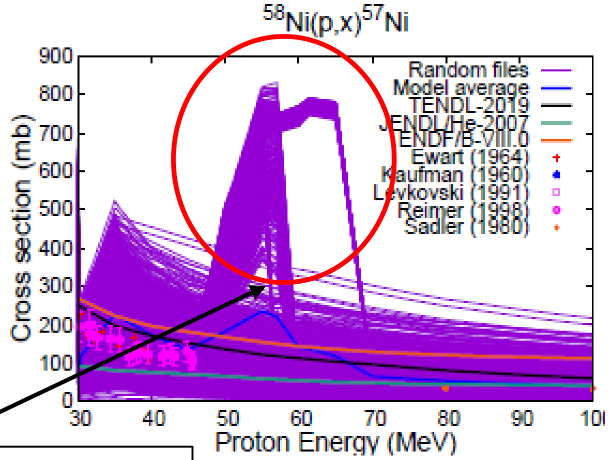
A simple average over all the models for a cross section at can be given as:

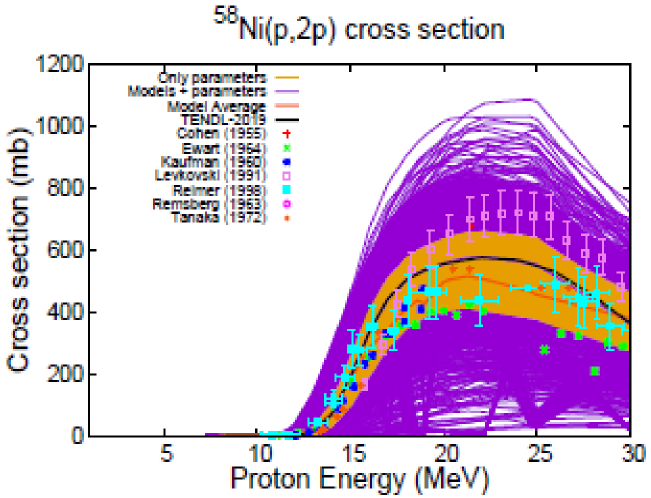
$$\overline{\sigma_E^k} = \frac{1}{n}\sum_{m=1}^{M}\sigma_E^k$$

There are bad models









'bad models can distort a simple average over the models

Note: Parameter variation in orange
Model + parameter variation in purple

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

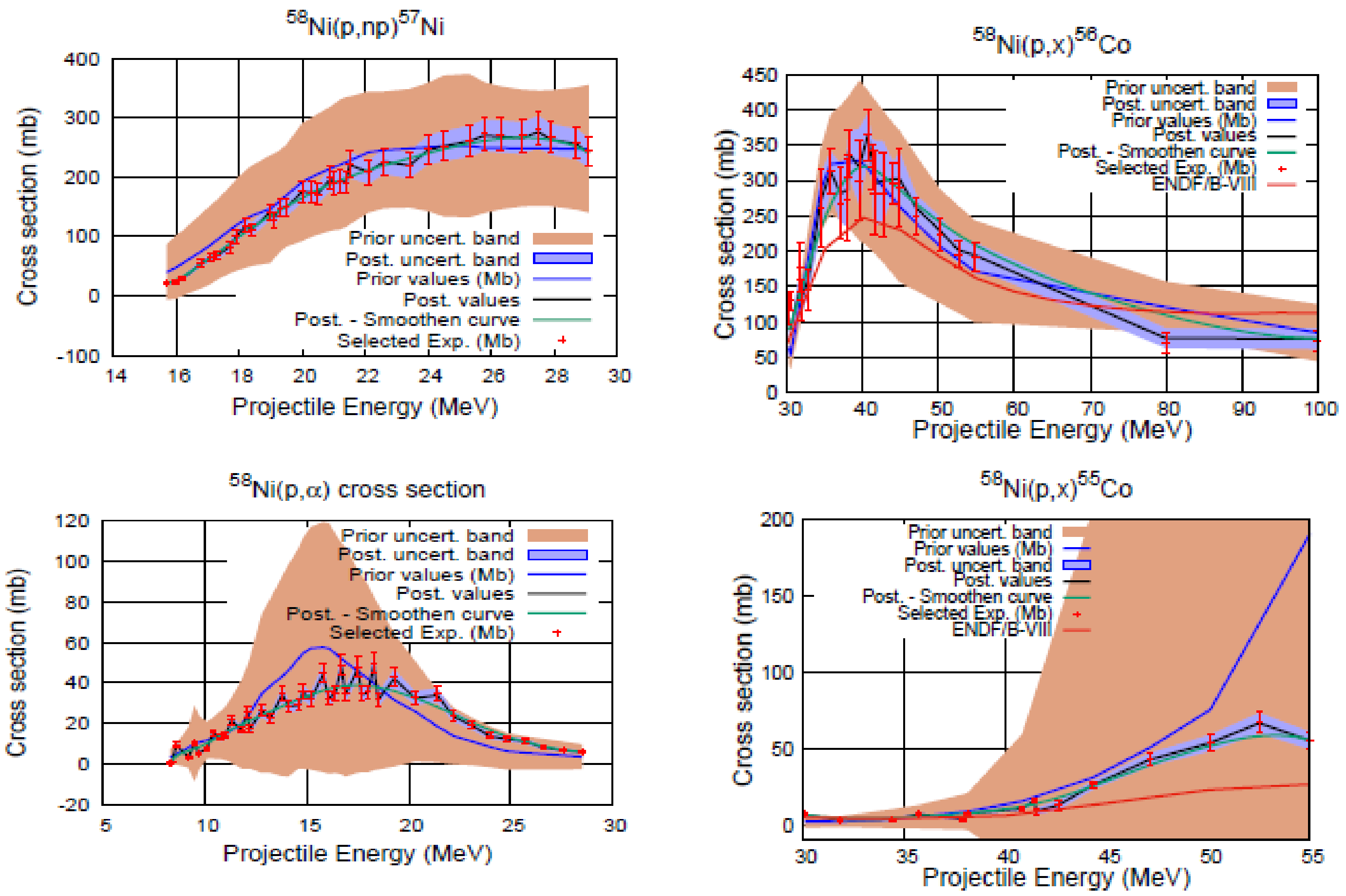
$$P\left(\overrightarrow{M_j},\overrightarrow{\sigma_{E_i}^{cal}} \middle| \overrightarrow{\sigma_{E_i}^{exp}}\right) = \frac{P\left(\overrightarrow{\sigma_{E_i}^{exp}} \middle| \overrightarrow{M_j},\overrightarrow{\sigma_{E_i}^{cal}}\right) * P\left(\overrightarrow{M_j},\overrightarrow{\sigma_{E_i}^{cal}}\right)}{P\left(\overrightarrow{\sigma_{E_i}^{exp}}\right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

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

Likelihood function:

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

Selection of experiments is very important here

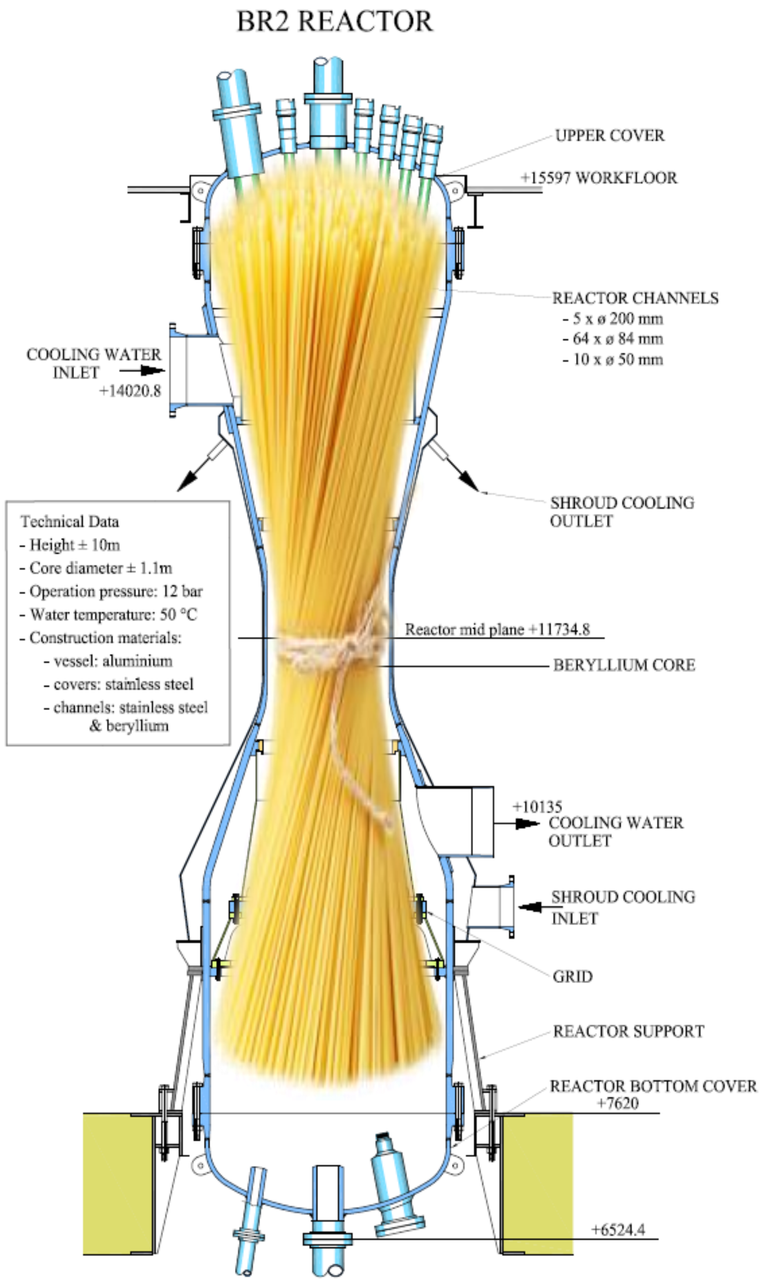


Reactor-based medical radioisotopes production

Thanks to **Geert Van den Branden** and **Steven Van Dyck**

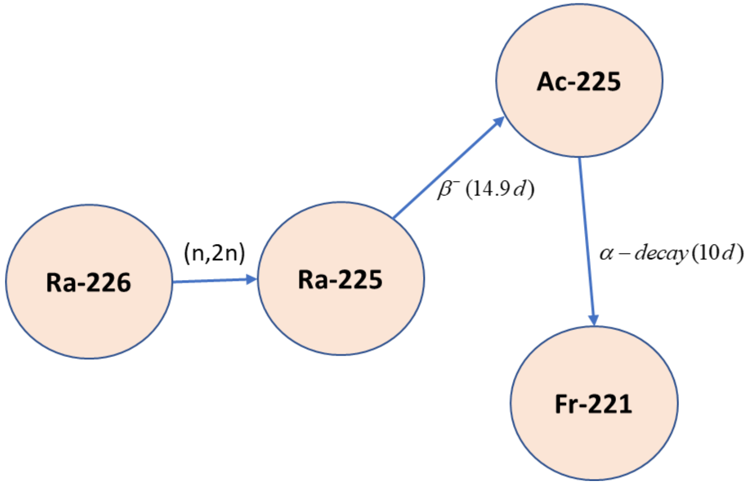
BR2 Main Features

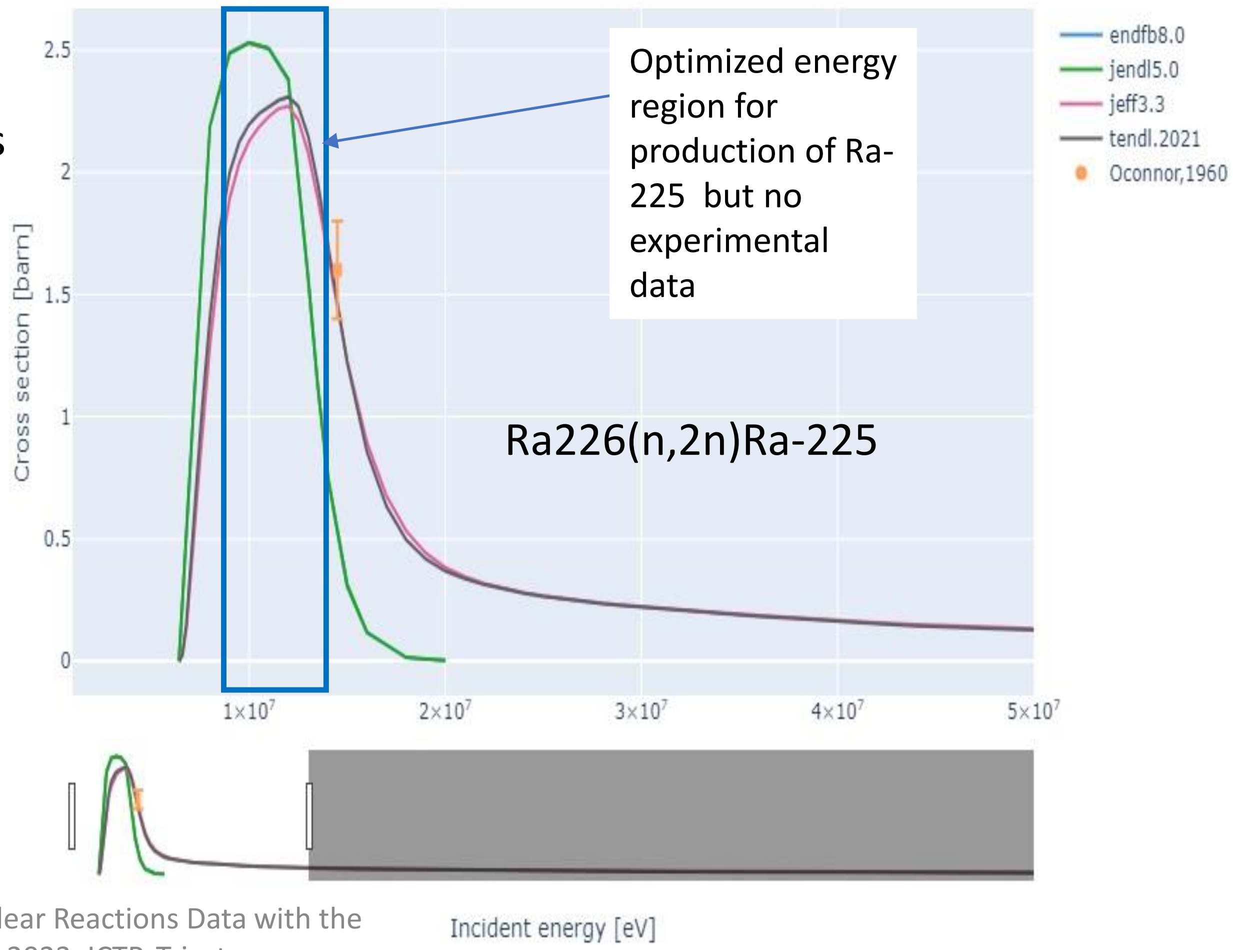
- Reactor core of hyperbolically arranged tubes
- Beryllium and water moderated
- Aluminium alloy fuel plate elements with HEU
- Water cooled
- BR2 has **very high** neutron fluxes
  - 1×10^{15} n/cm²/s thermal flux (E_n<0.5 eV)
  - 8×10^{14} n/cm²/s fast flux (E_n>0.1 MeV)
- BR2 has a **wide field of applications**
  1. Research & Development (fluxes/spectra/ temperatures)
  2. Radio-isotope production (Lu-177 (prostrate cancer), Mo-99/Tc-99m (imaging), Ir-192 (brachytherapy) , I-131 (thyroid gland), etc.
  3. Neutron transmutation doping of silicon
- High thermal power (for a MTR) 50MW – 100MW



Nuclear data needs for reactor-based medical radioisotope production: Ac-225 example

- Ac-225 is used in targeted alpha therapy (TAT) for prostate, breast and colon cancers, etc.
  - Ac-225 is attached to a carrier molecule that locks onto the cancer cell. Undergoes alpha decays ($t_{1/2}$=10 days) to Fr-221. The emitter high energy alpha particle kills the tumor locally.



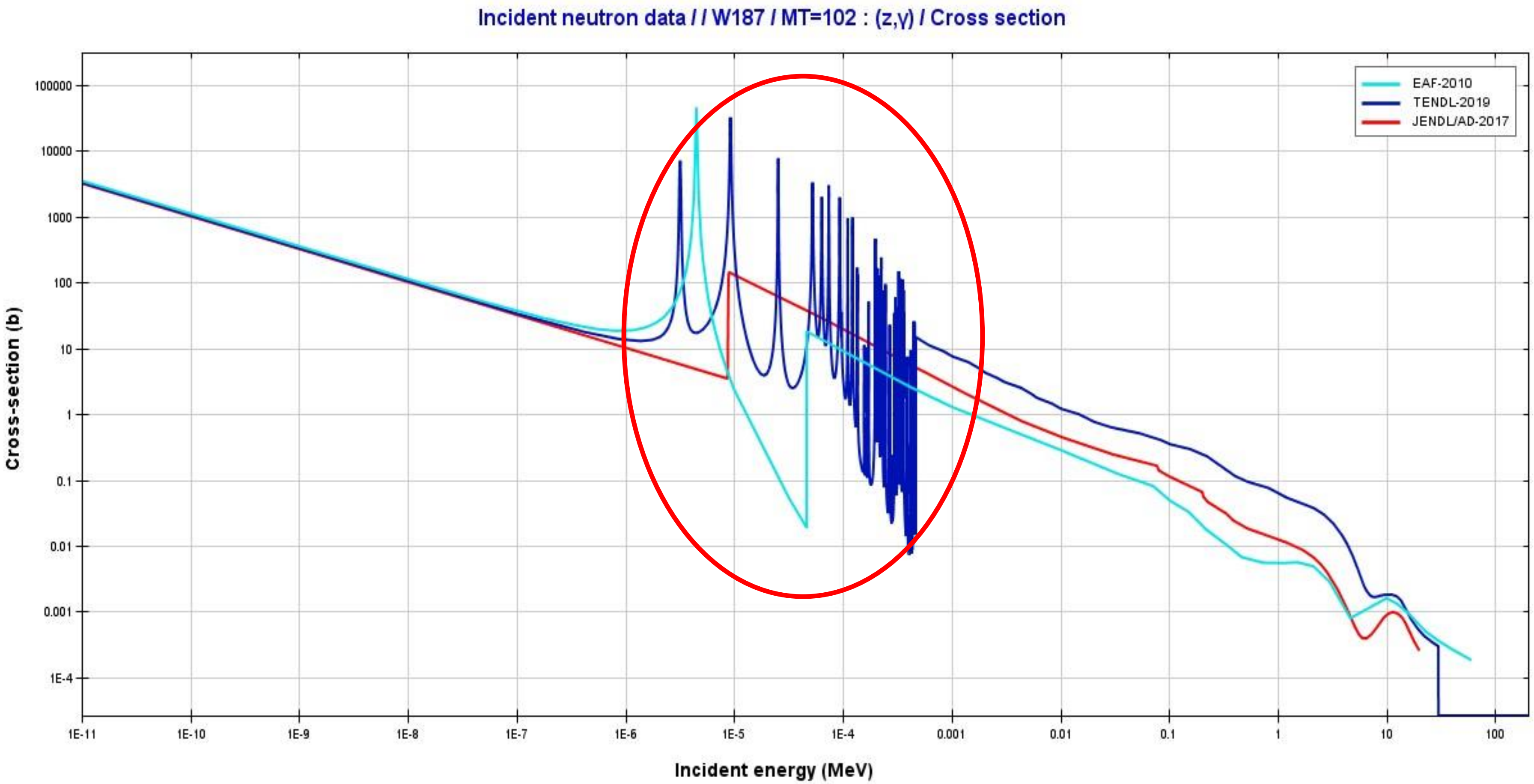


Problem: How to tailor reactor neutron flux to the energy region of interest

No experimental data for W-187(n,g)W-188

TENDL has resonances ??

Can we trust the evaluation??



Conclusion

- Bayesian Model Selection can be used to select ‘best’ nuclear reaction model set for nuclear data evaluation.
- Bayesian Model Averaging together with a smooth function can be used to reproduce experimental data within experimental uncertainties.
- The use of energy dependent weights in BMA would provide more flexibility. (Need to discuss this more with Arjan Koning)
- We need more attention to the nuclear data needs for reactor-based medical radioisotope production.

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