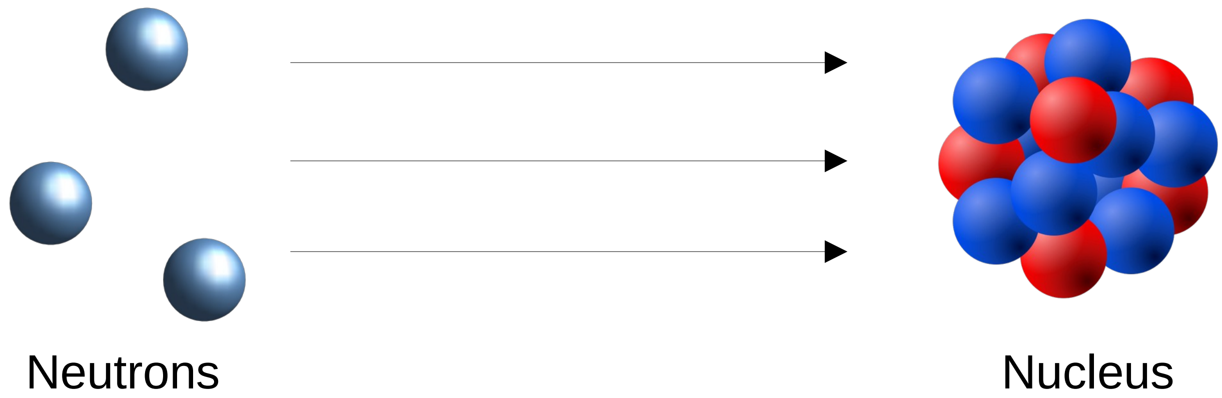
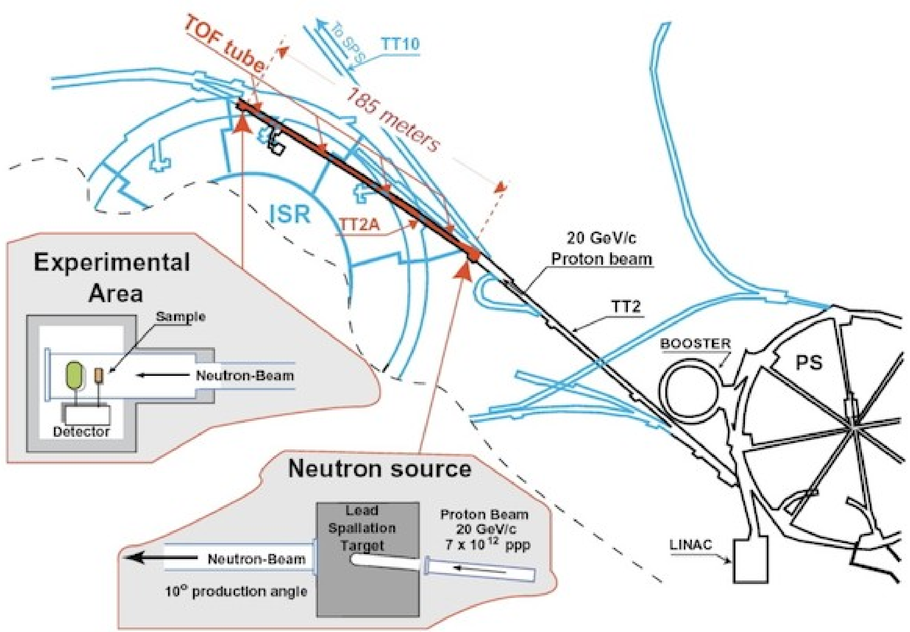
Modeling nuclear data relationships with Bayesian networks

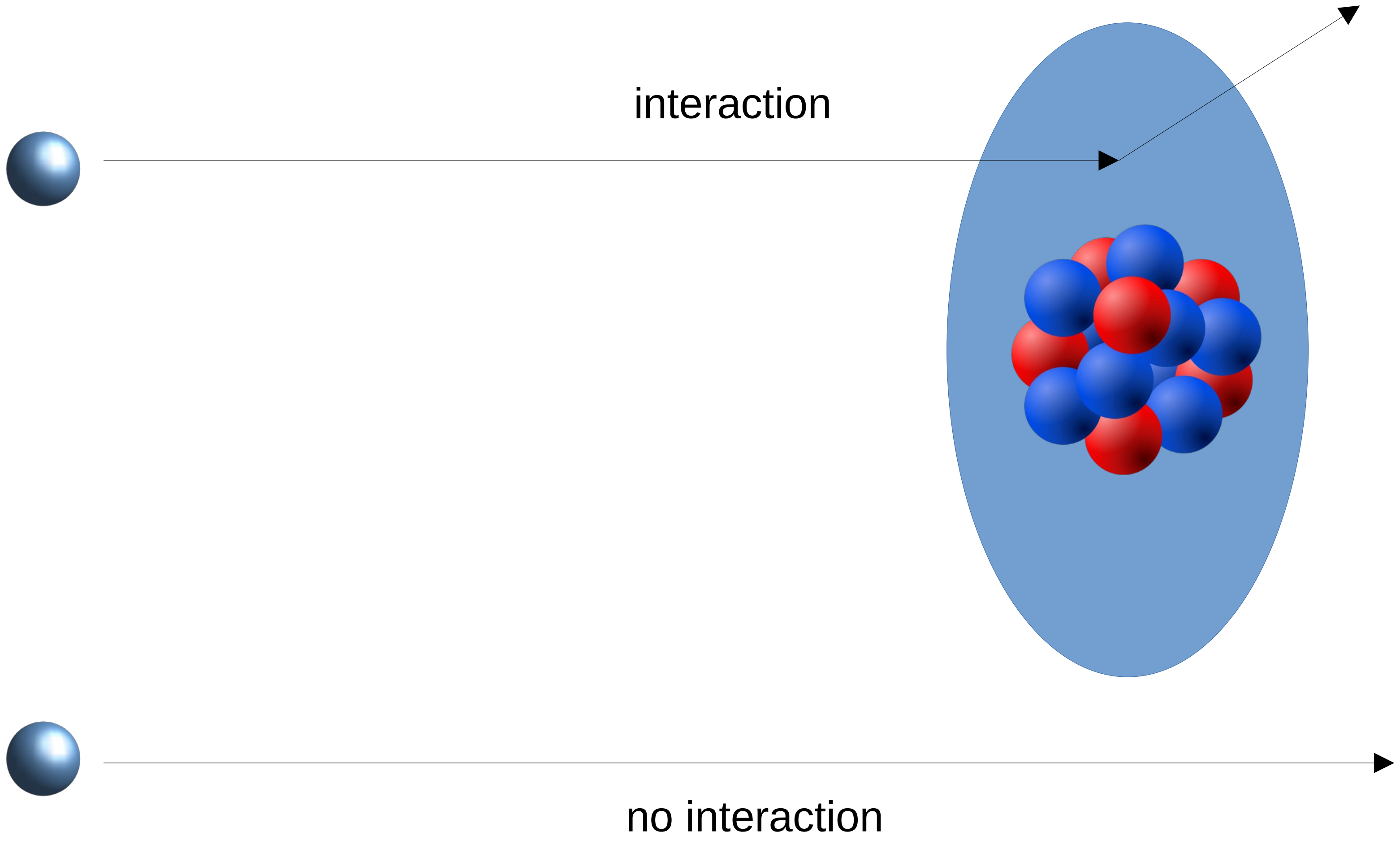
ML coffee breakfast club

Collision experiments



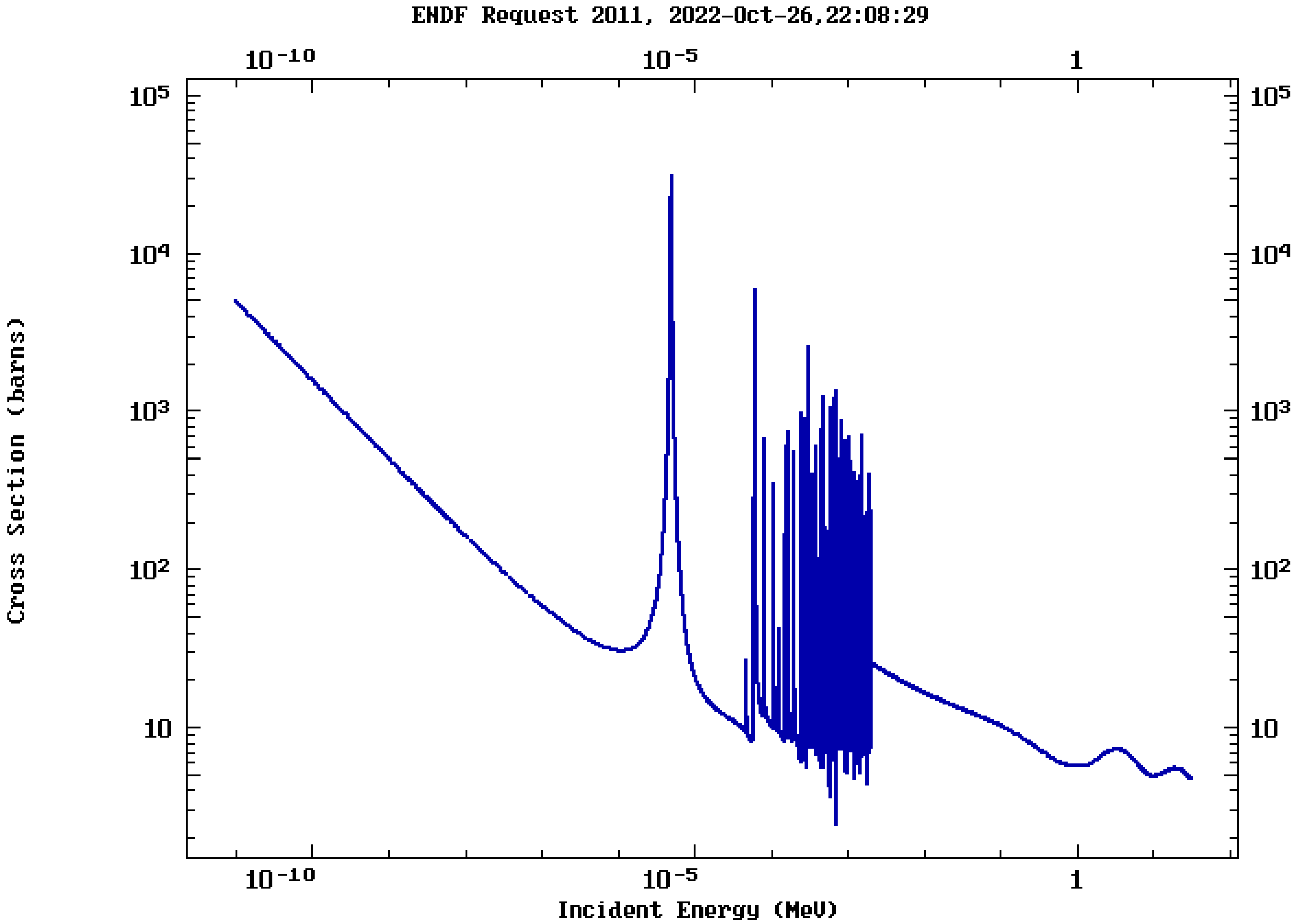


Total cross section



Velocity dependence of cross section

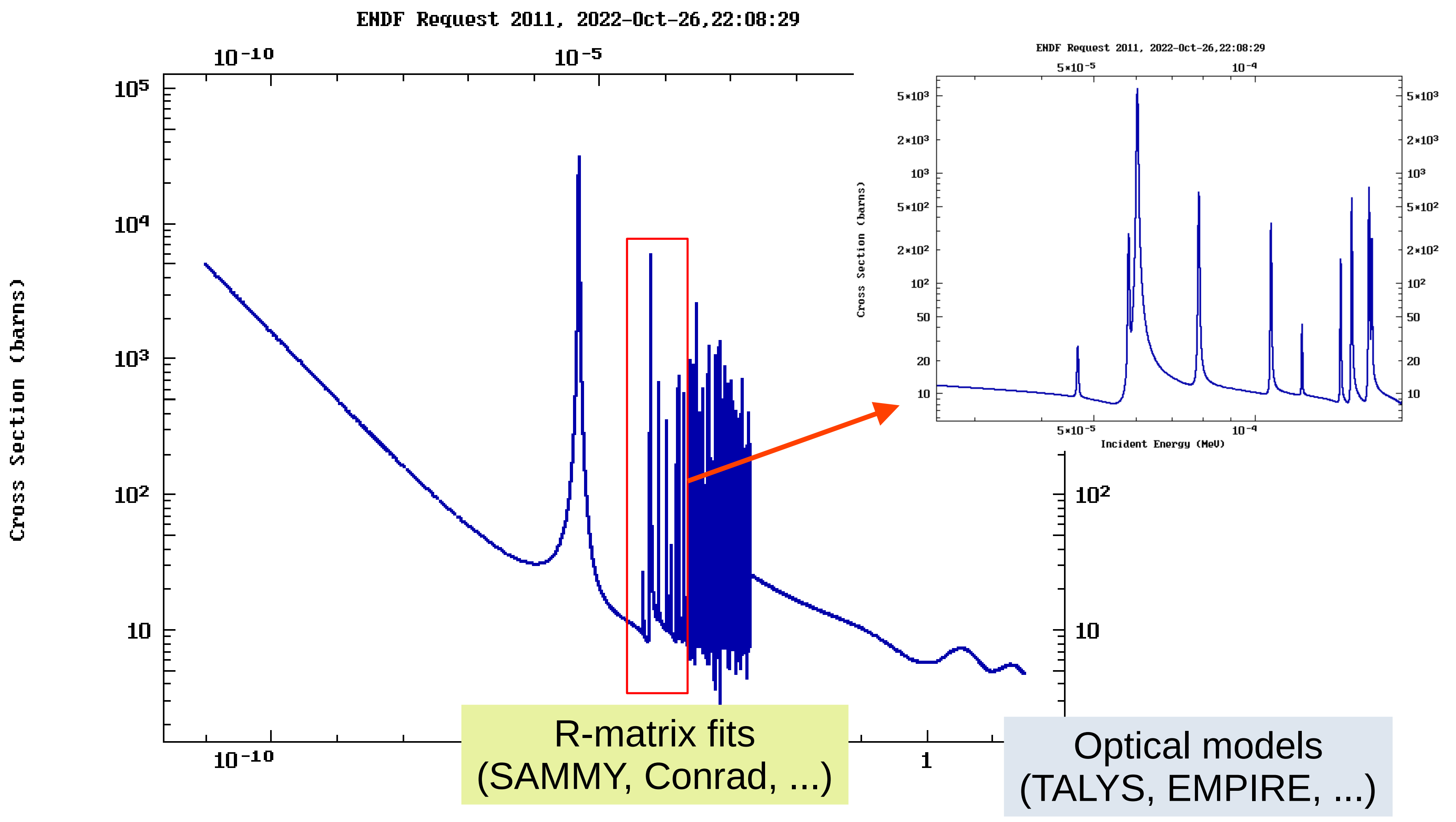
Total neutron-induced cross section of Au-197



1 barn = 10^{-28} m^2

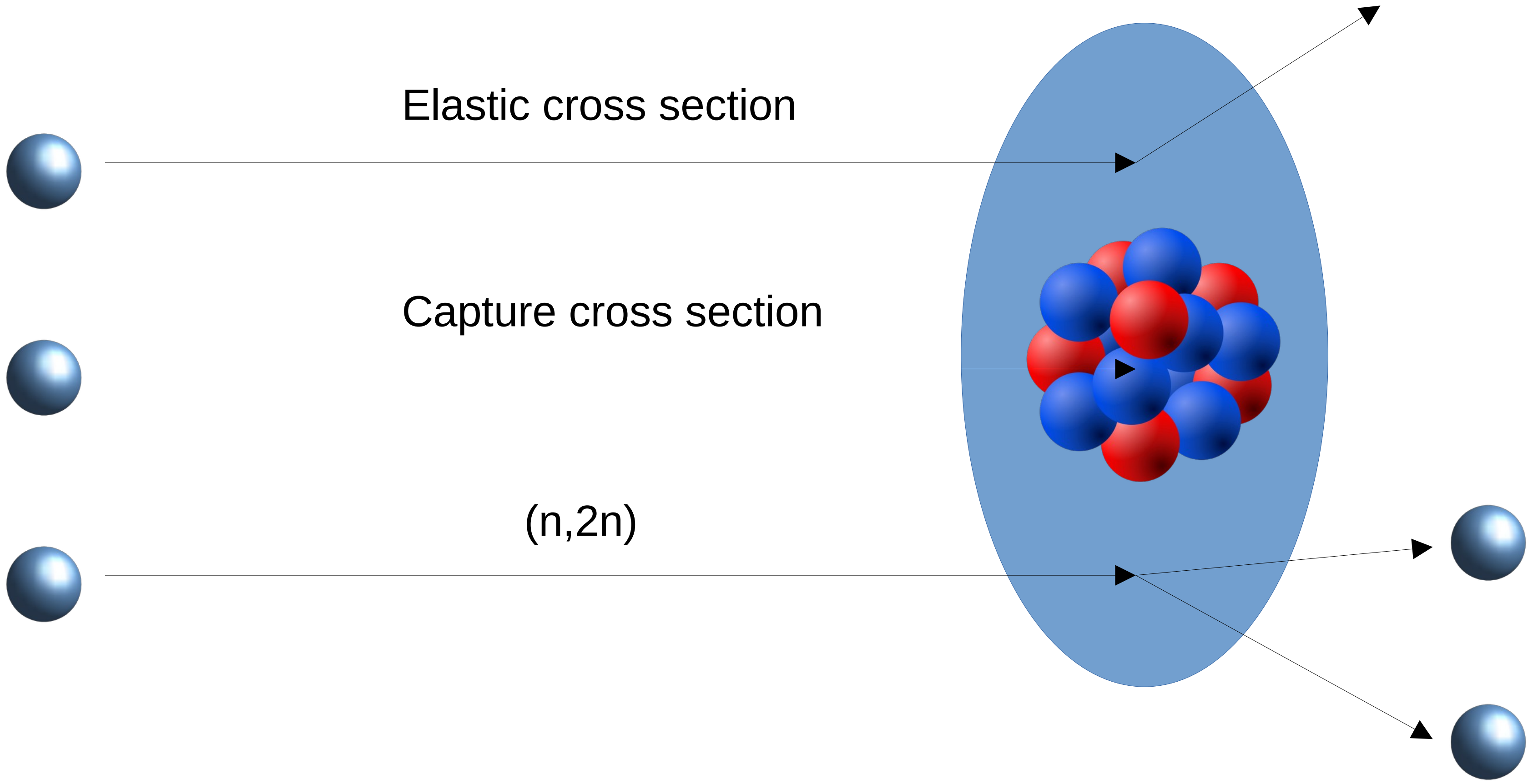
Velocity dependence of cross section

Total neutron-induced cross section of Au-197

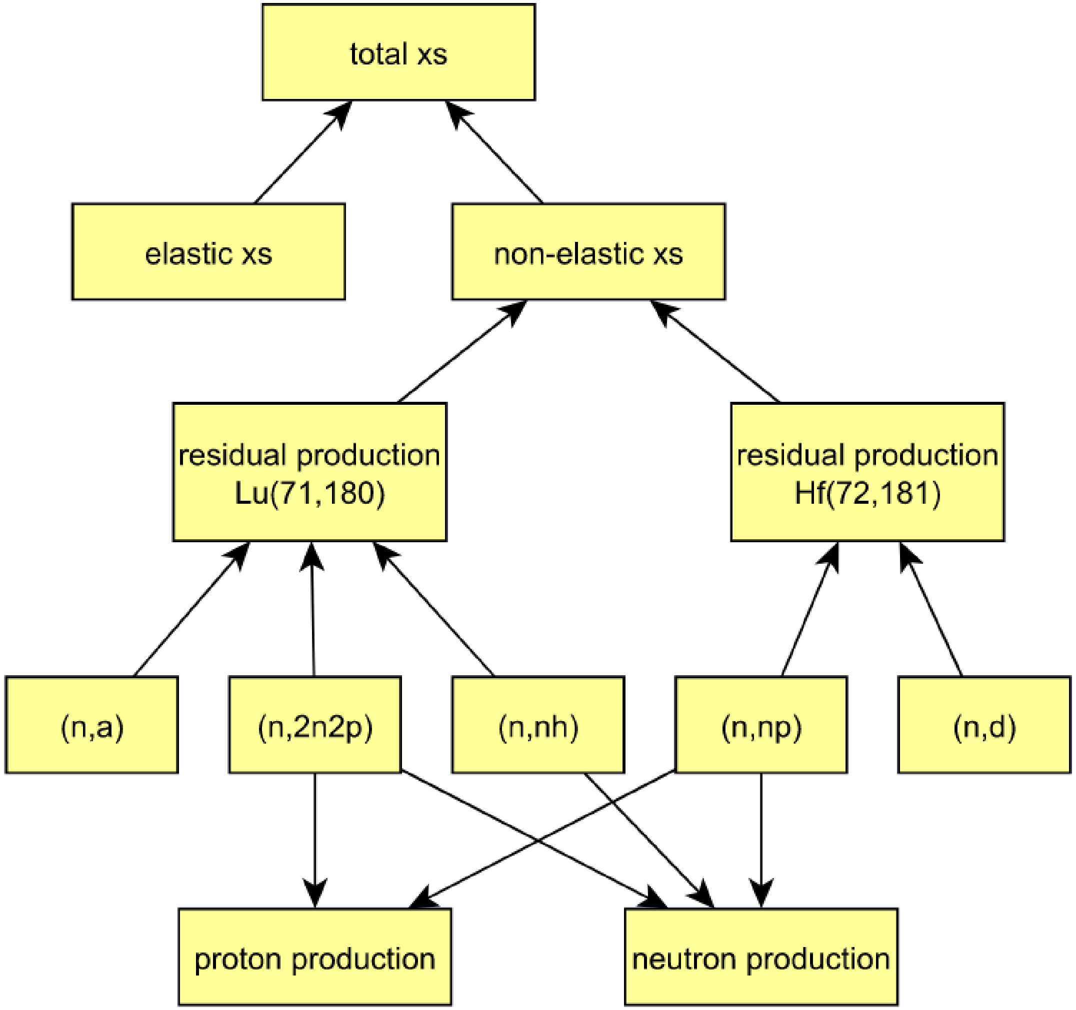


1 barn = 10^{-28} m^2

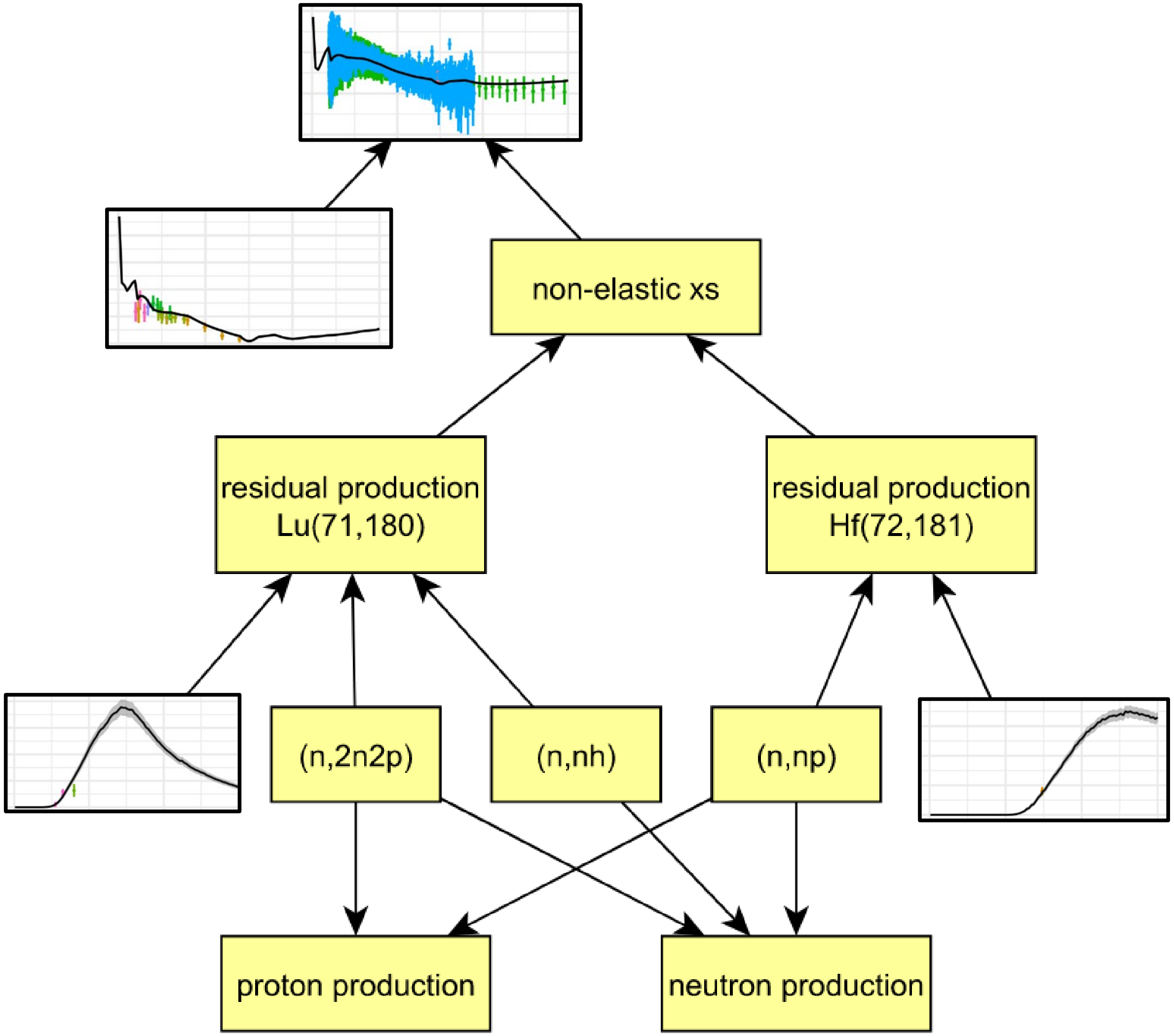
Different types of cross sections



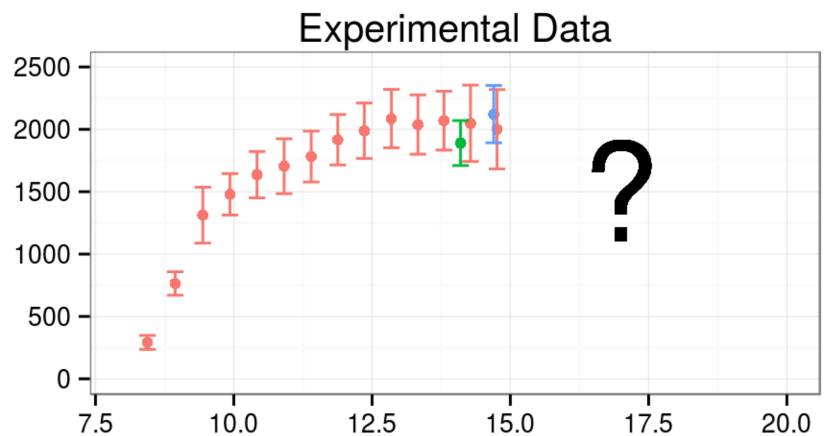
Relationship between cross section types

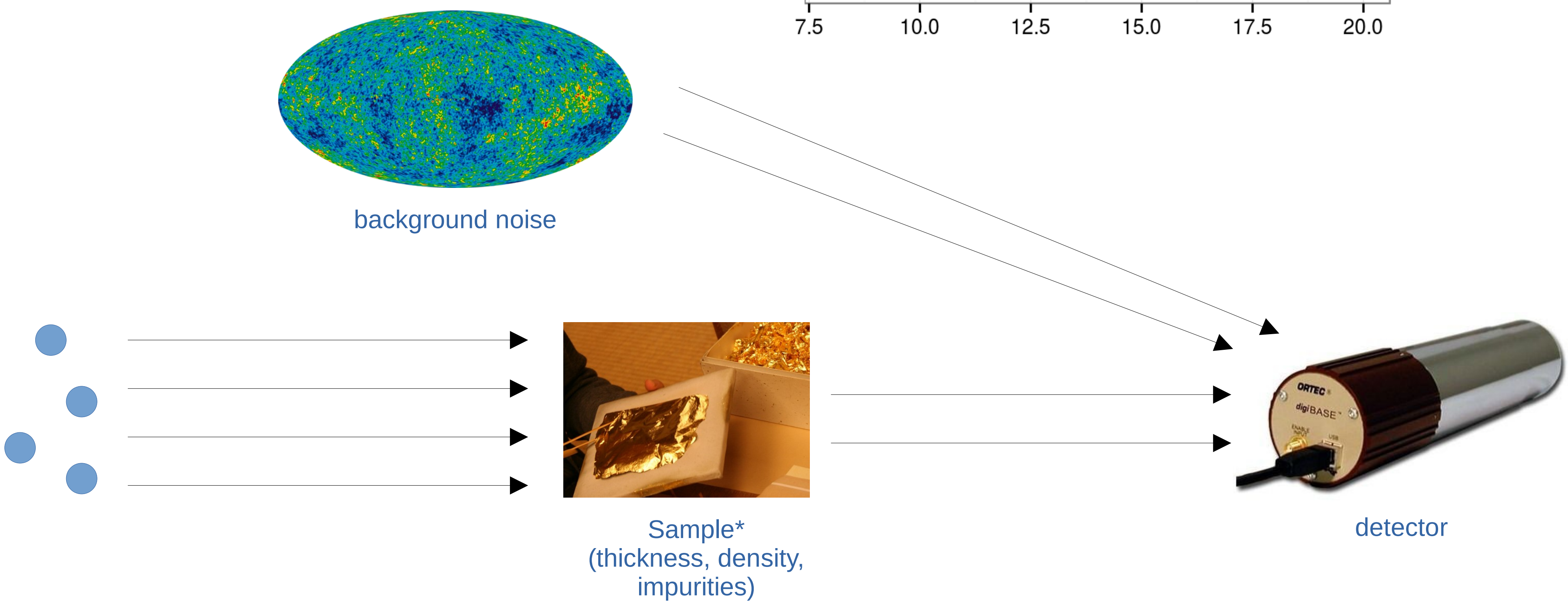


Network of functions



UQ of experimental data





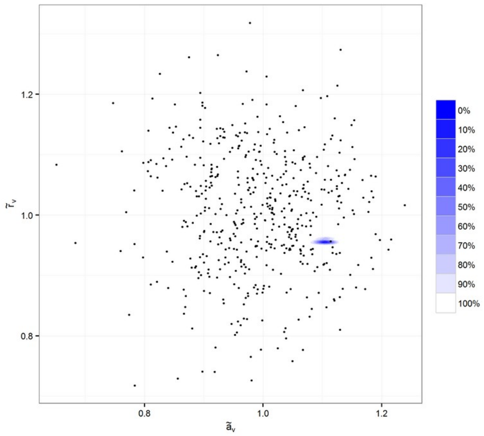
Scenarios in nuclear data evaluation

- Several nuclear physics models need to be consistently combined in an evaluation
- Nuclear models may be combined with non-parametric statistical methods to improve the description of available experimental data
- Sometimes we prefer to not use nuclear physics models and rely heavily on experimental data
- We want to incorporate uncertainty information of experiments into the statistical analysis

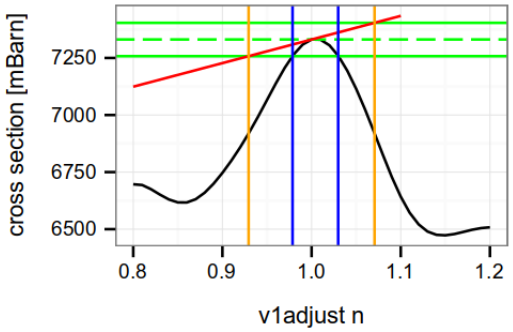
Bayesian inference

$$\pi(\vec{p}_{\mathrm{true}} \mid \vec{\sigma}_{\mathrm{exp}}, M) \propto f(\vec{\sigma}_{\mathrm{exp}} \mid \vec{p}_{\mathrm{true}}, M)\,\pi(\vec{p}_{\mathrm{true}} \mid M)$$

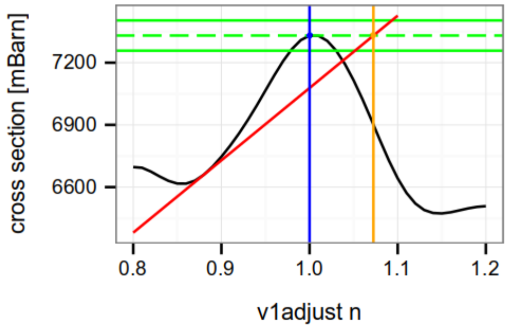
MVN MVN



Monte Carlo

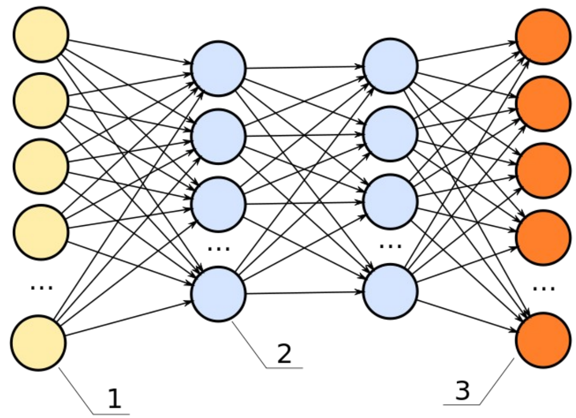


Optimization



GLS (sens.based)

An inspiration: composability of neural networks



TensorFlow

TORCH

K

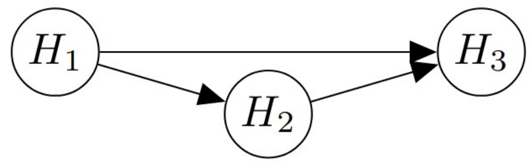
theano

Take simple building blocks (e.g., pooling layers, convolutional layers, etc.) and define their connection structure with a relatively simple language

Can we do the same for Bayesian models?

Bayesian networks

$$P(H_1, H_2, H_3) = P(H_1)P(H_2 \mid H_1)P(H_3 \mid H_1, H_2)$$



Thomas Bayes

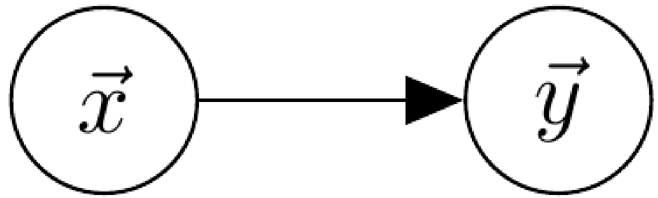
- Enable a more efficient way of storing information
- Enable a more efficient evaluation of the Bayesian update formula
- Preserve the identity of individual components
  (e.g., normalization errors and associated uncertainties)

Pierre-Simon Laplace

Judea Pearl*

* Photo credit: Better Than Bacon – Judea Pearl at NIPS 2013

Basic building block



$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

(e.g., model predictions)

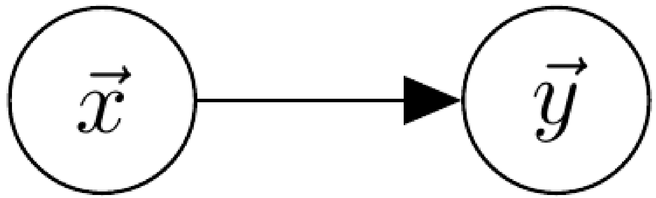
$$\boxed{\vec{y} = f(\vec{x})}$$

f may be non-linear

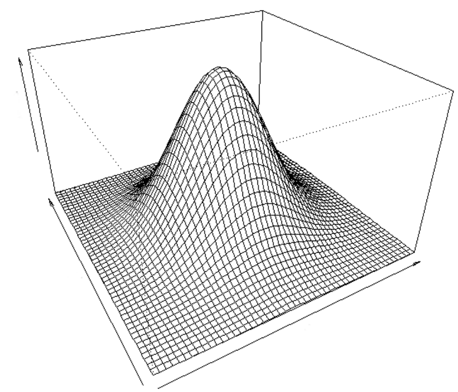
$$\vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

(e.g., convoluted model predictions)

Distribution assumption

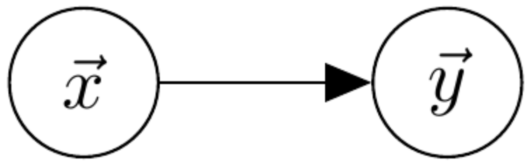


$$\vec{x} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$



Because of $\boxed{\vec{y} = f(\vec{x})}$ the distribution of $\vec{y}$ is not necessarily multivariate normal

Links between nodes



Log-normal distribution
(e.g., positive cross section)

$$y_i = \exp(x_i)$$

Truncated normal distribution
(e.g., non-negative cross section)

$$y_i = \max(0, x_i)$$

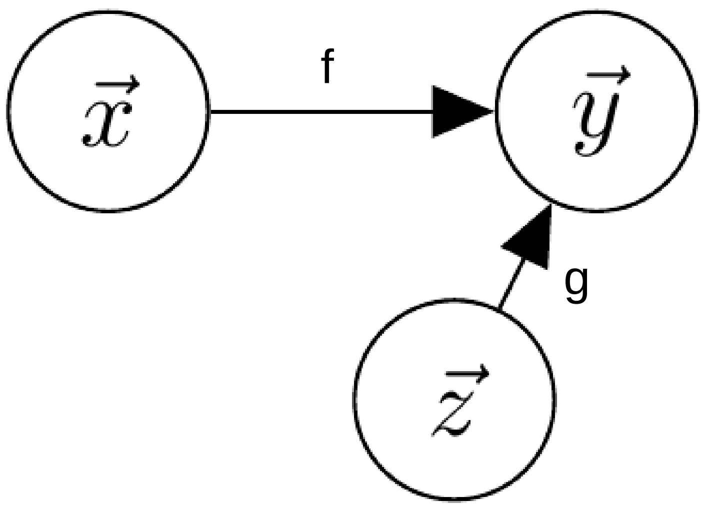
Linear interpolation
(e.g., model mesh to experimental mesh)

$$y_j = \left(\frac{E_{i+1} - E'_j}{E_{i+1} - E_i}\right) x_i + \left(\frac{E'_j - E_i}{E_{i+1} - E_i}\right) x_{i+1}$$

$$\text{if} \;\; E_i \leq E < E_{i+1}$$

Convolution
(e.g., model mesh to experimental mesh with finite energy resolution)

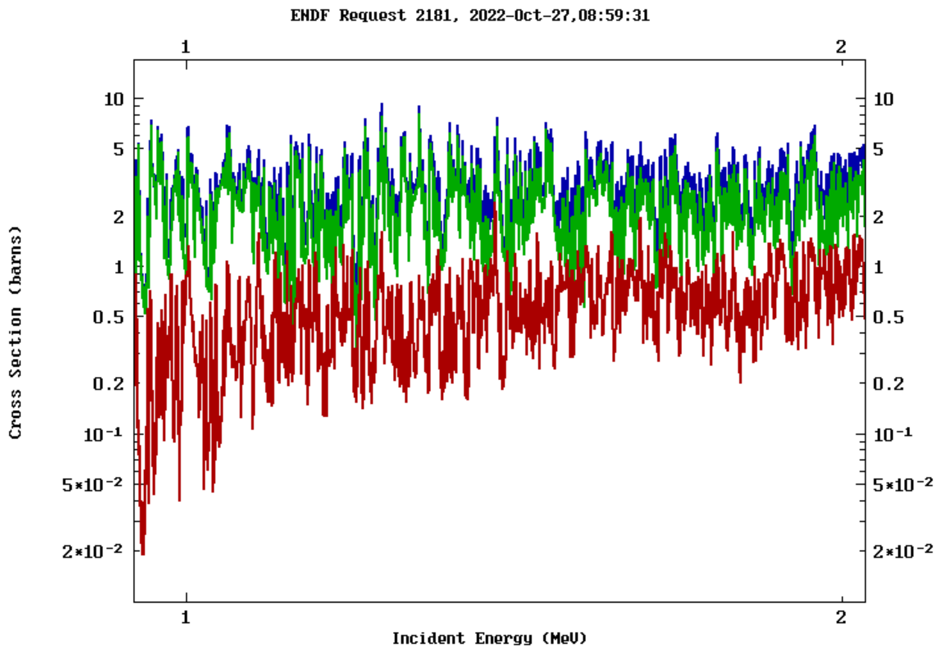
Combination of nodes

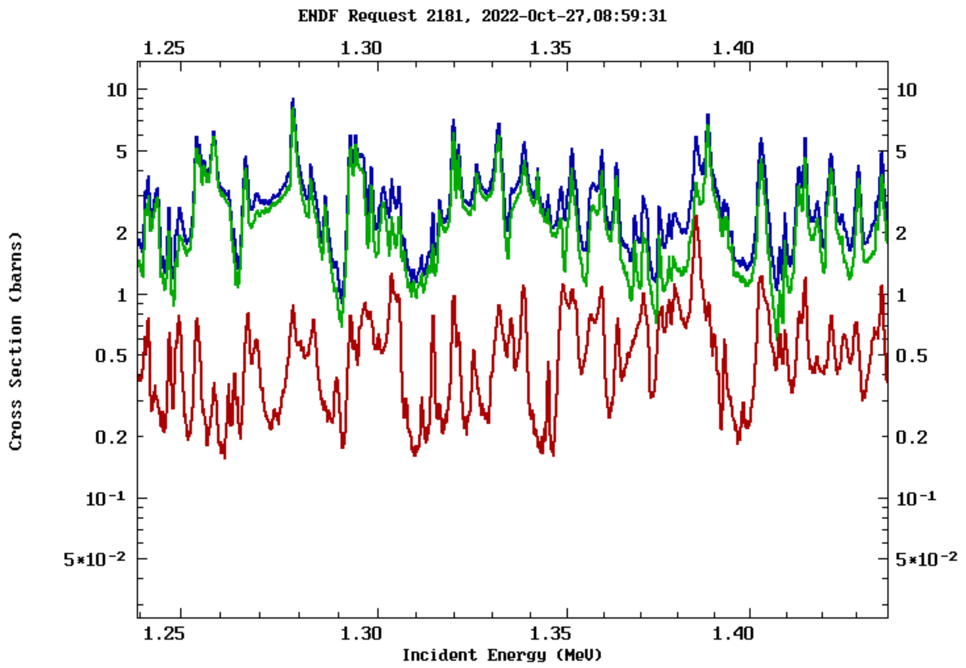


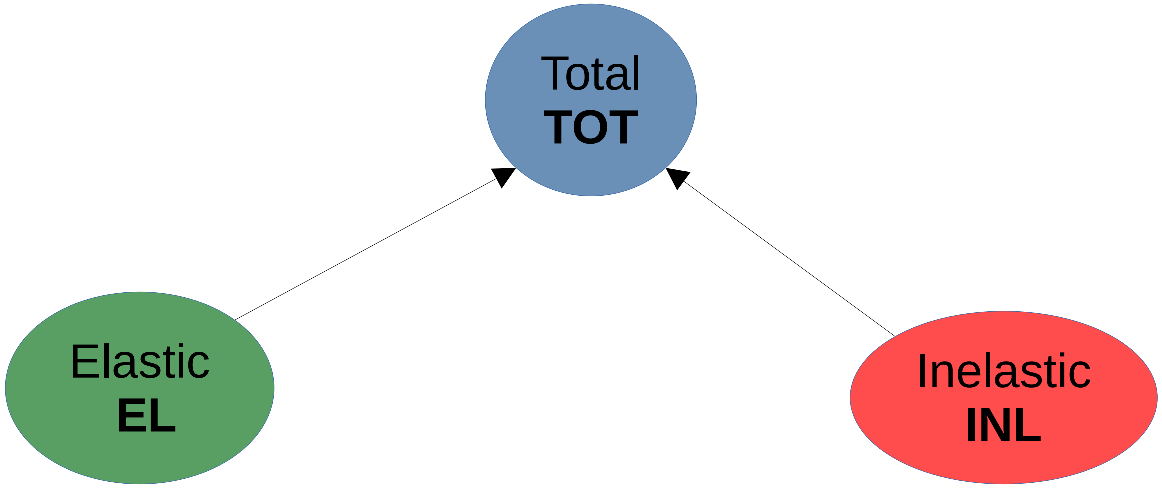
$$\vec{y} = f(\vec{x}) + g(\vec{z})$$

For example:
Experimental measurement is the sum of convoluted model prediction and statistical error

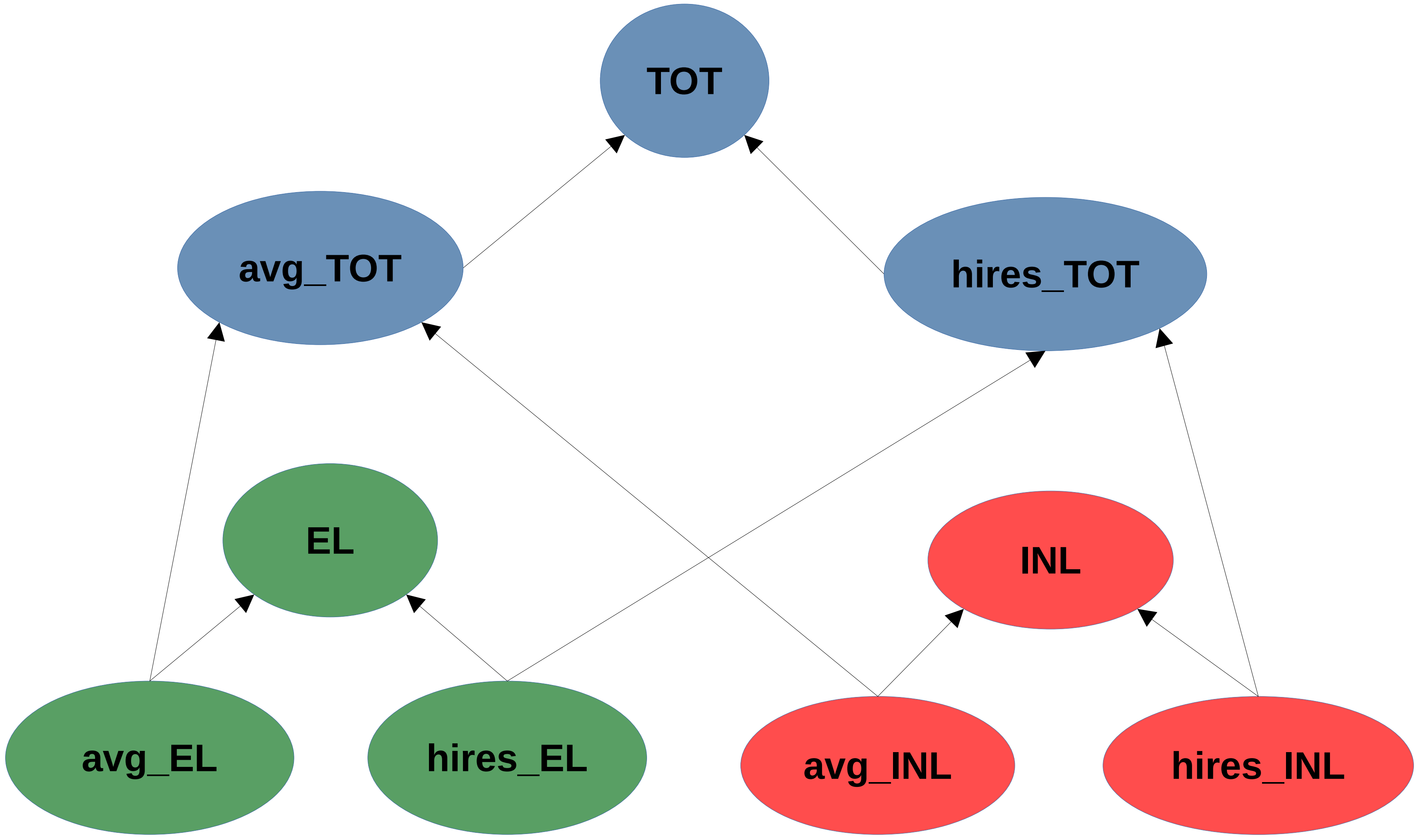
Example of Iron-56 between 1 and 2 MeV



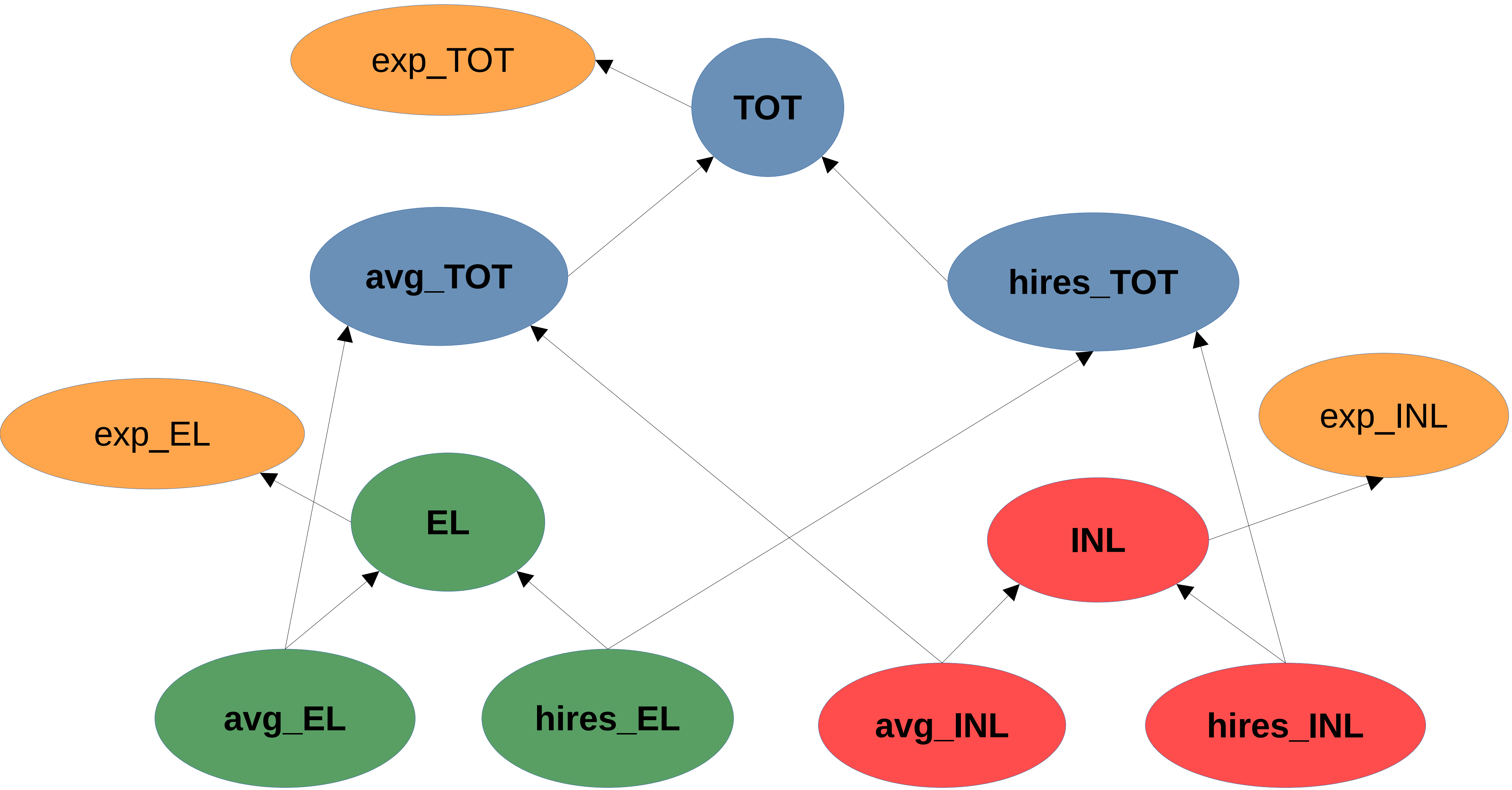




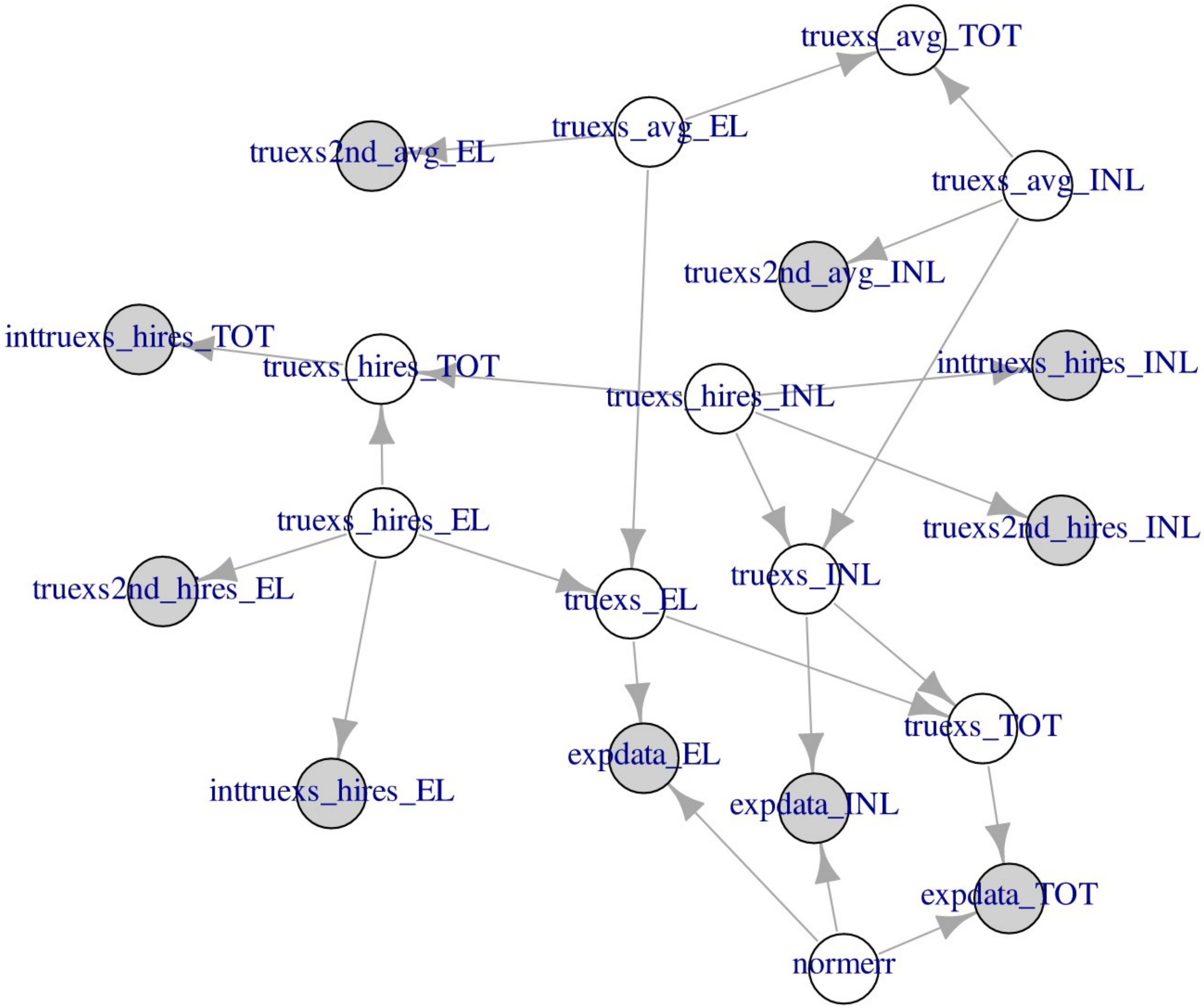
More fine-grained modeling



Coupling to experimental data

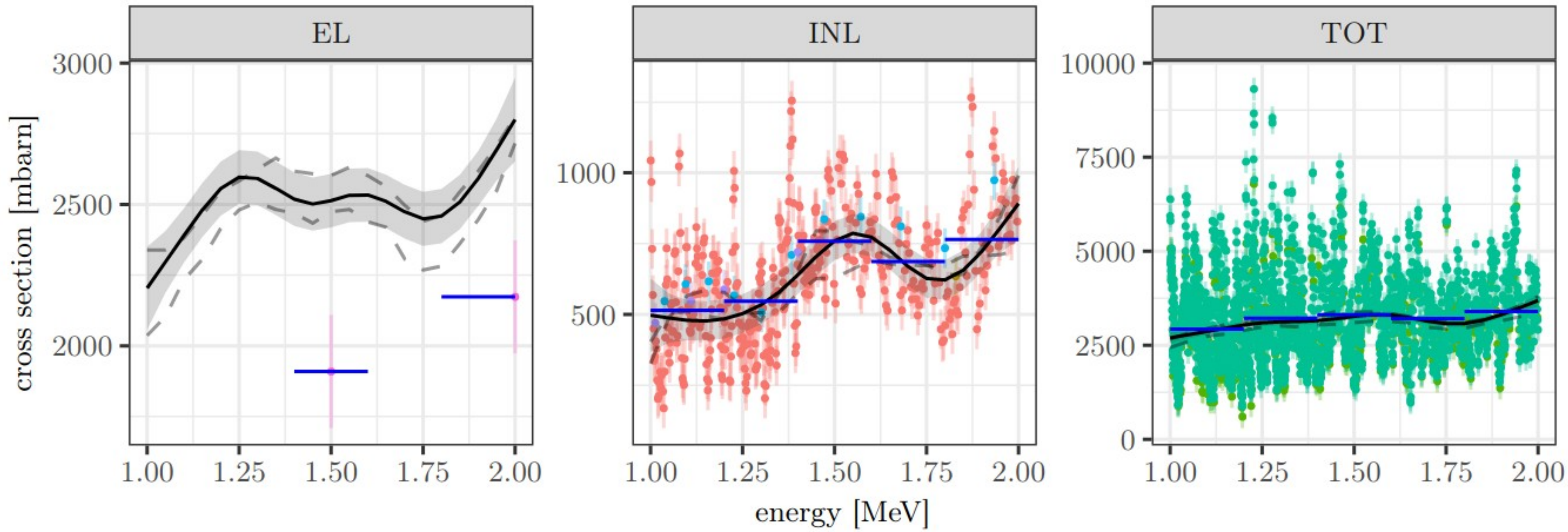


Final Bayesian network with many more regularizers



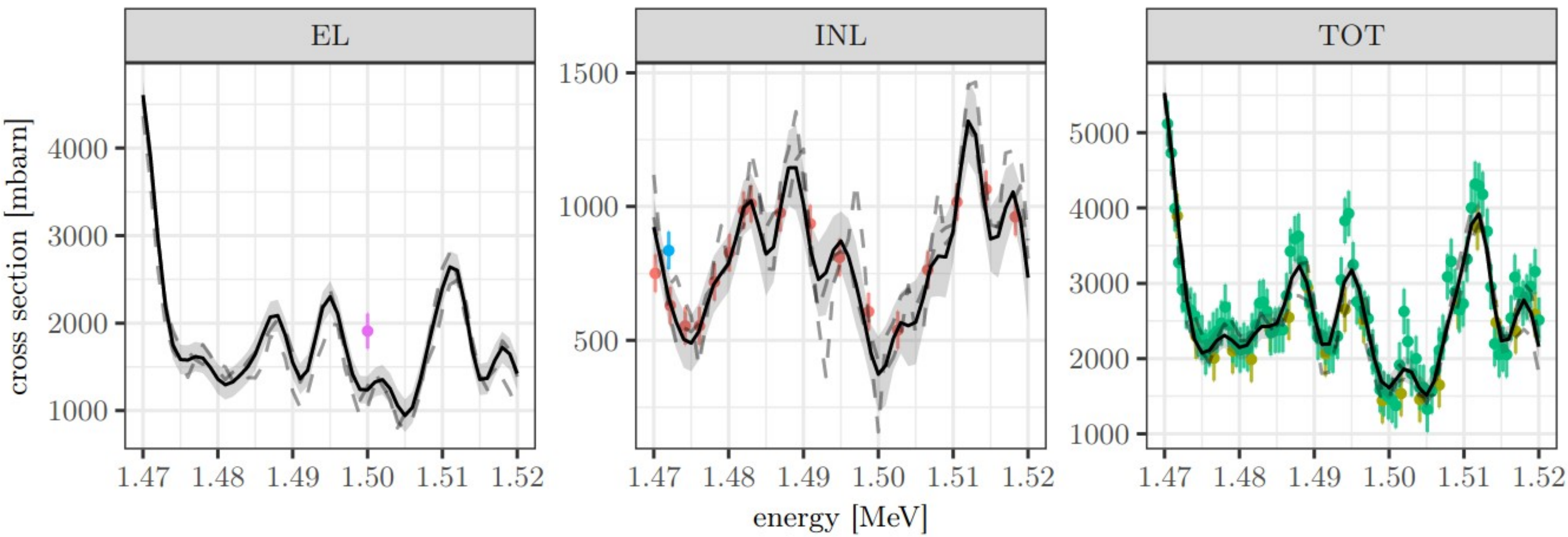
https://arxiv.org/abs/2110.10322

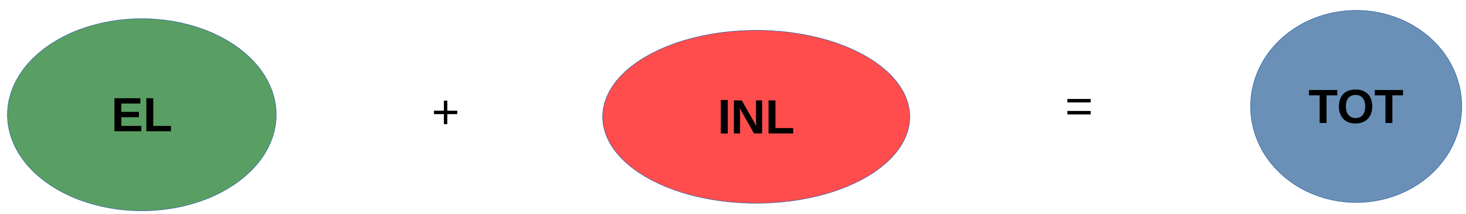
MAP estimates of average components



avg_EL + **avg_INL** = **avg_TOT**

MAP estimates of cross sections

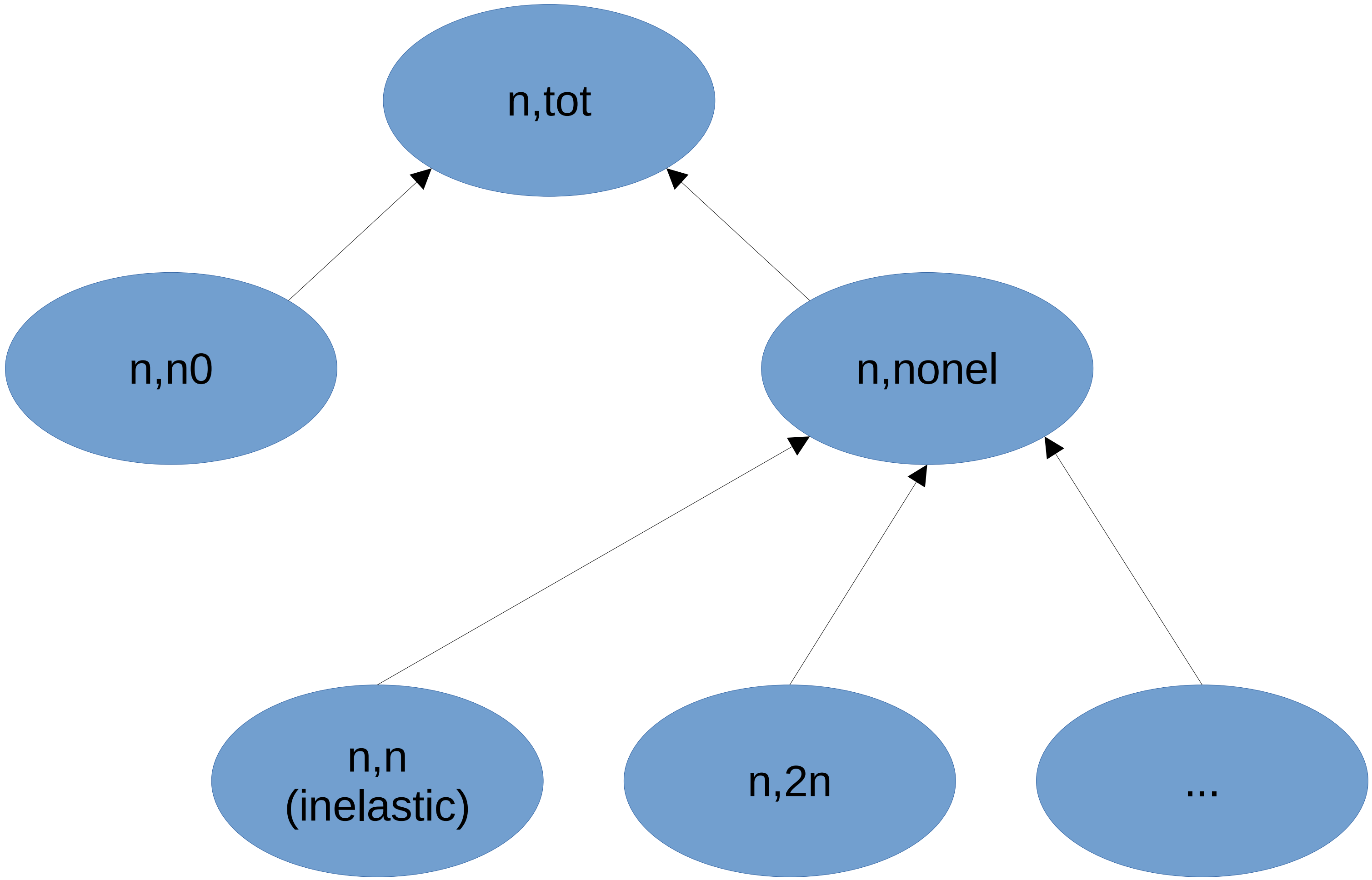




Motivation for another use case of Bayesian networks

- High-quality evaluations take a lot of time
- Final evaluations are stored in nuclear data libraries (JEFF, JENDL, ENDF/B, CENDL, etc.)
- If problems with an evaluation in a nuclear data library are detected (e.g. discovered by new experimental data), it can take again a lot of time to update the evaluation
- **Idea**: Employ Bayesian networks to *quickly and consistently* update evaluations in nuclear data libraries

Construction of Bayesian network, e.g. Ni-58



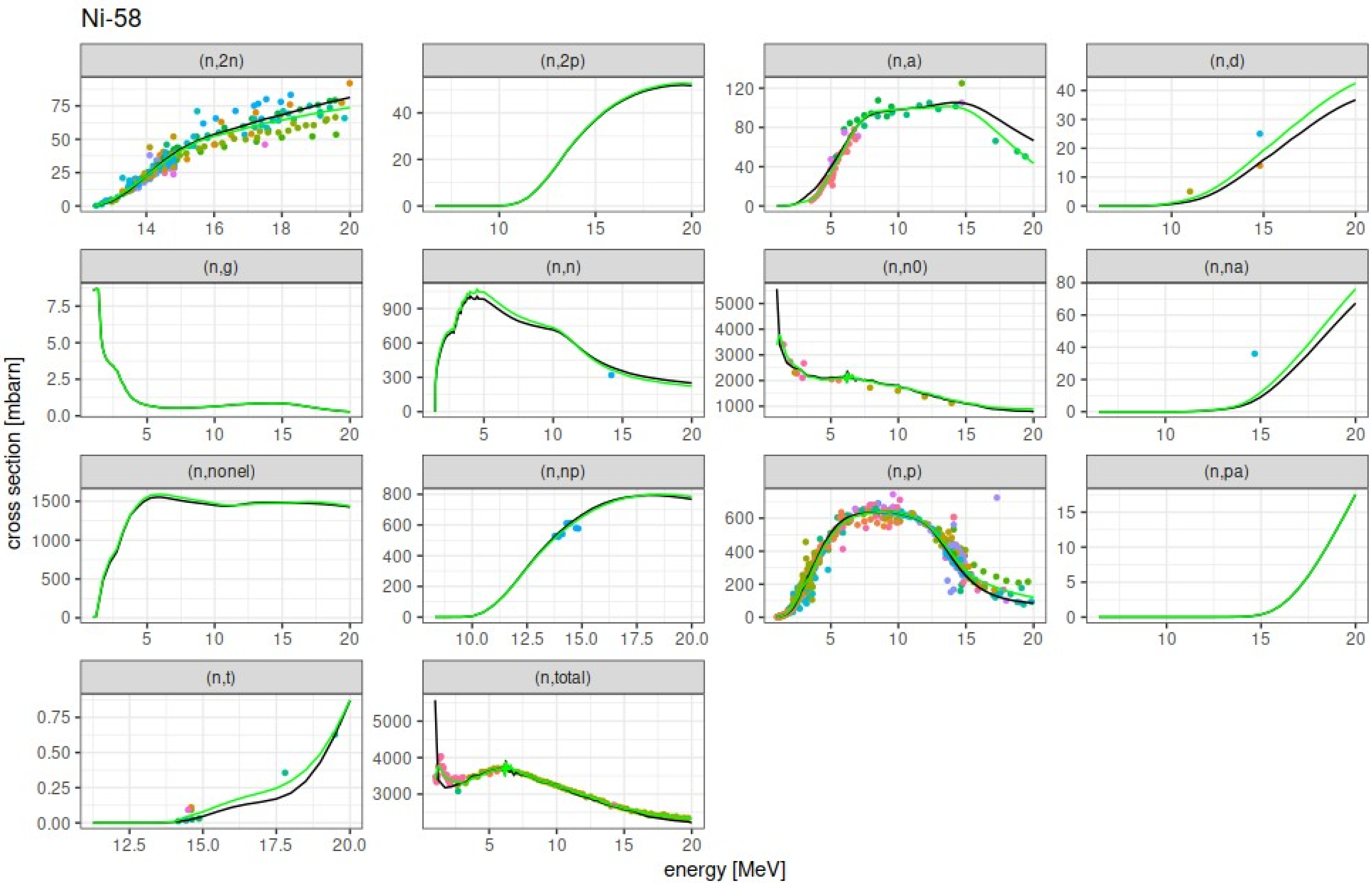
Prior assumptions

- ENDF/B-VIII.0 cross sections were used as prior mean values
- Prior uncertainty: 30% of prior cross section value
- **Introduction of prior for second derivative**
  - Prior values of 2nd derivative taken from ENDF/B-VIII.0
  - Prior uncertainty: 30% of 2nd derivative of prior values

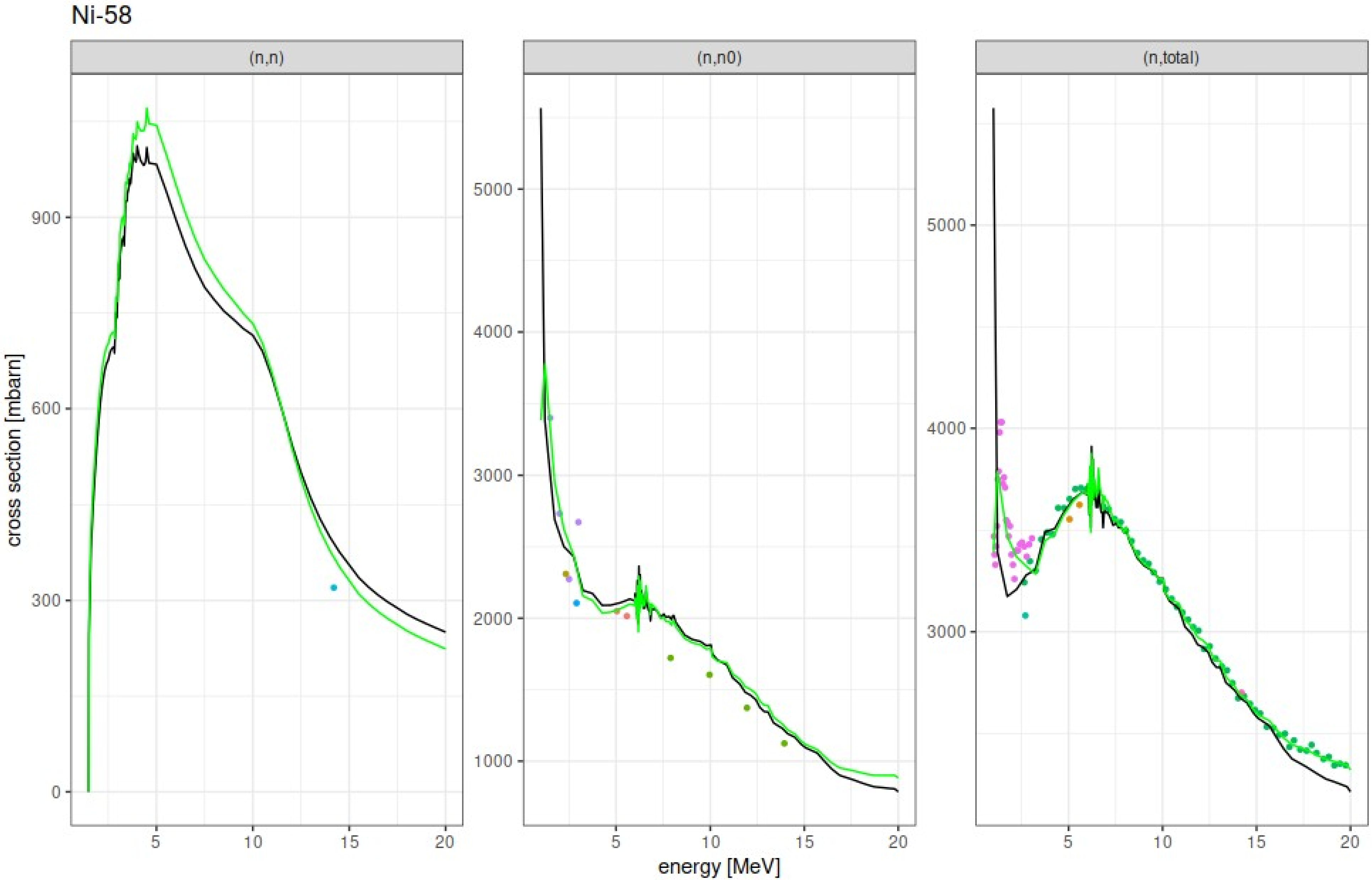
Evaluation starting point

- The Ni cross section evaluations in ENDF/B-VIII.0 (MF3) were used as a starting point (i.e., as pior mean values)
- Not considering inelastic level scattering for the time being
- Limited energy range 1 to 20 MeV for this demonstration
  - All data are linear-linear interpolated
  - MT5 is absent in this energy range in all files and in the one where it is present has negligible cross section
- No energy mesh unification was done (for simplicity)
- In total 19704 mesh points (all isotopes and reaction channels)
- Reduced mesh size of elastic and total cross sections by averaging over 0.5 MeV bins (after reduction 3817 mesh points remaining)

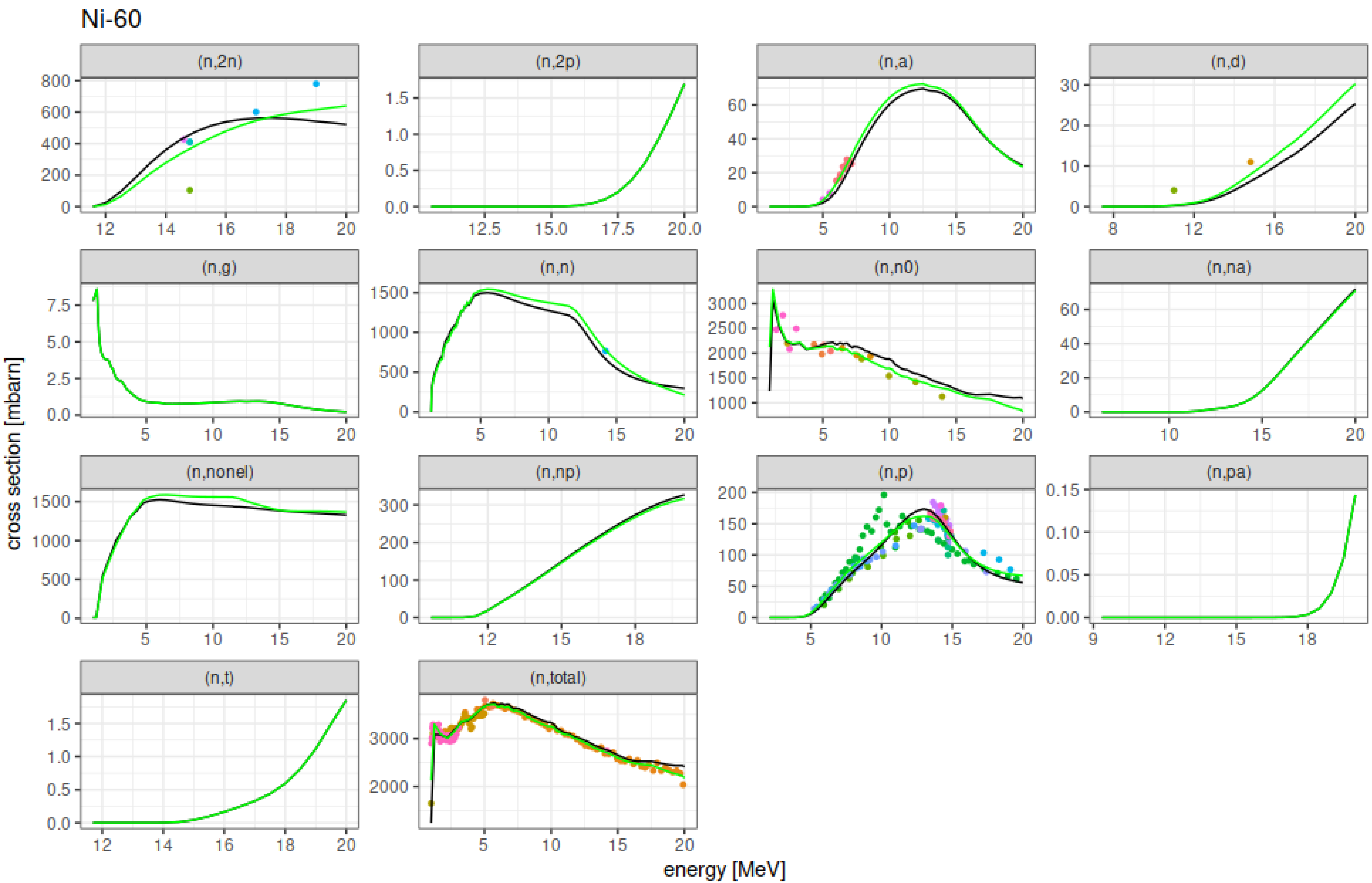
Ni-58 evaluation



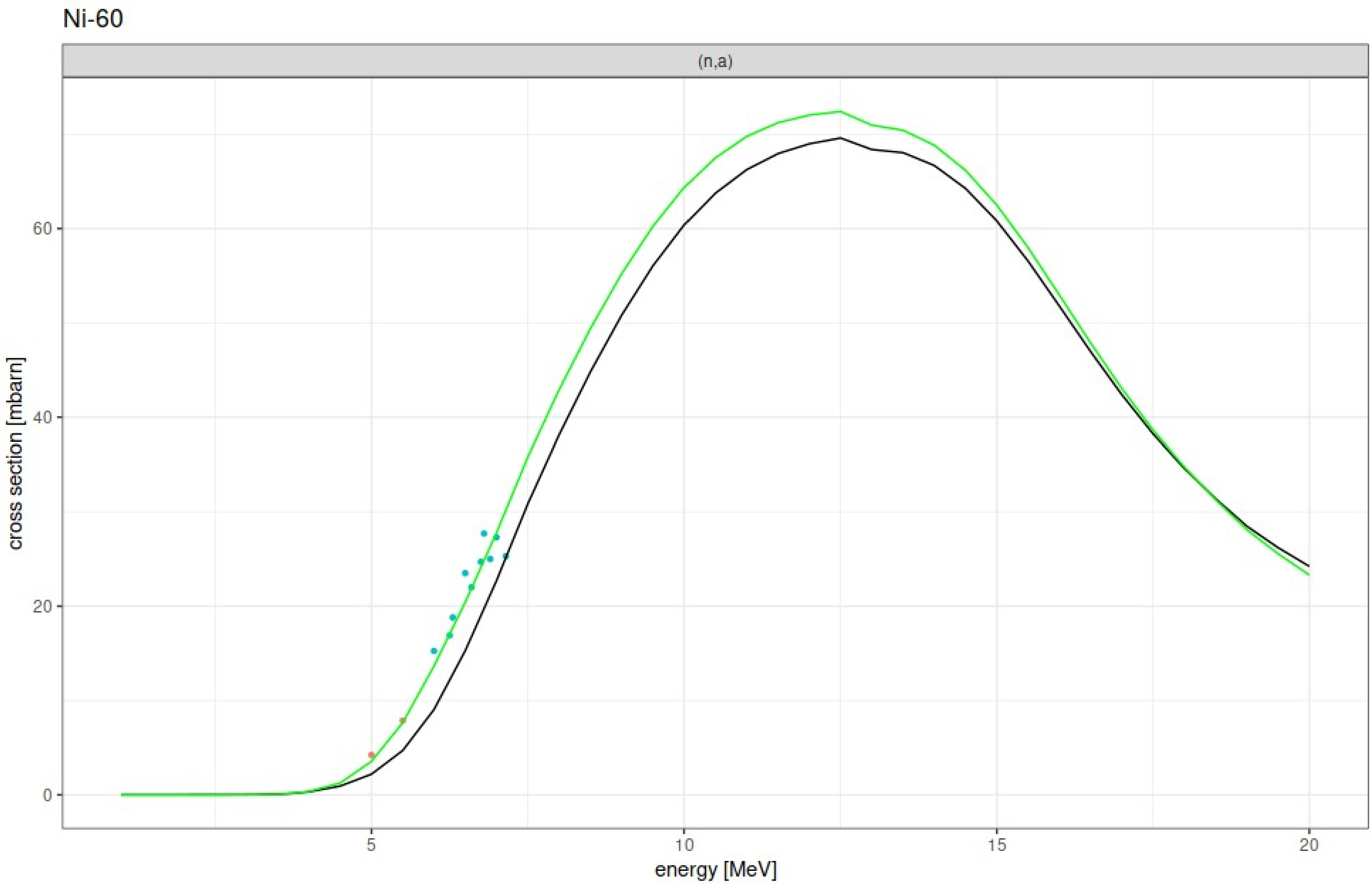
Ni-58 evaluation: (inl, el, tot)



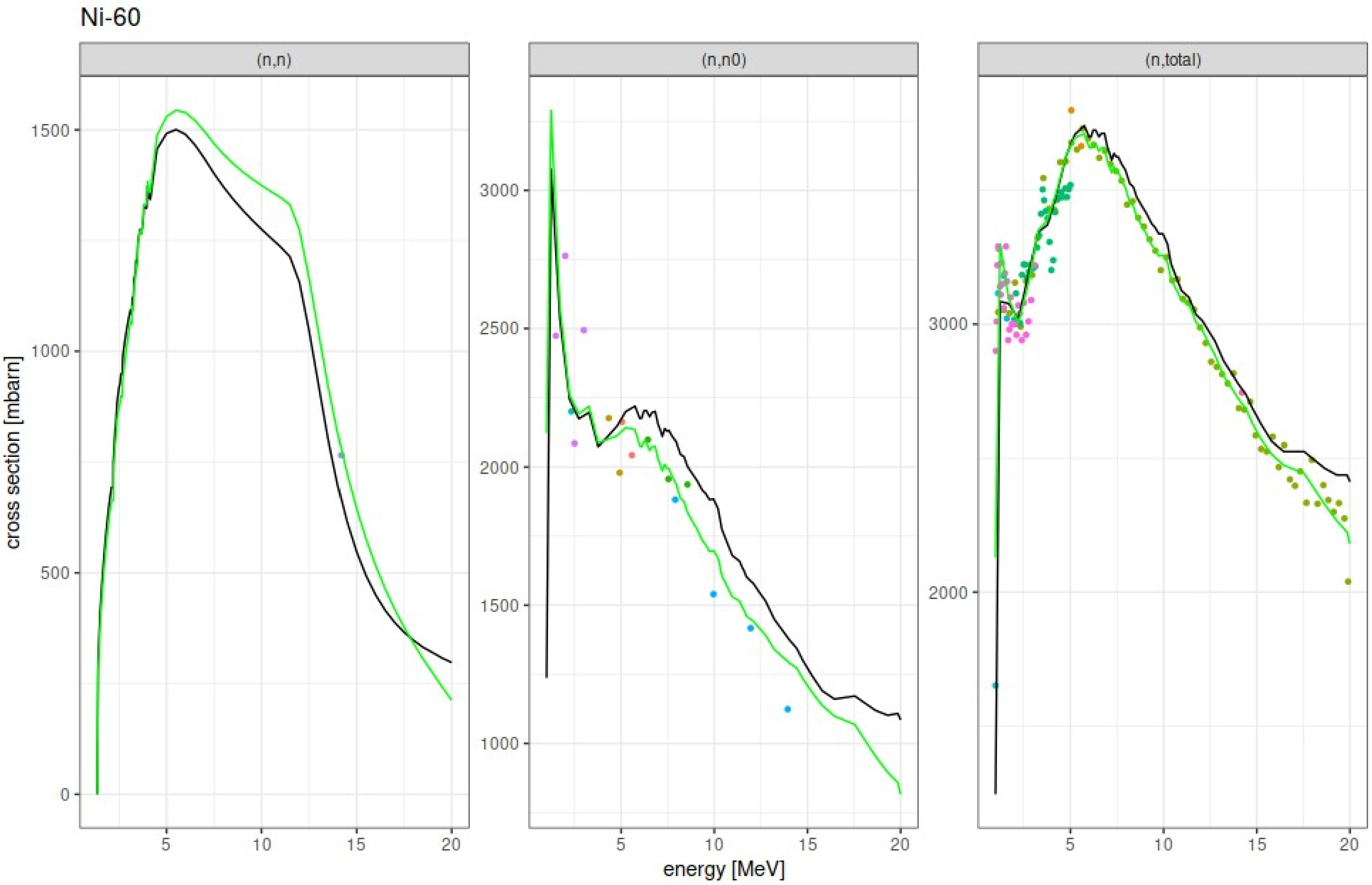
Ni-60 evaluation



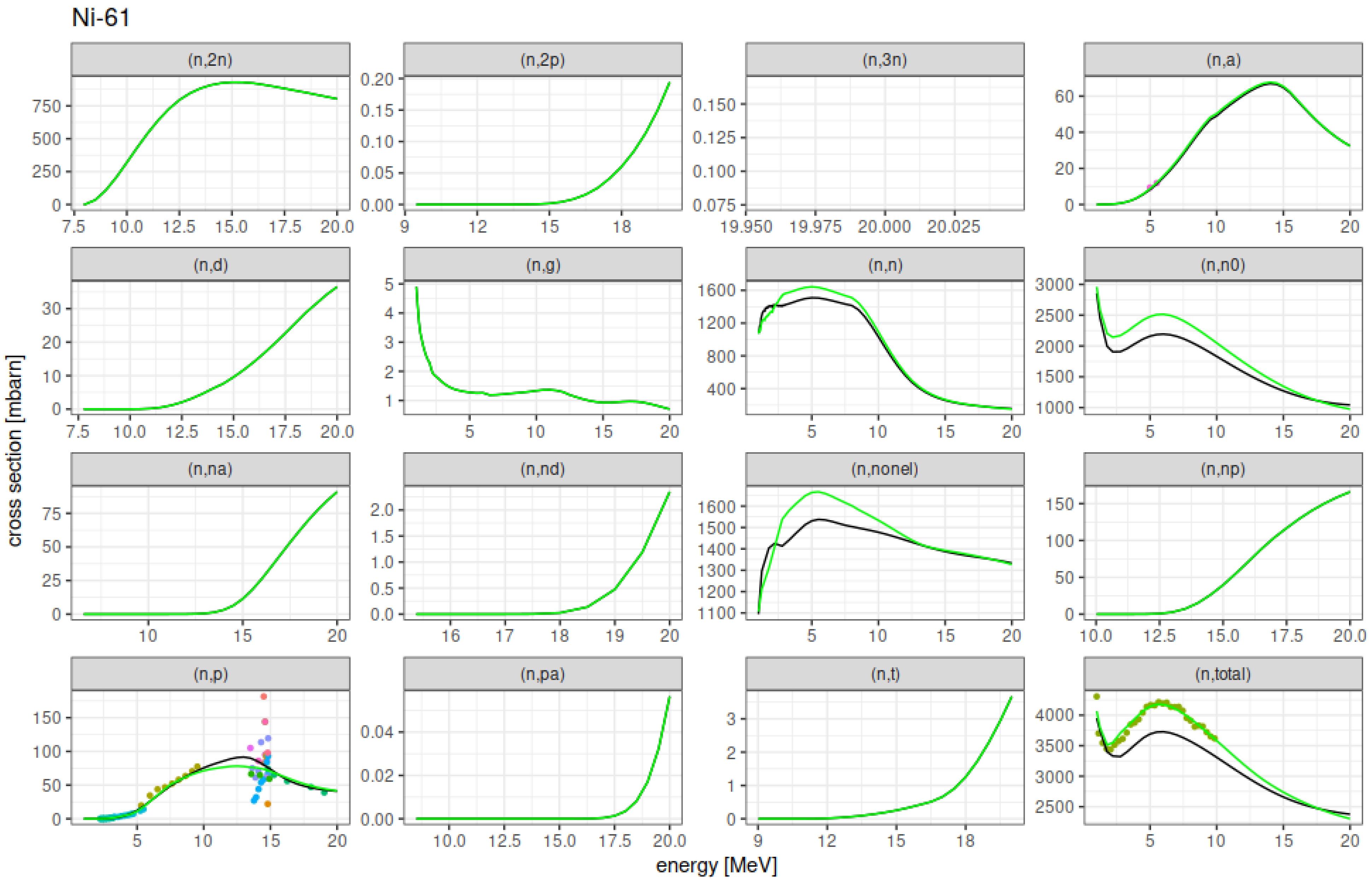
Ni-60 evaluation: (n, alpha)



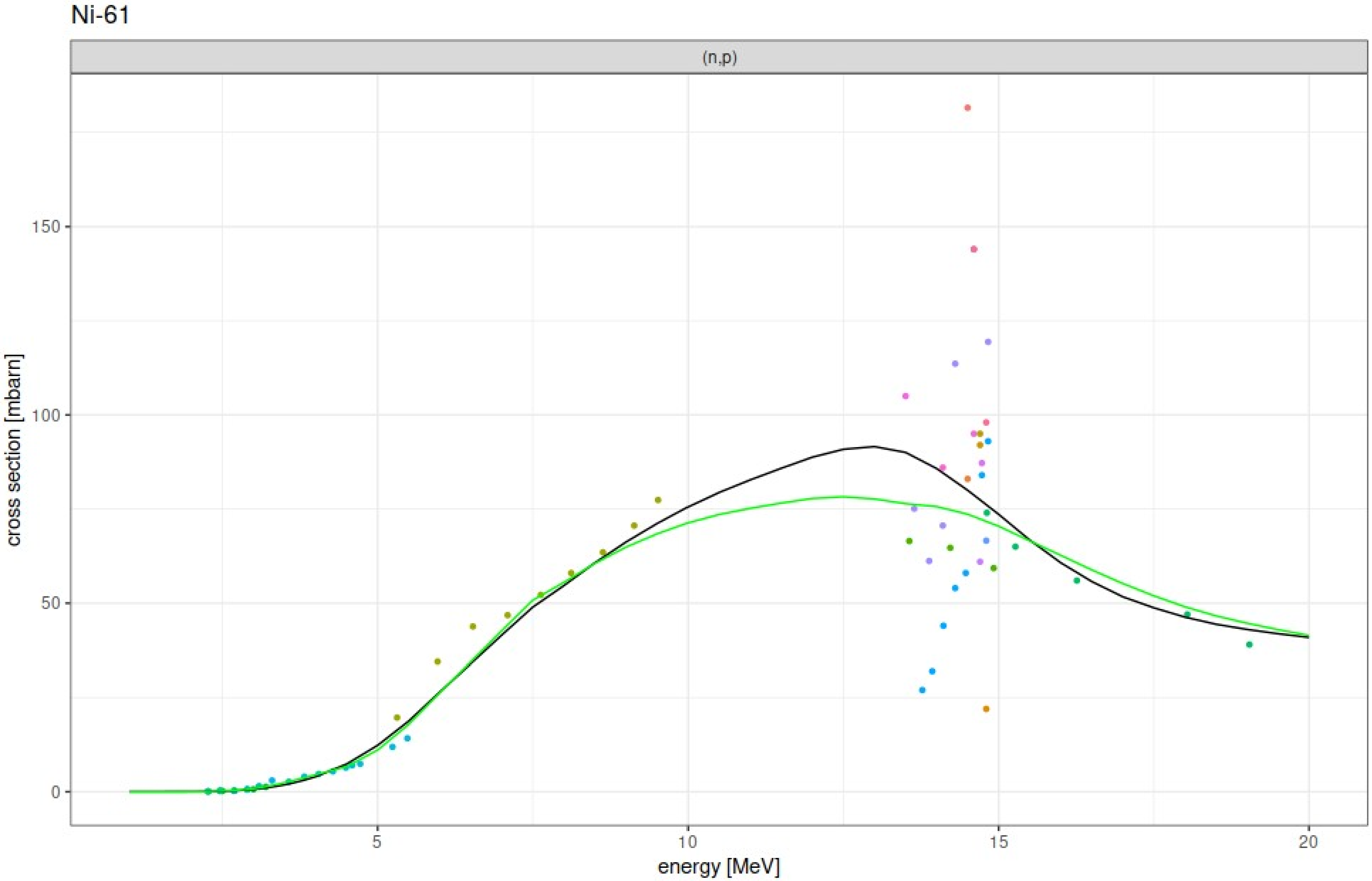
Ni-60 evaluation: inl, el, tot



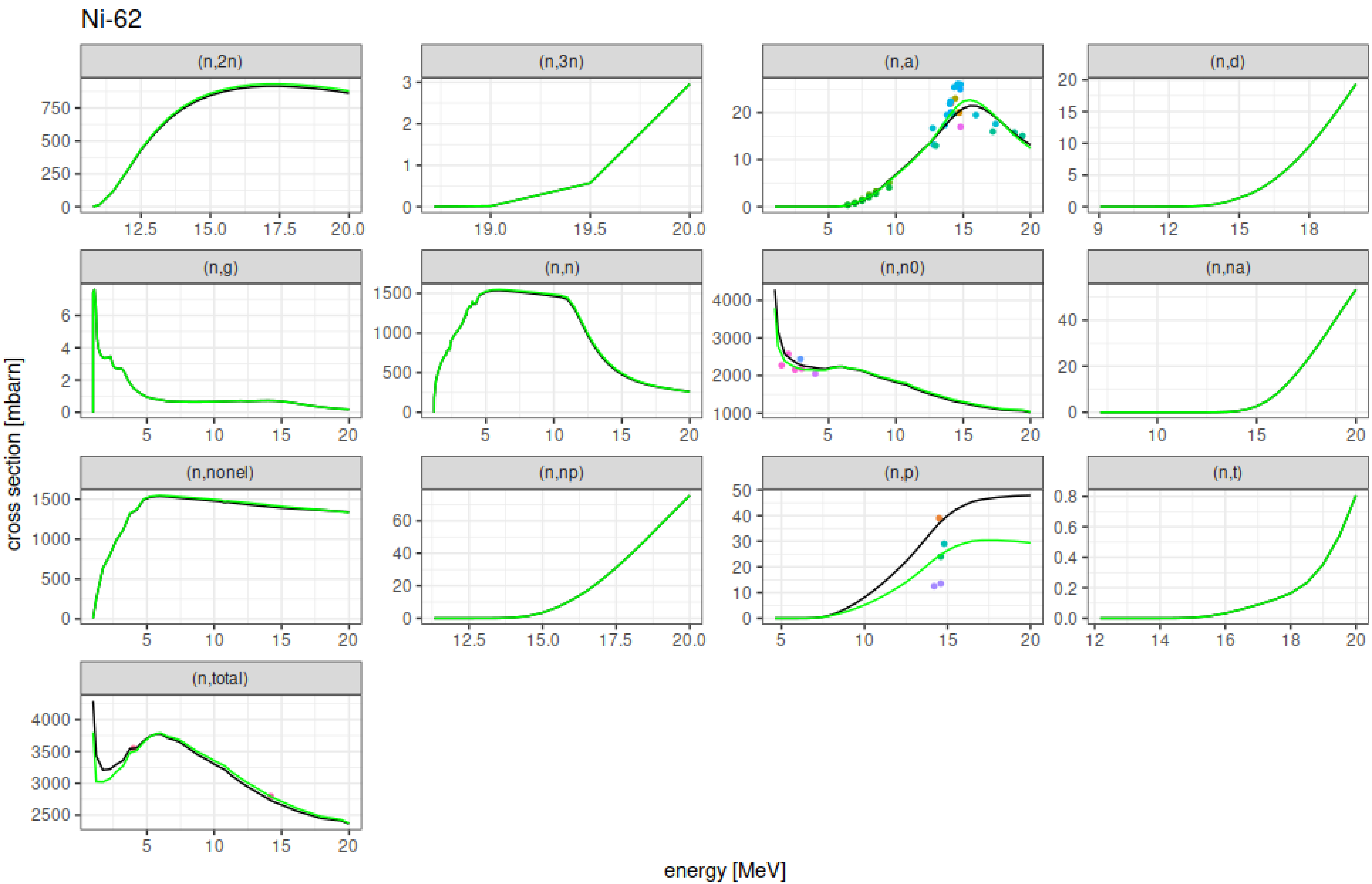
Ni-61 evaluation



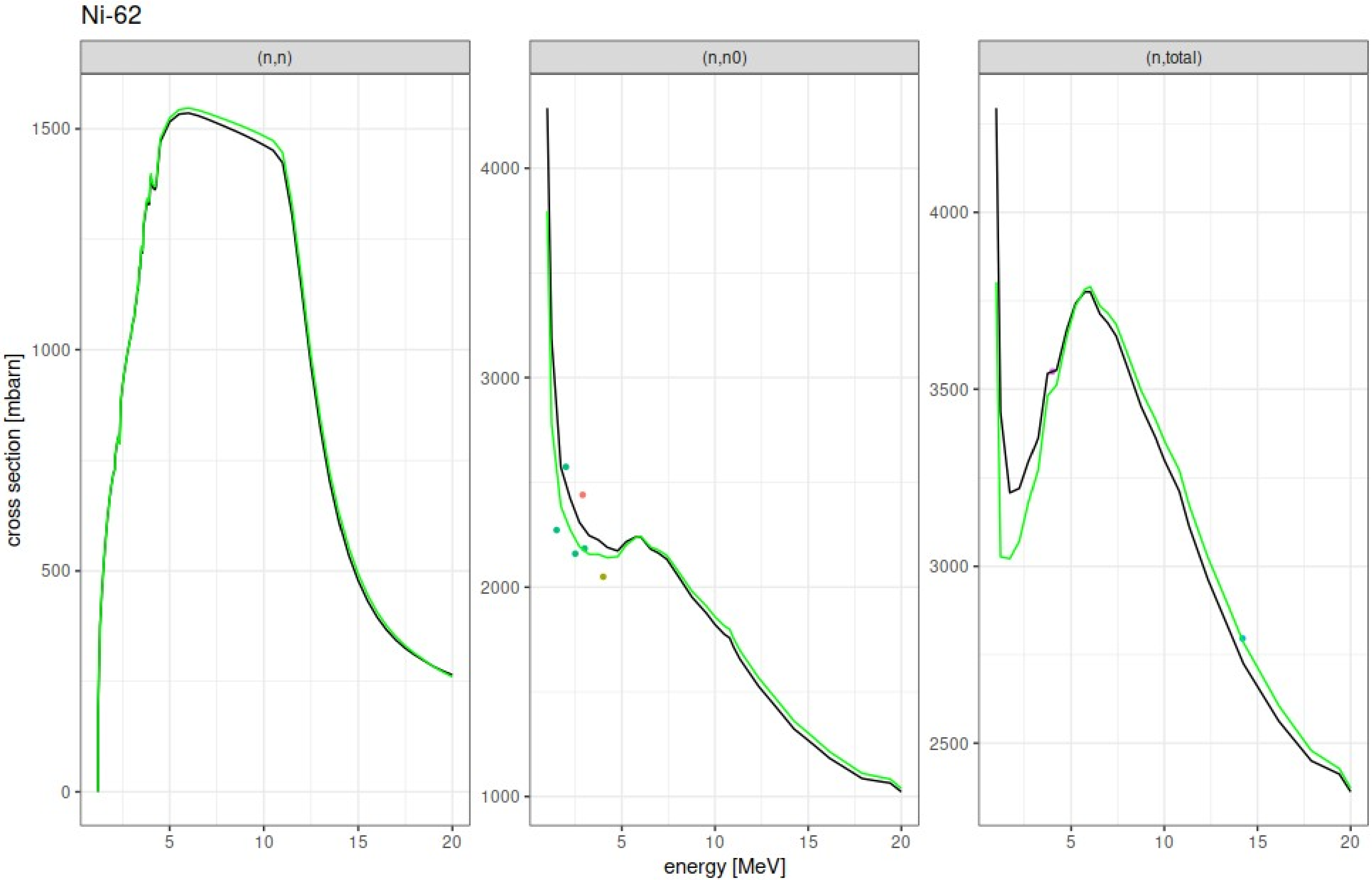
Ni-61 evaluation: (n,p)



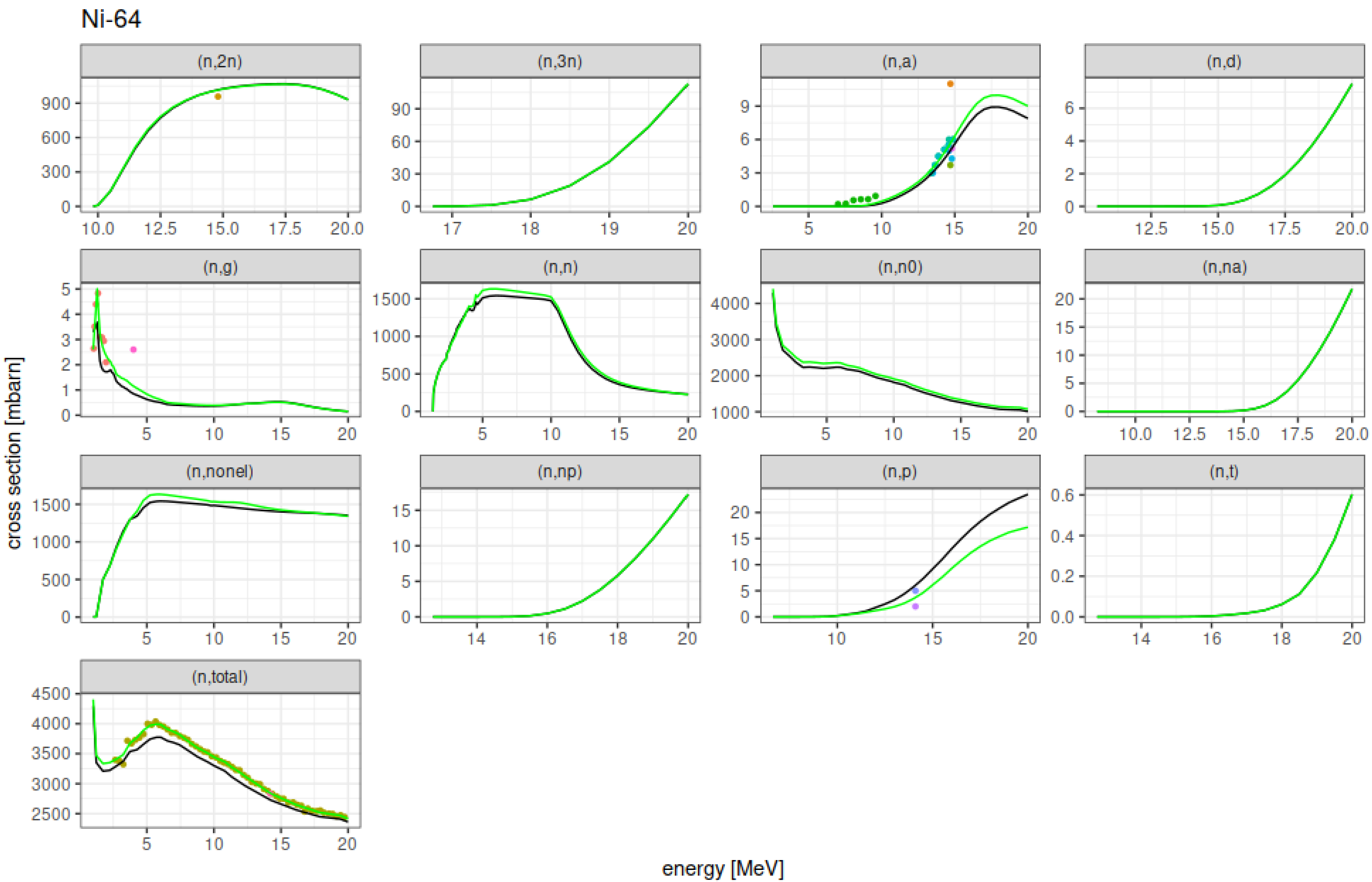
Ni-62 evaluation



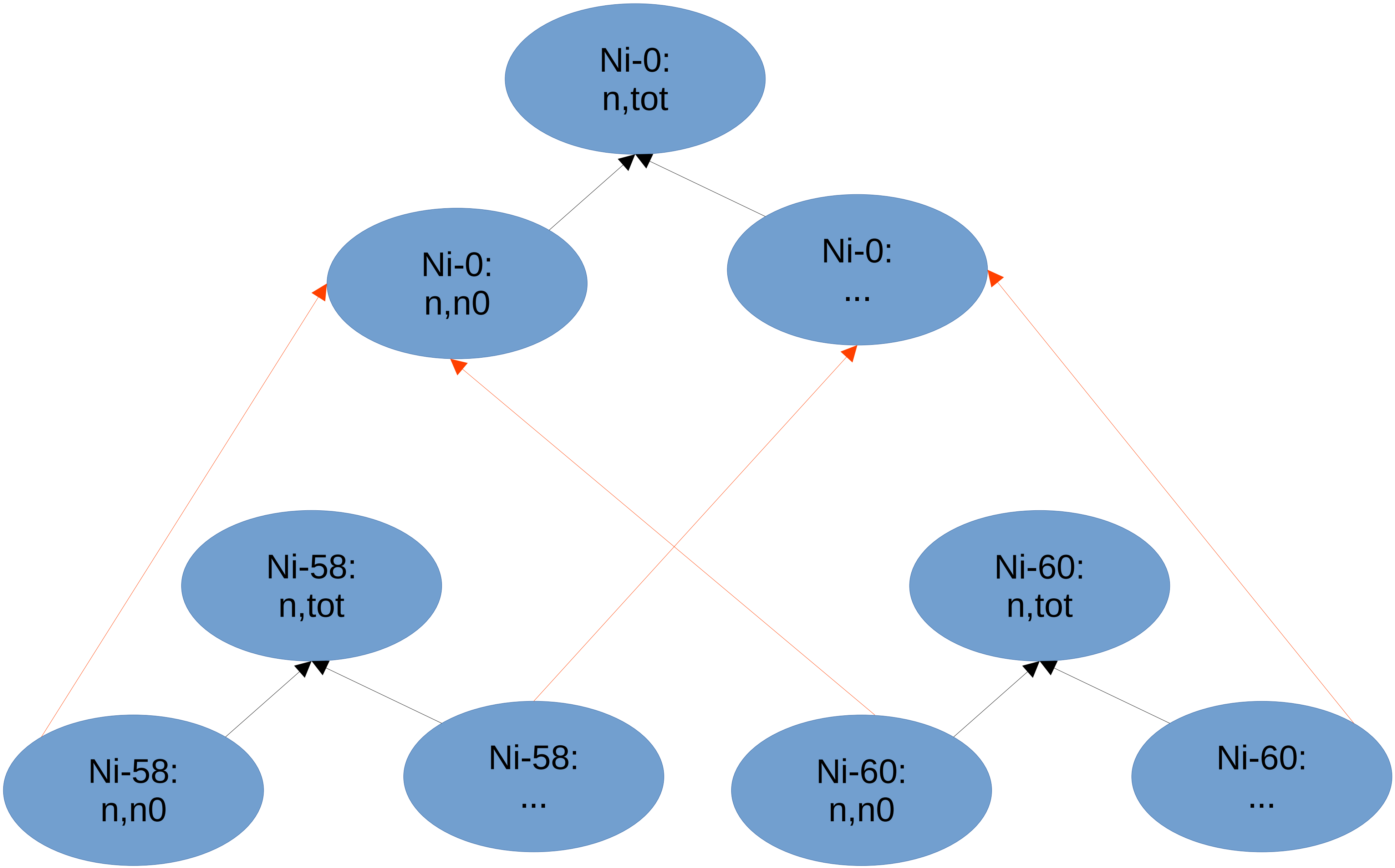
Ni-62 evaluation: inl, el, tot



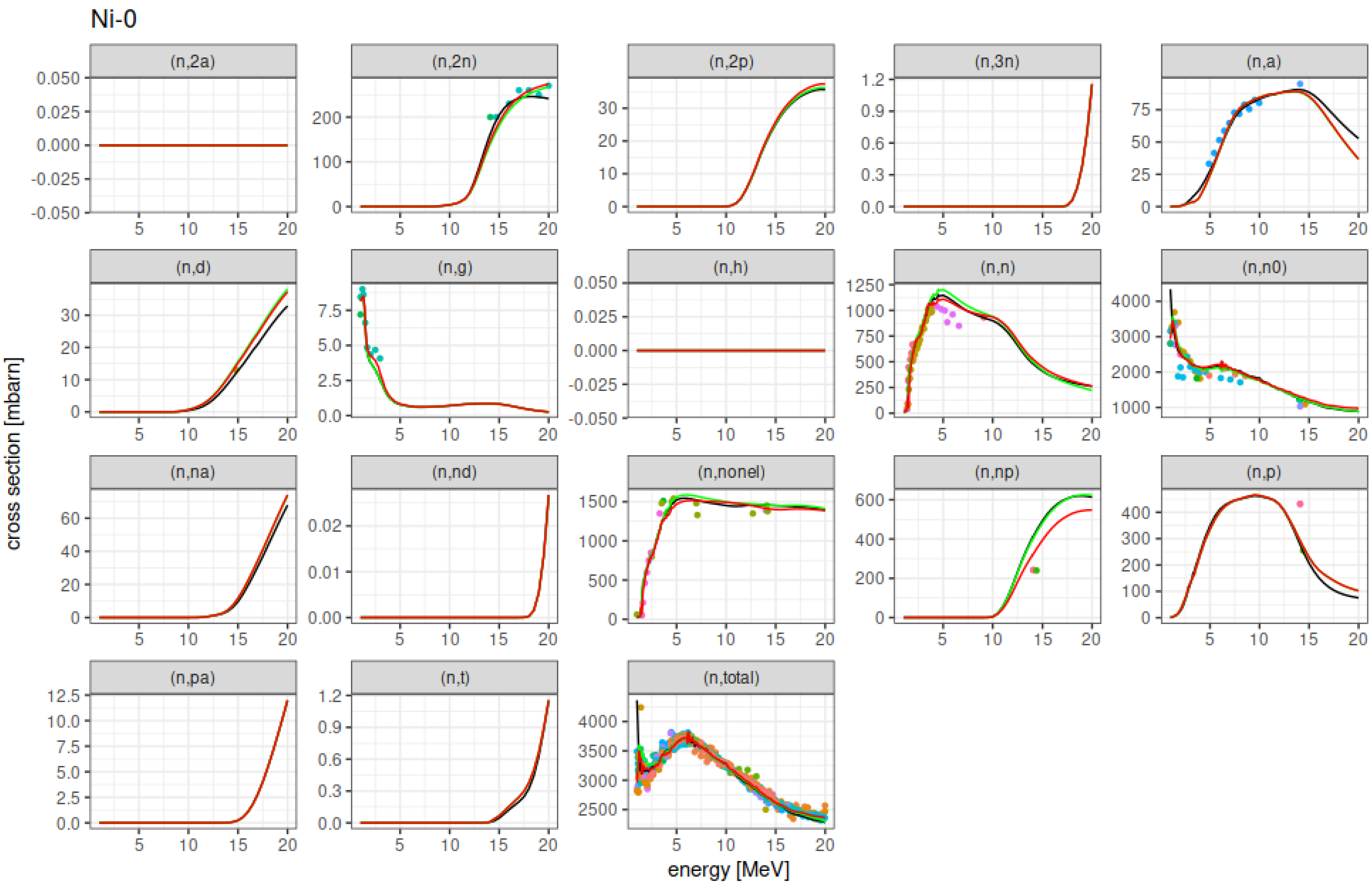
Ni-64 evaluation



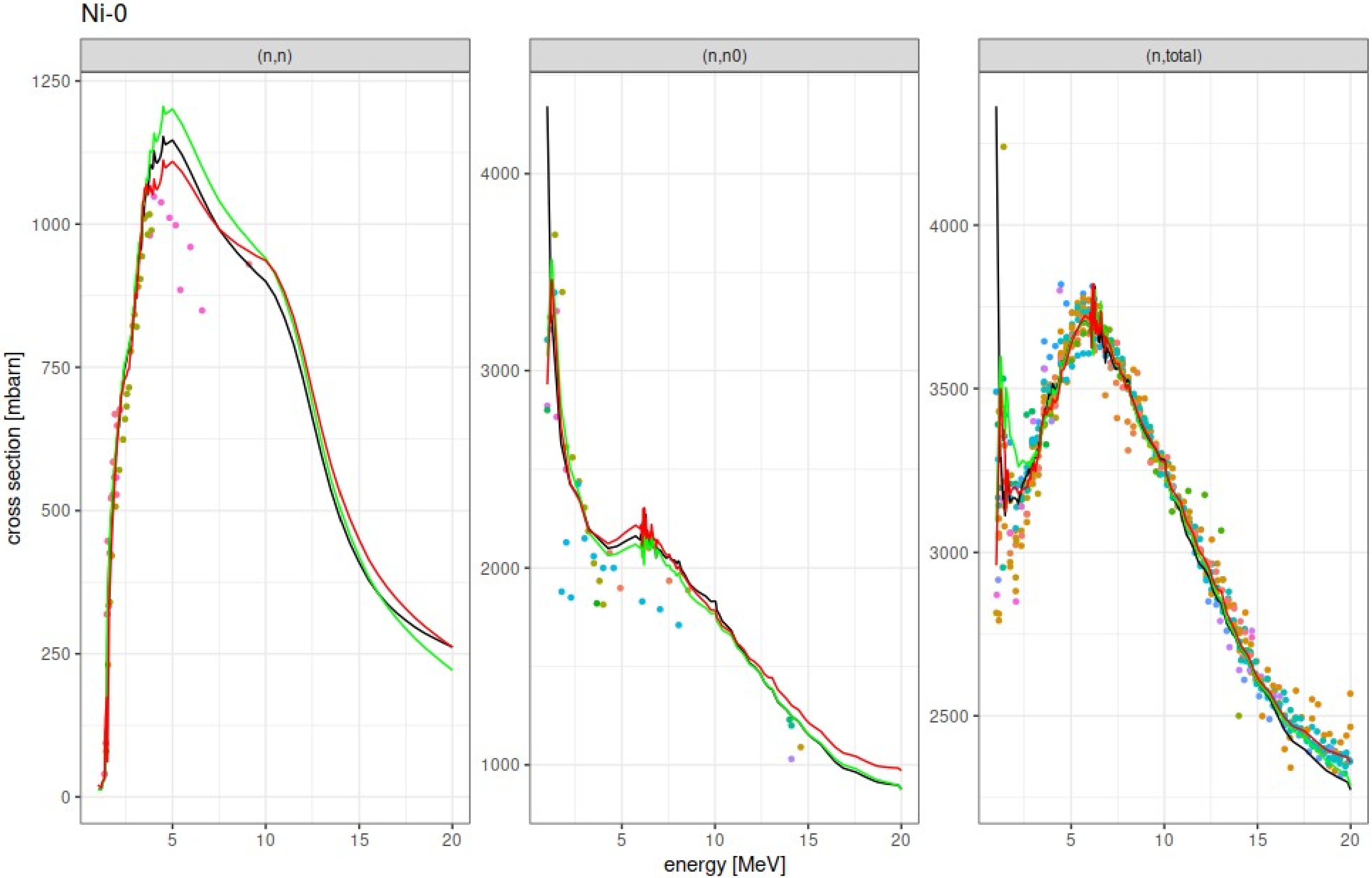
Connecting the individual Bayesian networks for consistent treatment of nat-Ni data



Evaluation of Ni-0 (coupled)

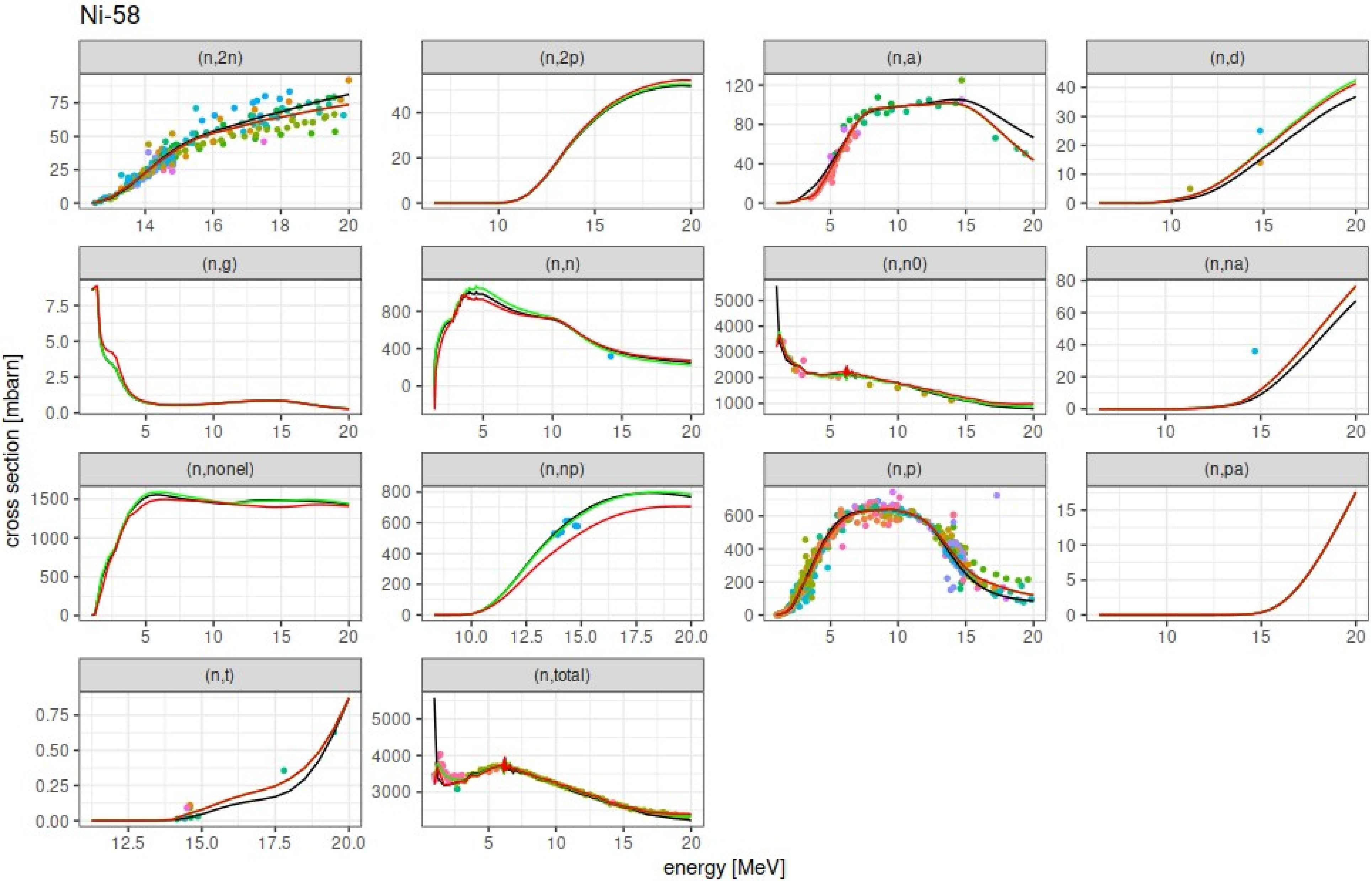


Evaluation of Ni-0 (coupled): inl, el, tot

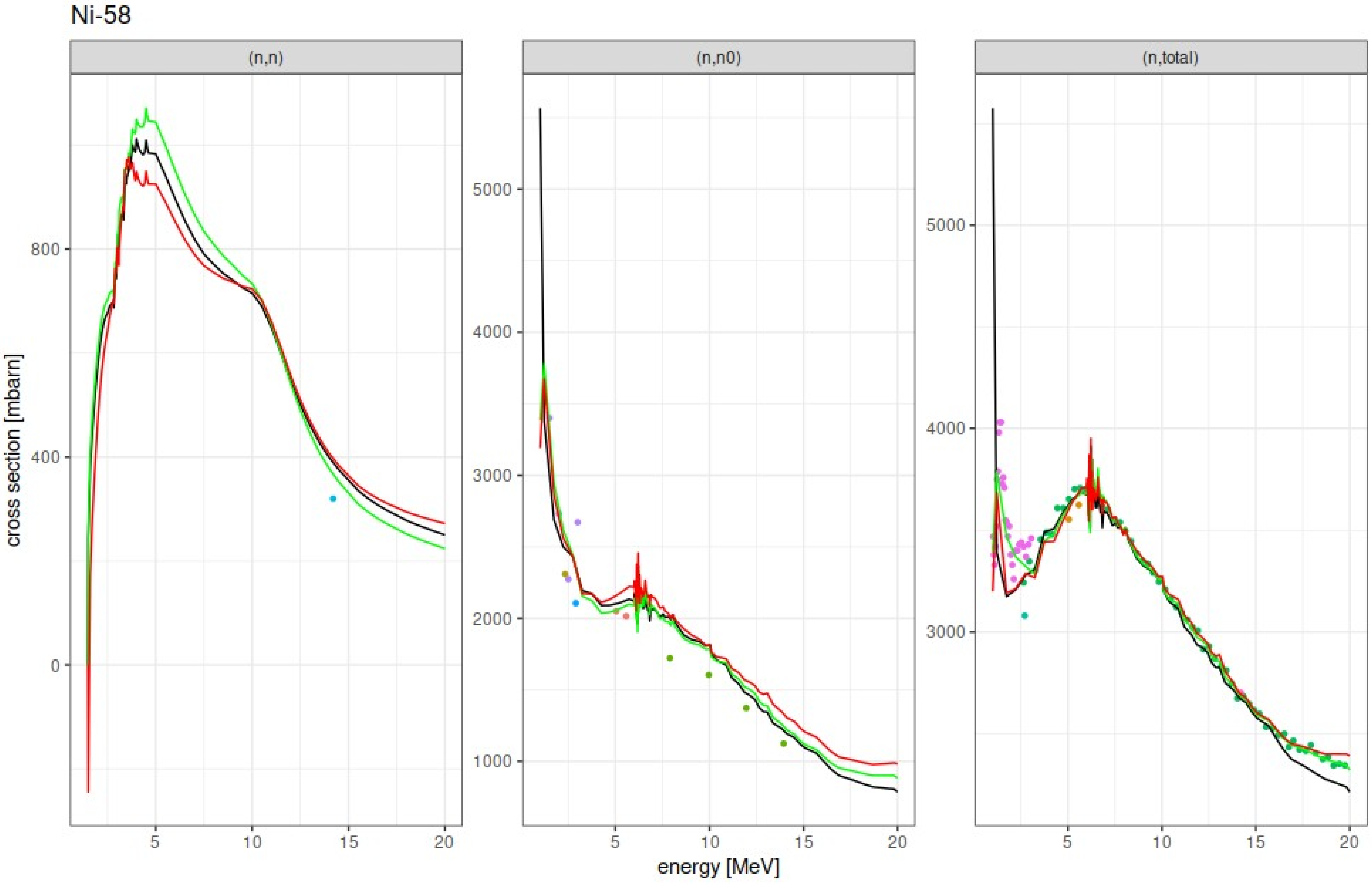


Pay attention to how the discrepant data in (n,total) near 1 MeV affects the other isotopes!

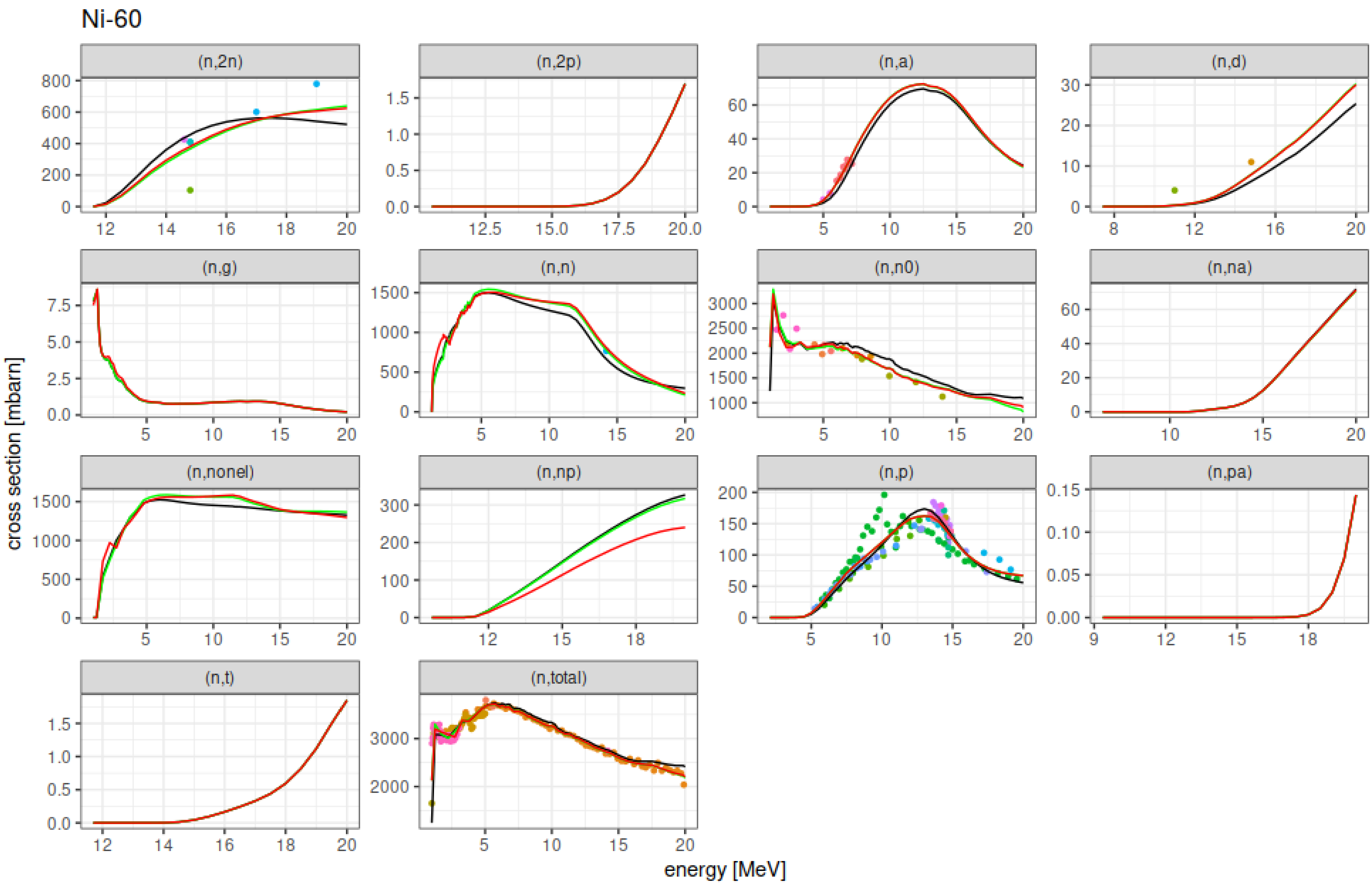
Evaluation of Ni-58 (coupled)



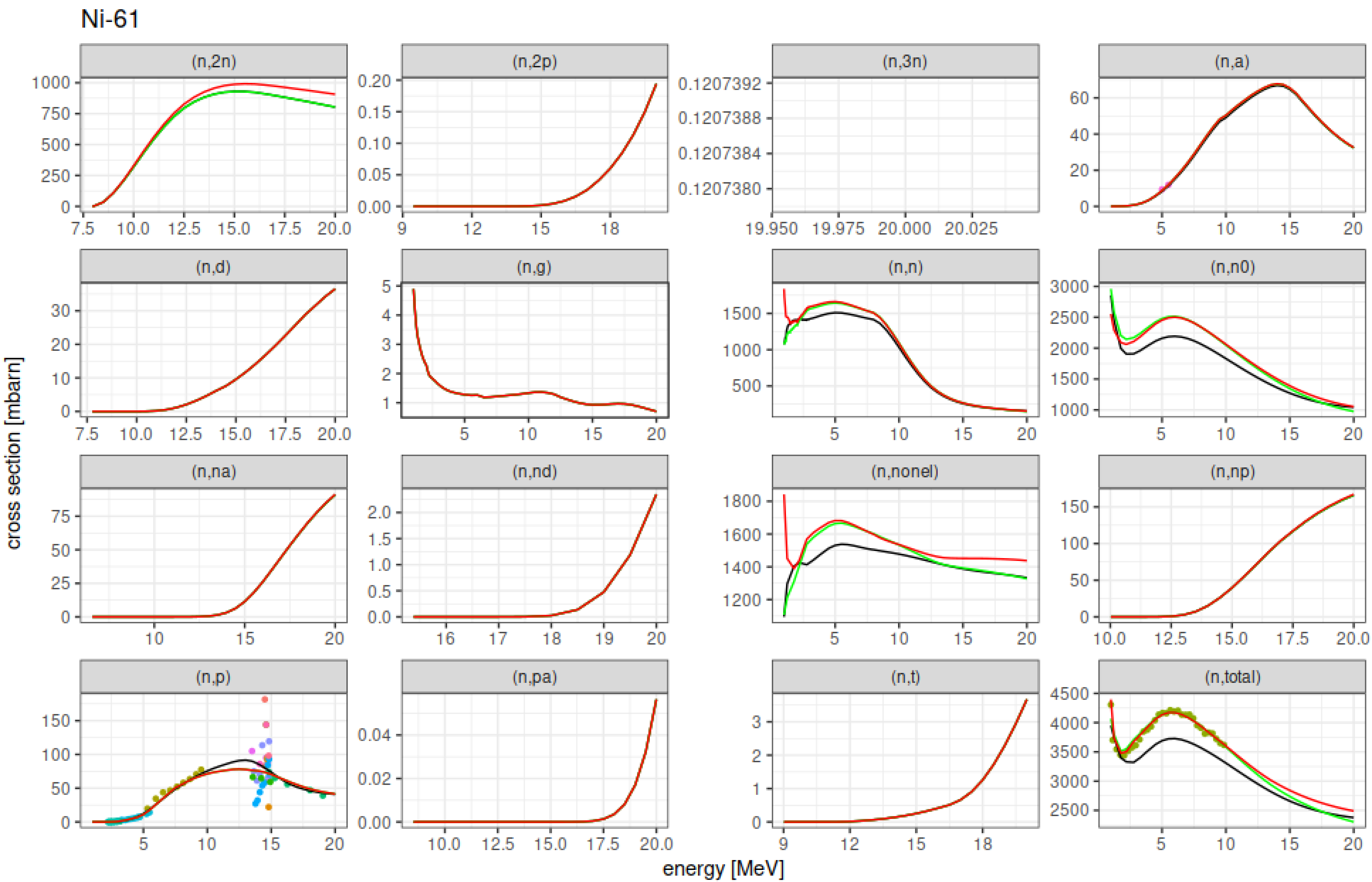
Evaluation of Ni-58 (coupled): inl, el, tot



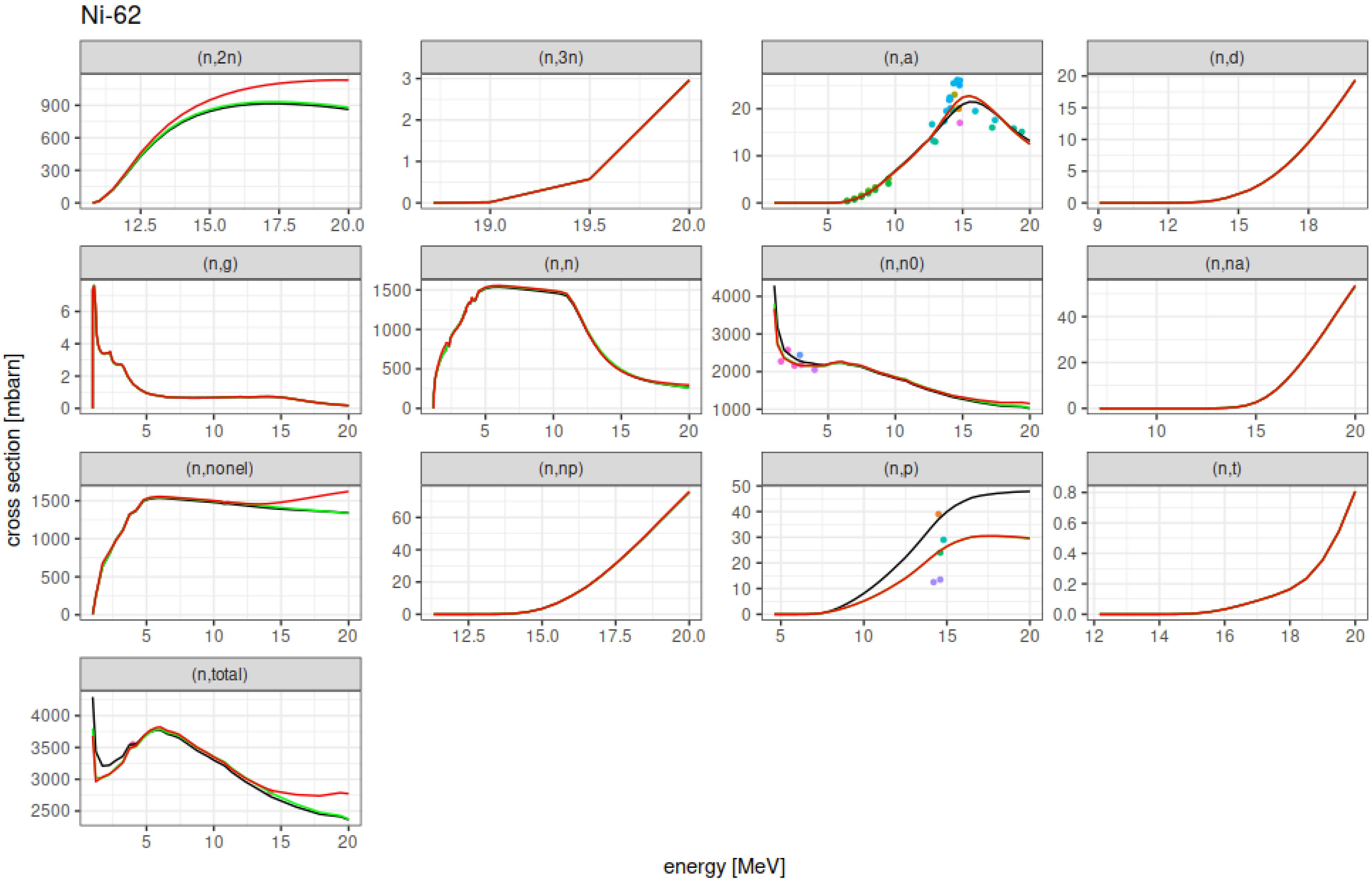
Evaluation of Ni-60 (coupled)



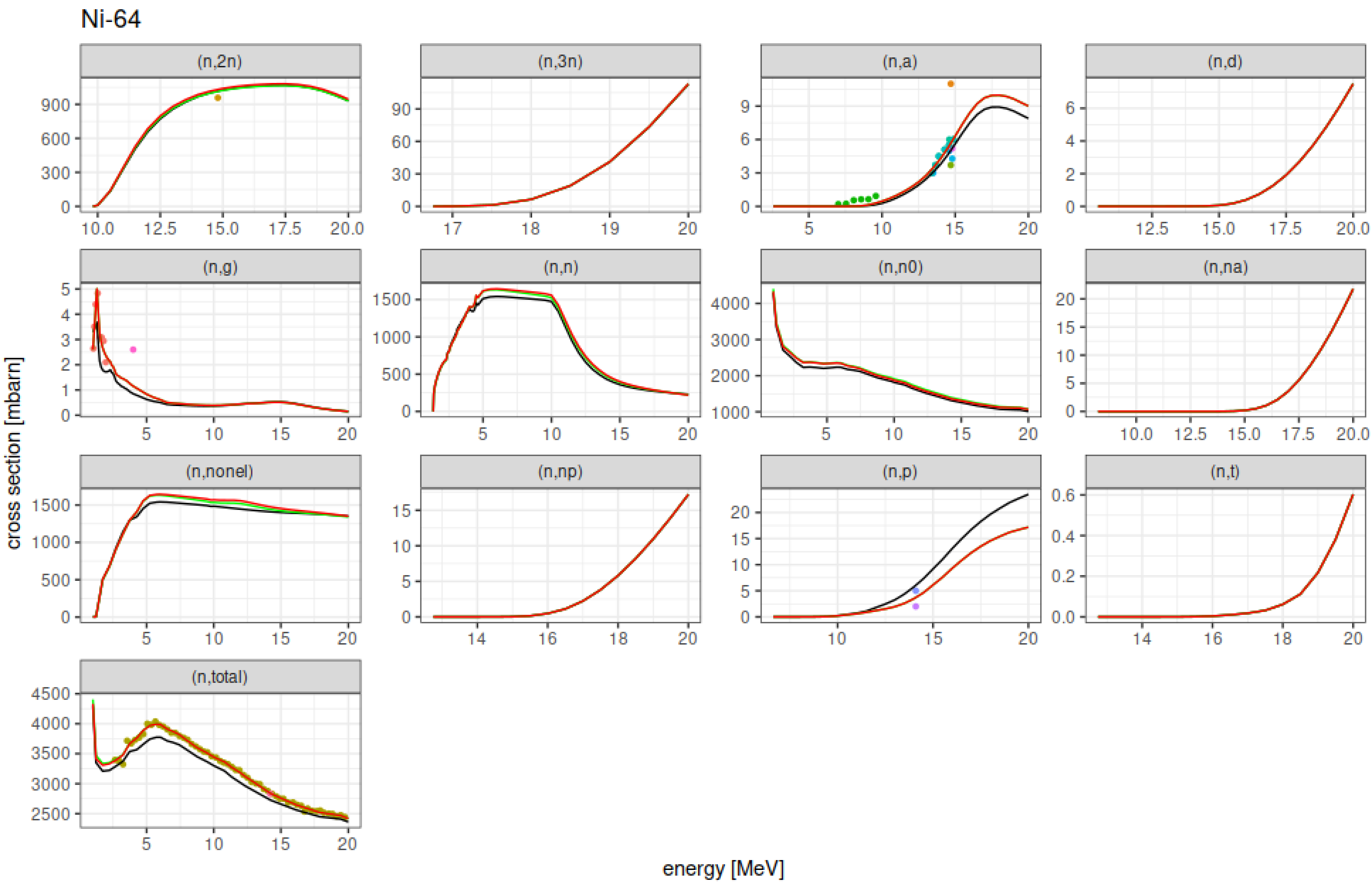
Evaluation of Ni-61 (coupled)



Evaluation of Ni-62 (coupled)



Evaluation of Ni-64 (coupled)



Ideas for discussion

- What is important to consider from the nuclear physics perspective? (e.g., constraints)
- Where do you anticipate difficulties in the application of Bayesian networks in the nuclear data context?
- Ideas for useful building blocks? (linked to experiments, nuclear models, constraints)
- Regarding making Bayesian network inference available as an online service or software package, any thoughts on APIs, frameworks, technology, design for a good user experience?