Uncertainty quantification of neutron induced cross-section of Zr-90 with model defect treatment using Nuclear Data Evaluation Pipeline of Uppsala (NEPU)

The Curious Case of the Biased Zr-90 Fit

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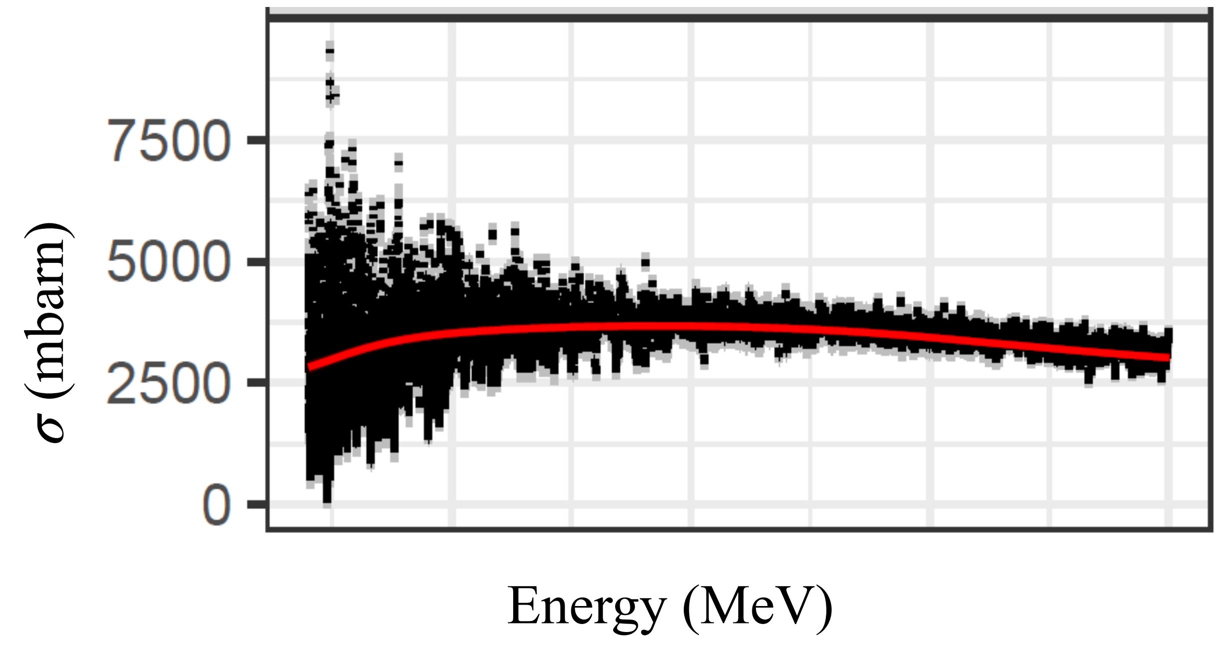
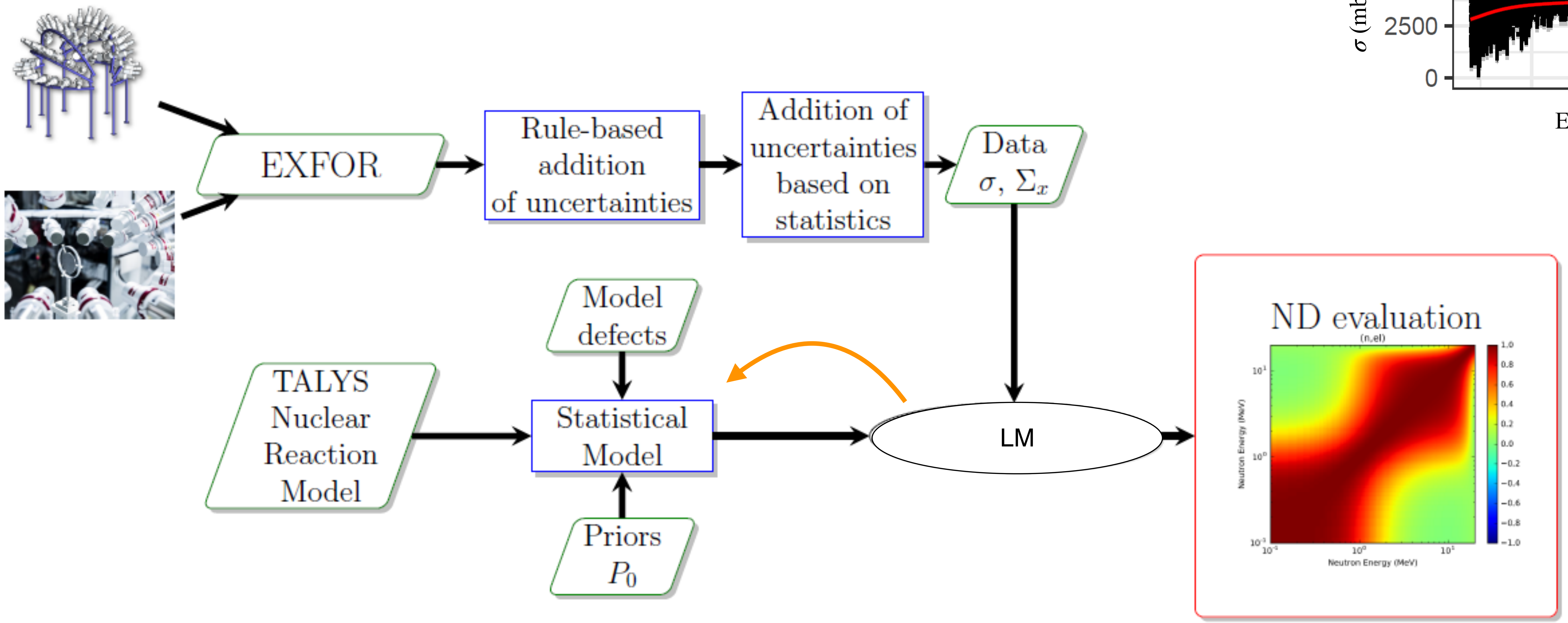
NEPU: Nuclear Data Evaluation Pipeline of Uppsala

A pipeline for nuclear data evaluation that implements (and further develops) methodology to treat model defects and inconsistent experimental data that has originated in research activities at UU.
Goal: Automatization, Reproducible.

G. Schnabel, H. Sjöstrand, J. Hansson, D. Rochman, A. Koning, R. Capote Nucl. Data Sheets 173, 239 (2021)
A.Göök, E. Andersson-Sundén, J. Hansson, and H. Sjöstrand, EPJ Web of Conf. 294, 04005 (2024)

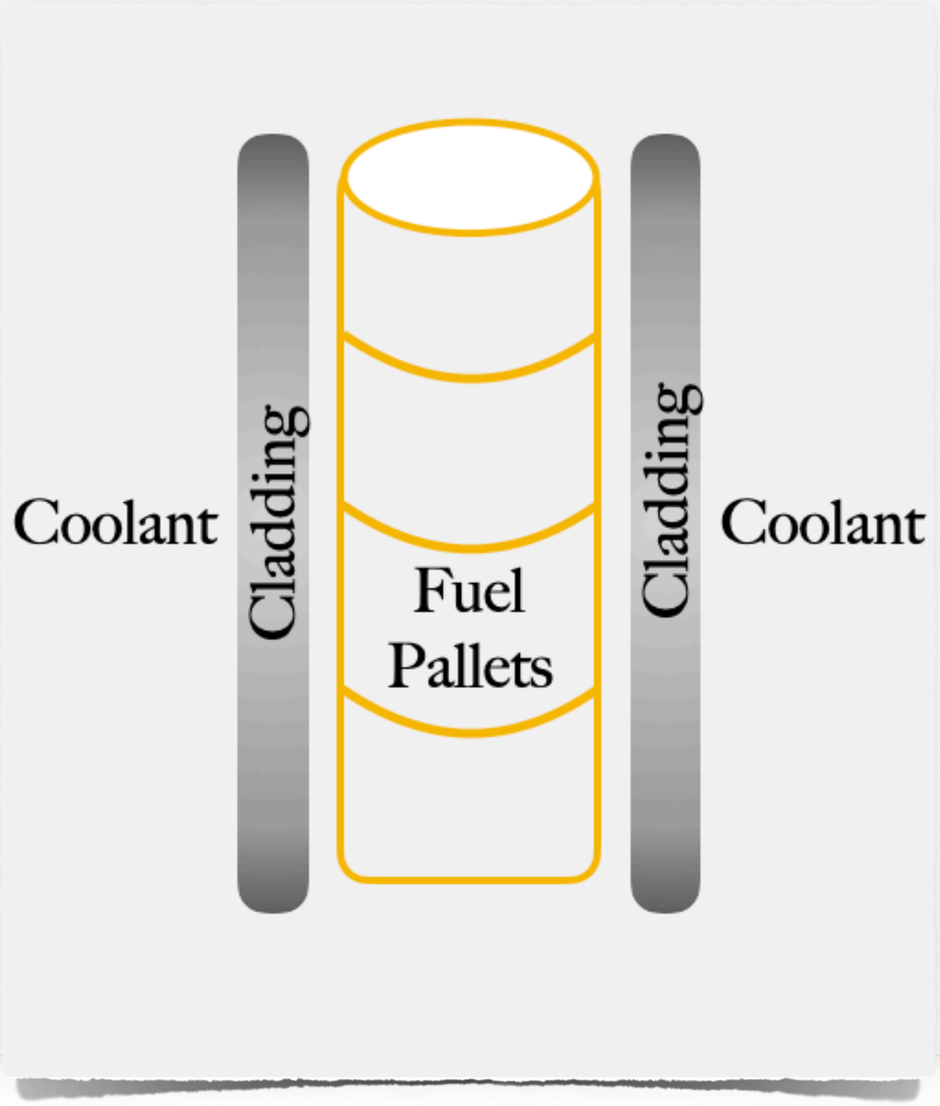




Zr-90 on NEPU - Input setup

Why Zr-90?

- Assembly structure & cladding material
- Isotopic abundance of Zr-90 ~ 51%



For Zr-90 we have used TENDL-2019 input and TALYS-1.95 version.

We plan to use latest TENDL input with TALYS-2.2

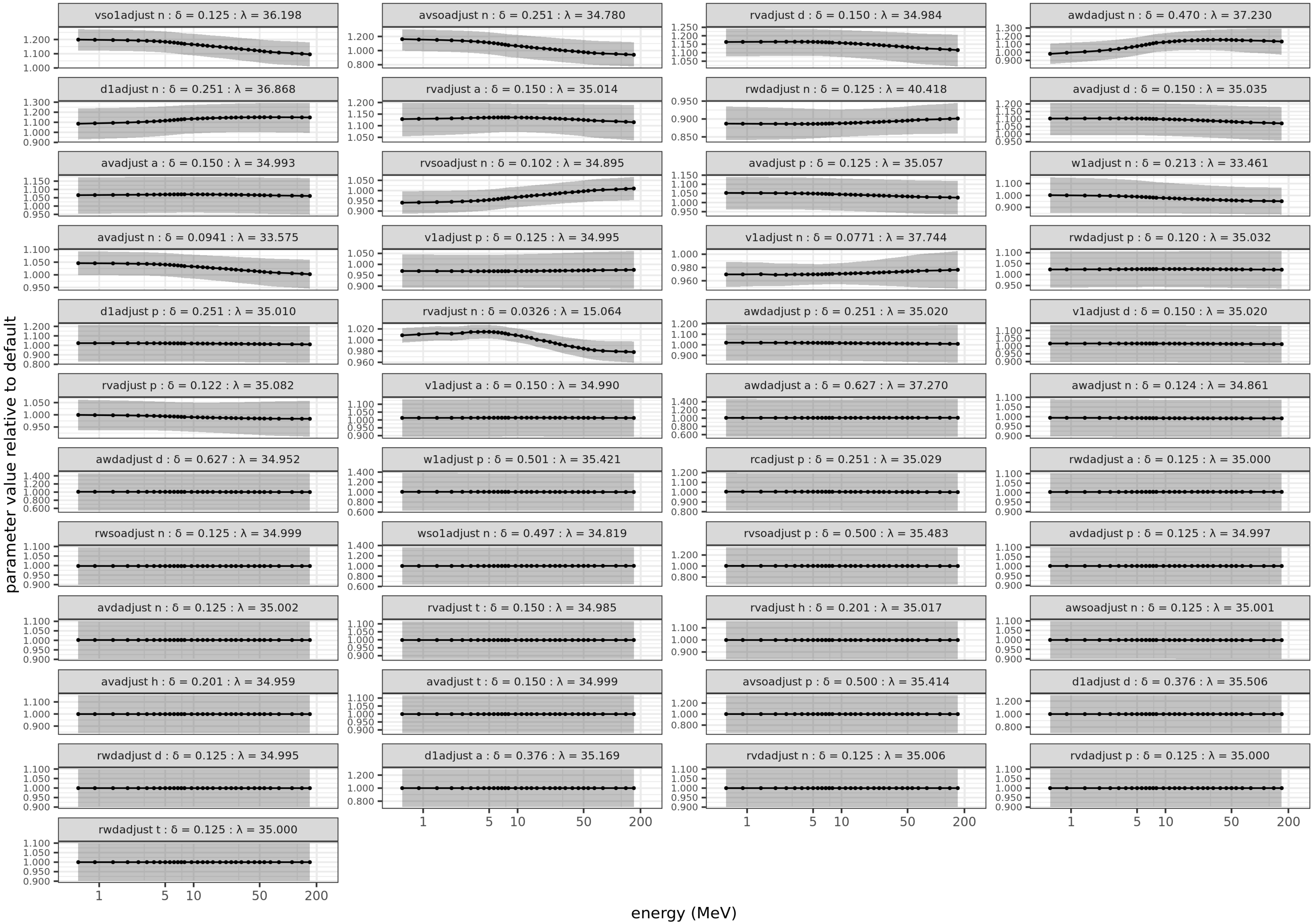
Total experimental data: 1727 across 9 reaction channels

Energy range: 1-150 MeV

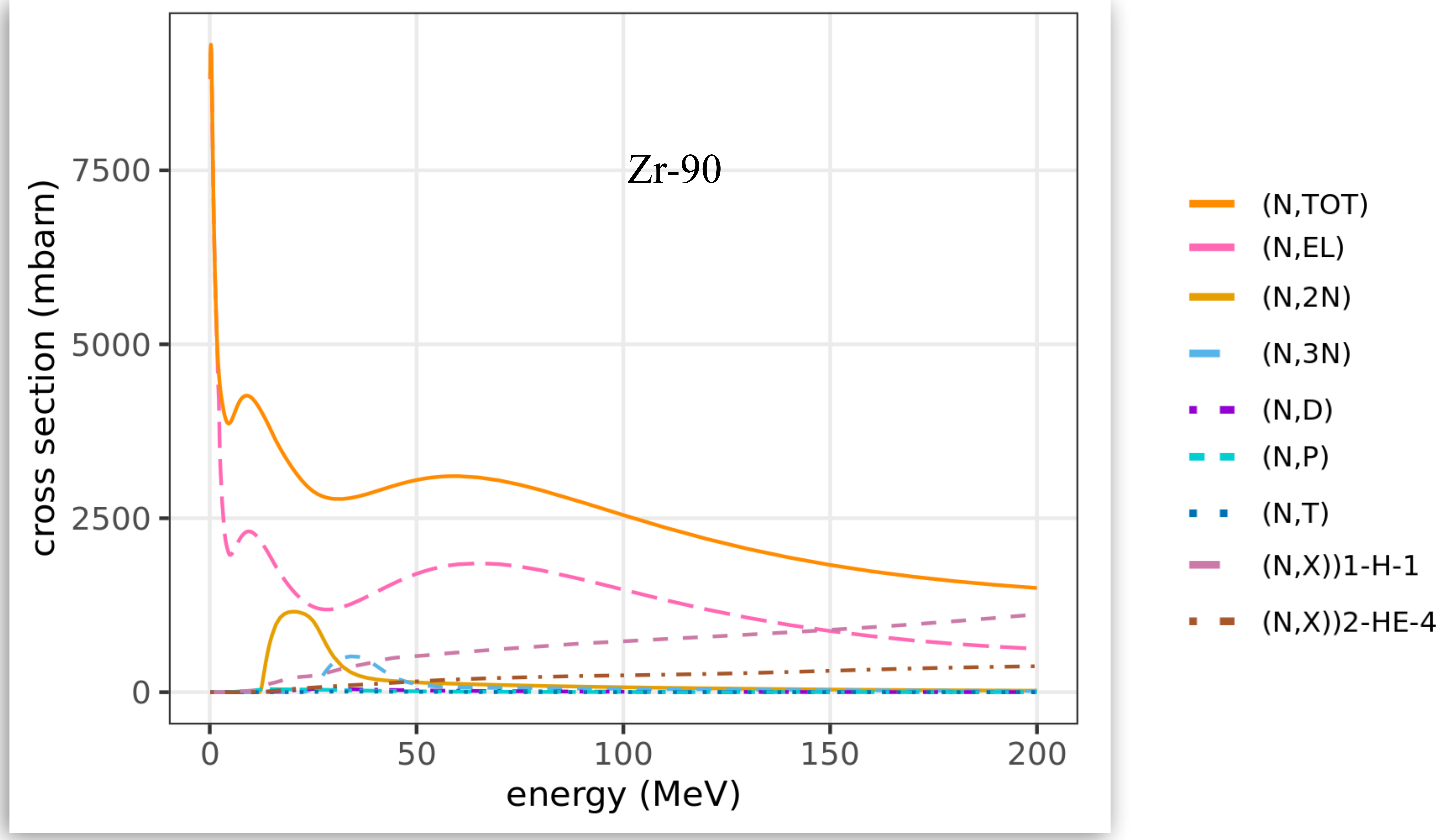
Free TALYS parameters: 3834, including energy dependence

Selected for LM fit: 1614 / 3834

GP treatment on energy dependent model parameters (preliminary)

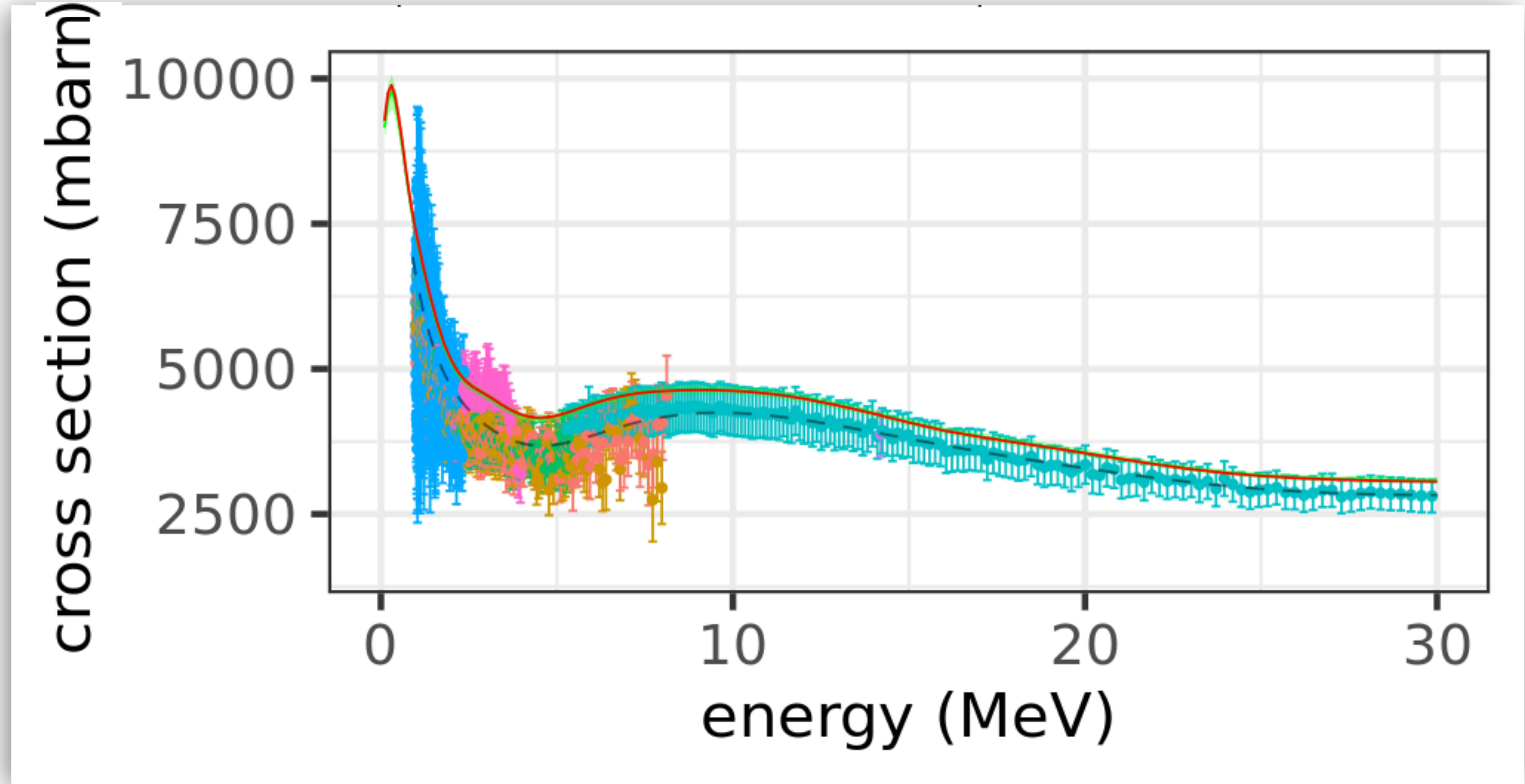


Posterior cross-section for neutron-induced channels (preliminary)



The Anomaly

TALYS looks better : but the numbers say otherwise



n = 1535 data points

	χ^2	χ^2/n
TALYS default	**944 119**	**615**
Posterior fit	**209 144**	**136**

TALYS is visually better — yet $\chi^2/n = 615$

Rule-based addition of uncertainties in NEPU

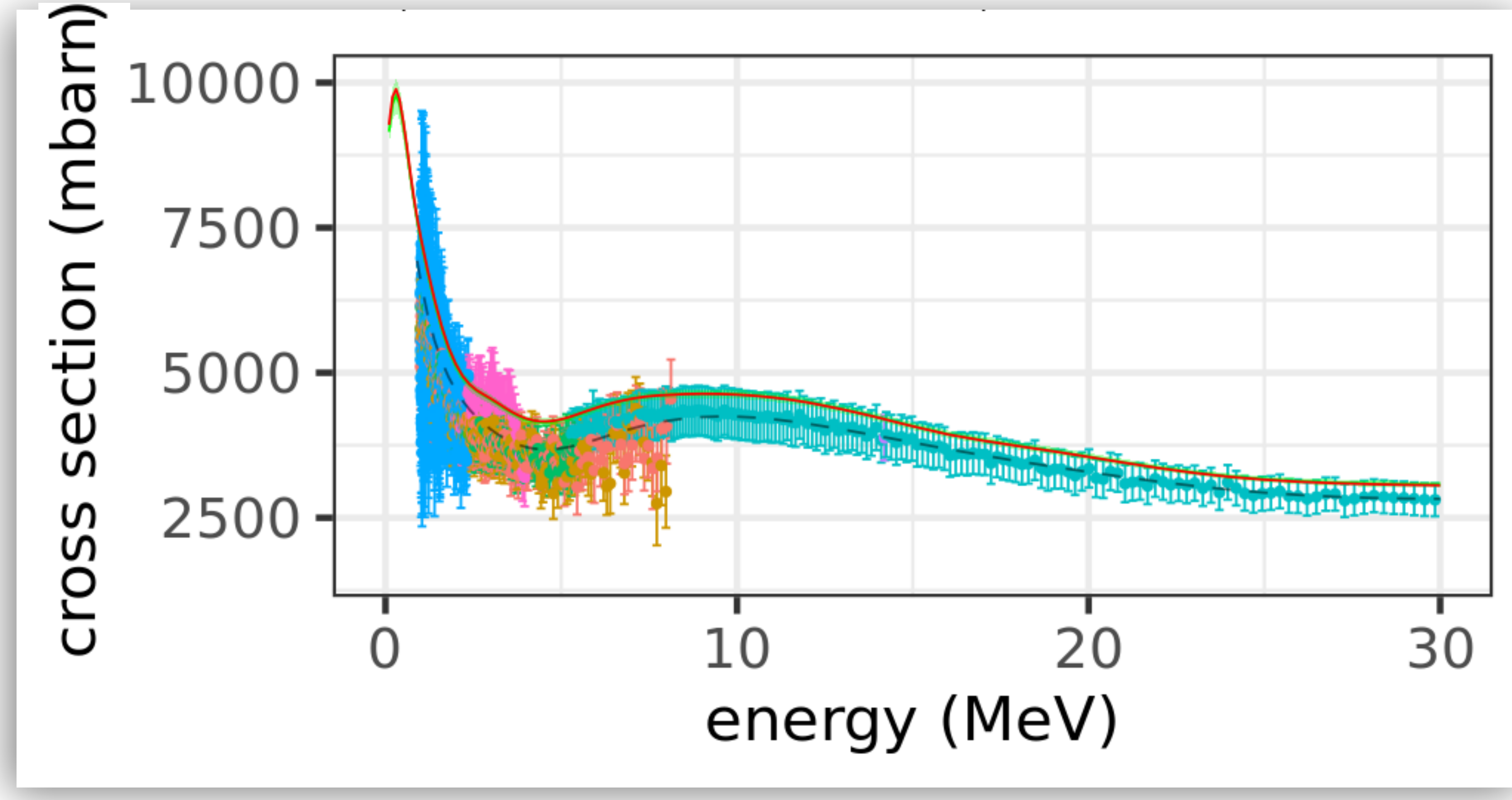
NEPU on what EXFOR reports

1. **Statistical unc. reported**
   → use as random (diagonal)
   → use reported sys, or 10% penalty

2. **Total unc. + systematic components reported**
   → random = sqrt[(σ²_tot − σ²_sys)]
   → use reported sys

3. **Only total unc., no breakdown reported**
   → random = total unc. (as given)
   → add 10% systamtic unc

4. **No uncertainty reported**
   → random = 10%
   → sys = 10%



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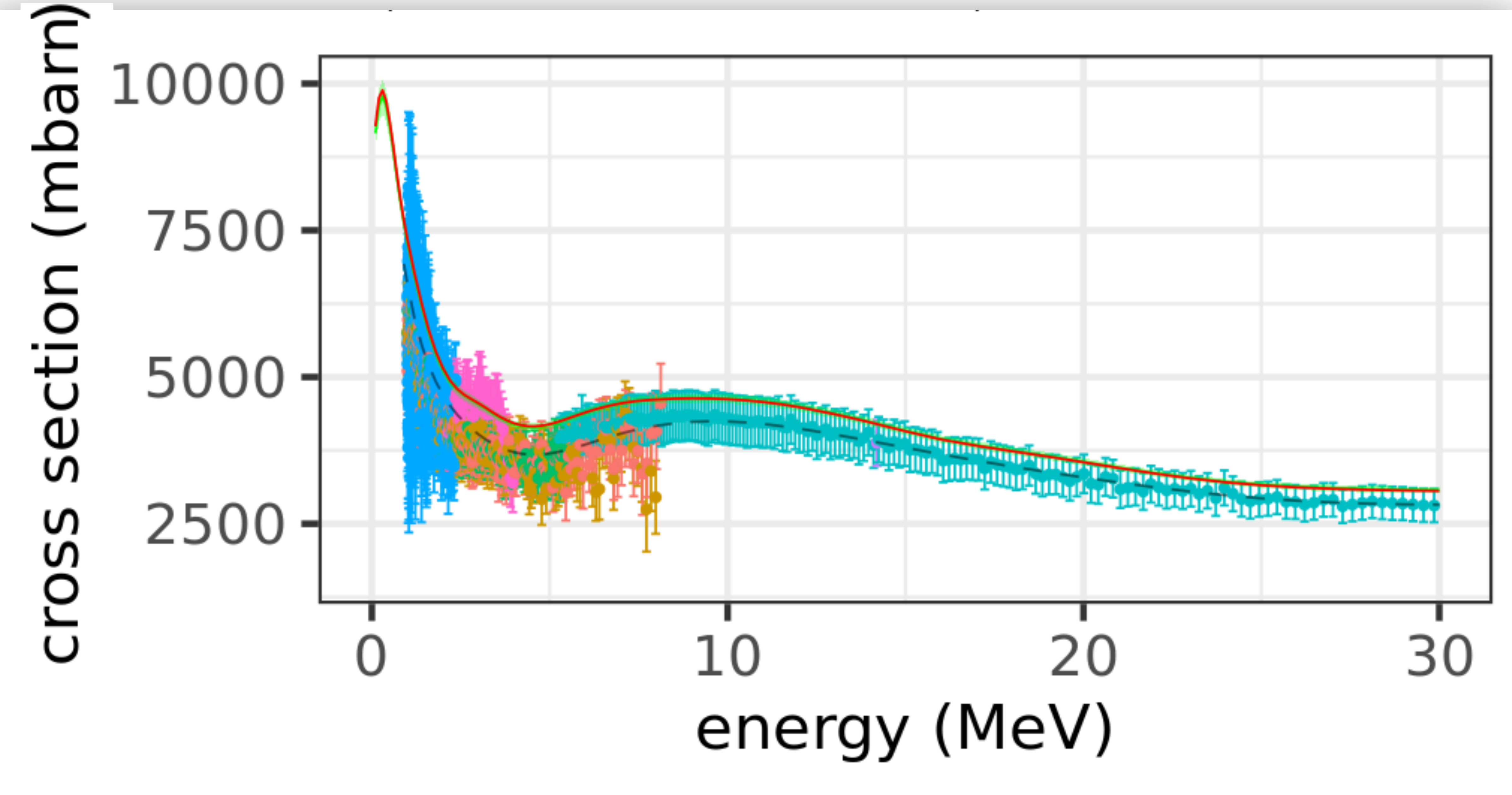
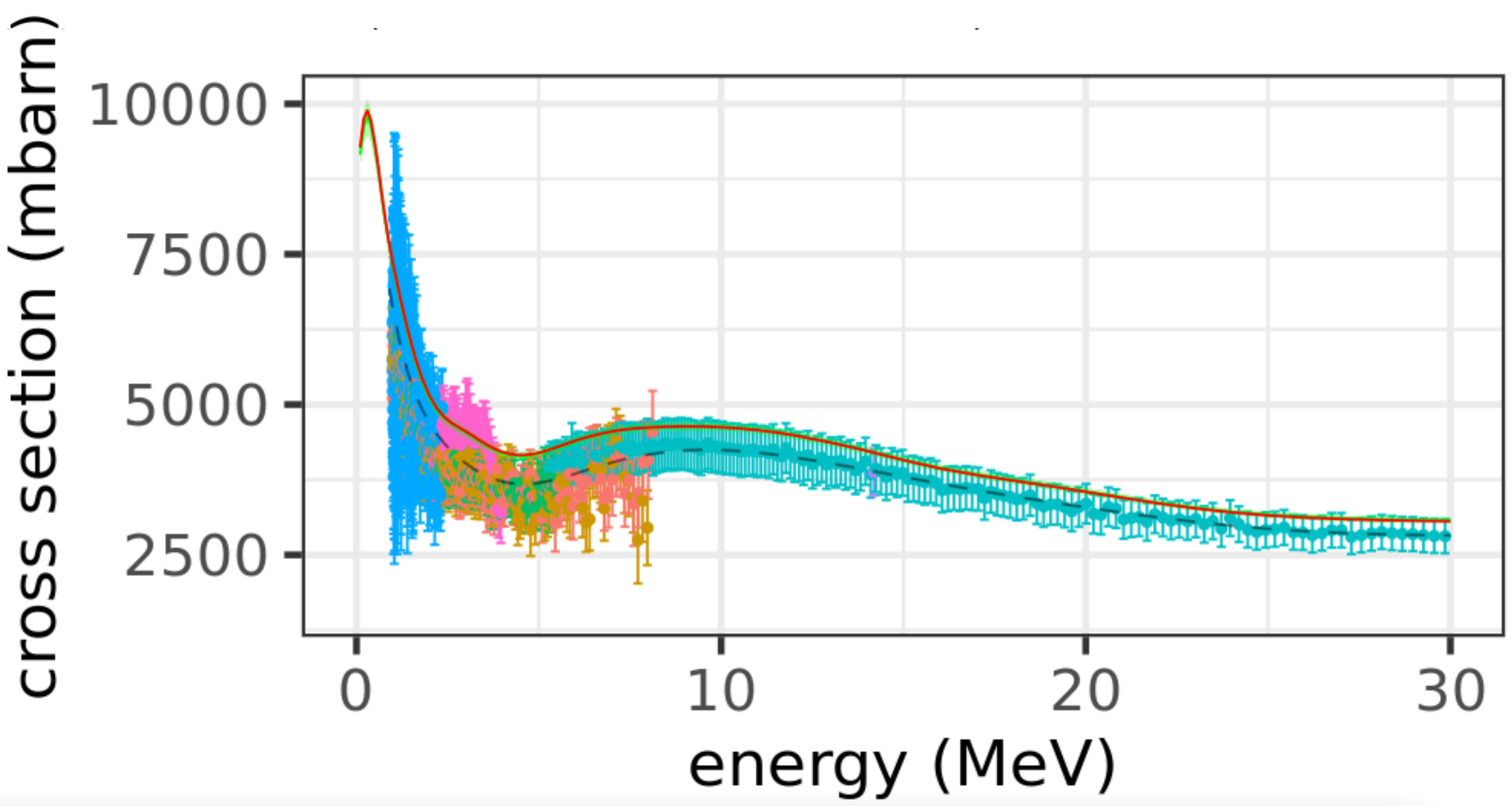


The Covariance Model

What does GLS actually minimise?

$$\chi^2 = (y - f)^T C^{-1} (y - f)$$

where $C_{ij} = \sigma^2_{i,\text{rand}}\delta_{ij} + \sigma_{i,\text{sys}}\sigma_{j,\text{sys}}$



Random uncertainty

- Diagonal: $C_{ij} = \sigma_i^2\delta_{ij}$
- Each data point residual penalised independently
- GLS is sensitive to individual point offsets
- A curve displaced upward pays a cost at every point

Systematic (fully correlated)

- Off-diagonal: $C_{ij} = \sigma_{i,\text{sys}}\sigma_{j,\text{sys}}$
- all points move together mode
- A coherent level shift costs almost nothing in χ^2
- GLS minimizes shape mismatch - not the overall offset

When C is dominated by large correlated systematics, GLS optimises shape. A systematic level bias is invisible to χ^2.

Reconstructing the uncertainty

Before

Uncertainties almost entirely assigned as fully correlated systematic (to penalise inconsistent experiments)→ level offset → high posterior bias

After

Partial reallocation to random component → individual point residuals now penalized

Random Unc: Maximum of reported or 1% of data
Systematic Unc: Maximum of reported or 5% of data

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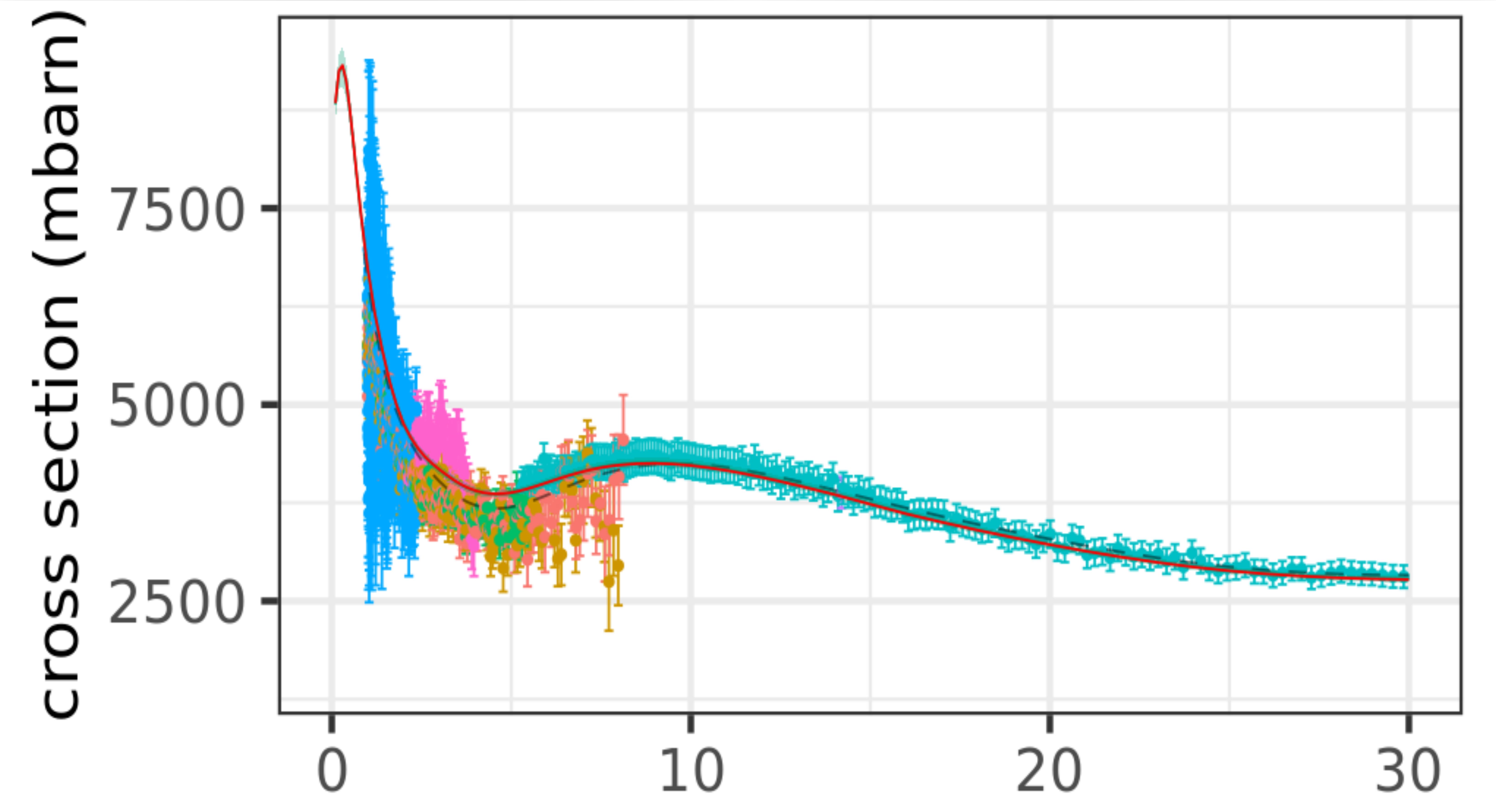
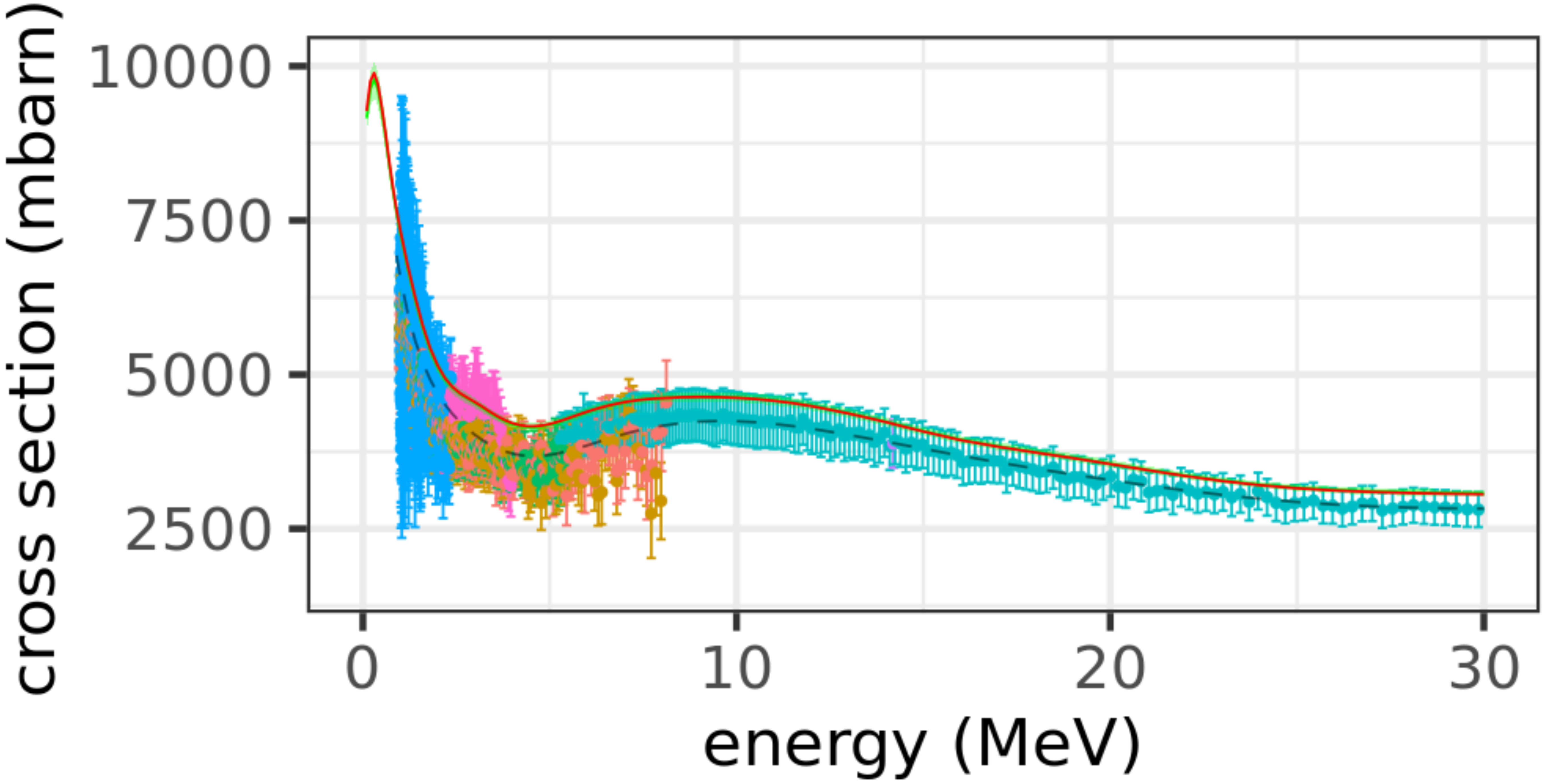
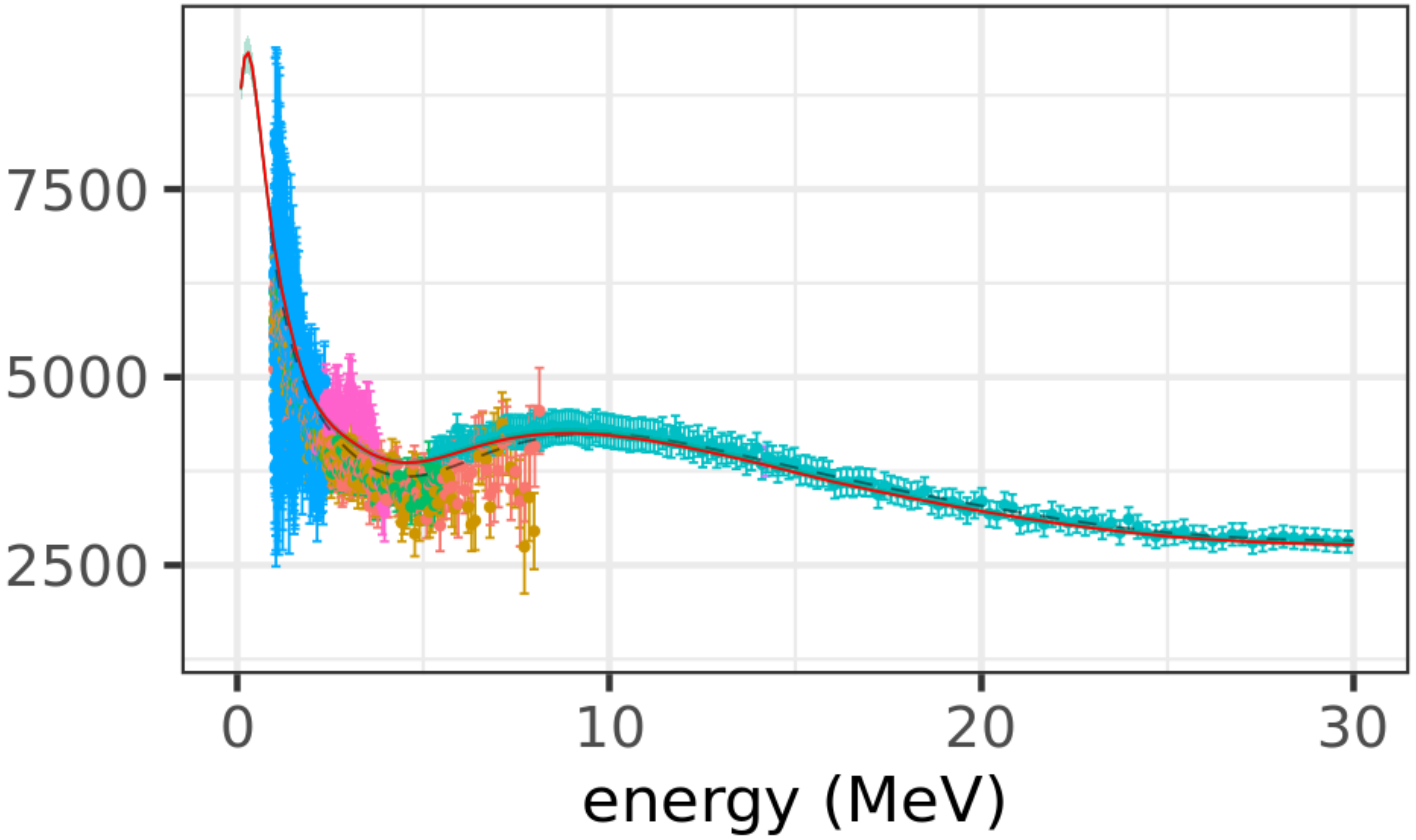
→ **Better fit**



Before vs. After





Large χ^2/n | large correlated unc.

$\chi^2/n \approx 1.01$

Uncertainty quantification of $\sigma_{(N,*)}$ for Zr-90 (preliminary result)

Peelle's Pertinent Puzzle

Relative uncertainties should be converted to absolute before entering the covariance matrix.

The PPP bias (without correction)

$$\sigma_{\mathrm{abs,i}} = p_i \times y_i$$

If relative uncertainty p_i is quoted on the measured value y_i, and y_i scatters above the true value, σ is inflated — the uncertainty correlates with the fluctuation.
GLS gives them less weight → the result is biased downward

The standard fix

$$\sigma_{\mathrm{abs,i}} = p_i \times f(E_i)$$

Replace measured y with a smooth reference f (e.g. TALYS default).
Breaks the correlation.

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When PPP renormalization goes wrong

Example

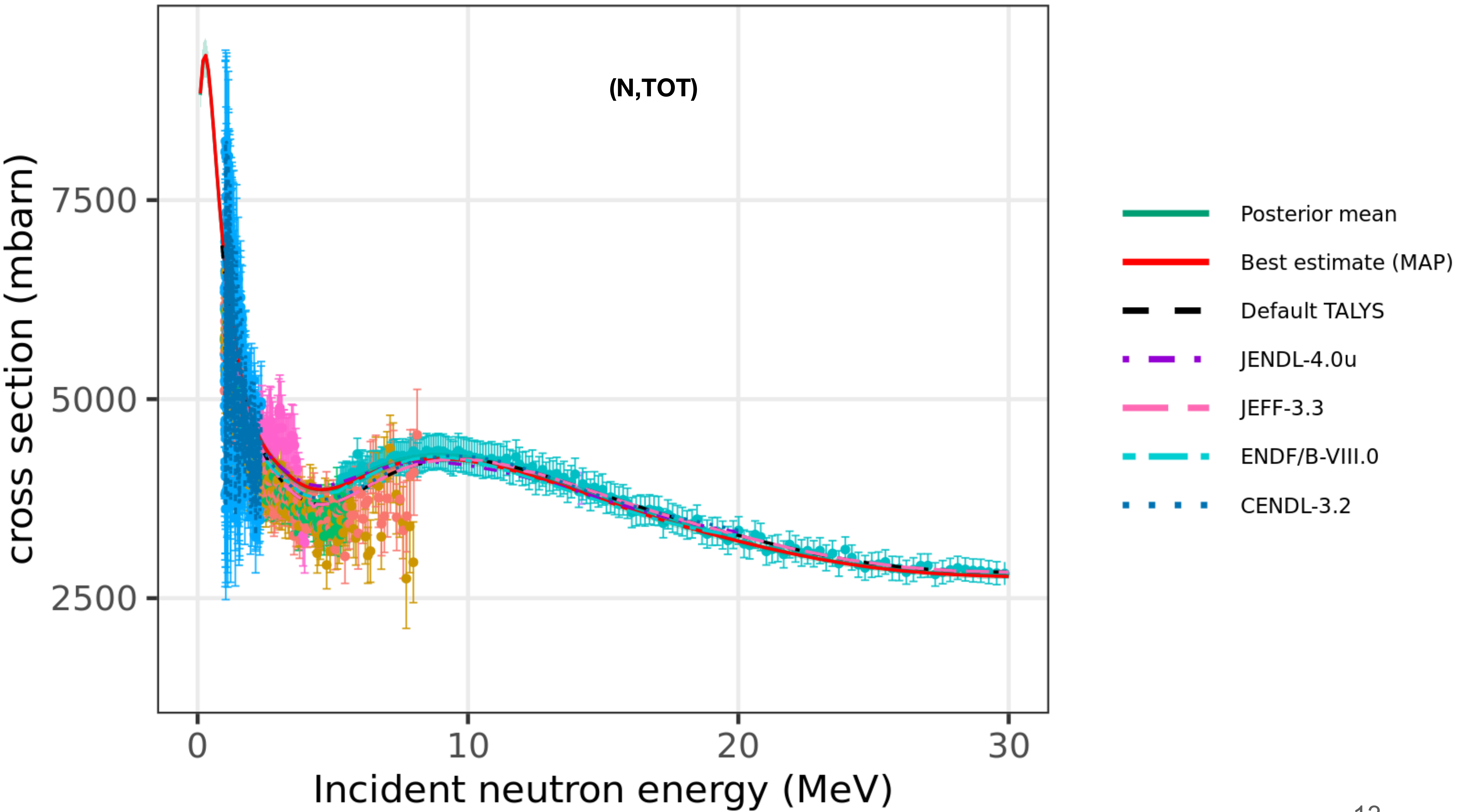
Experiment: y = 5000 mb, p = 10% → σ = 500 mb
TALYS reference: f = 1000 mb
→ after PPP fix: σ = 100 mb
Uncertainty reduced by factor 5.

In resonance regions and in outliers

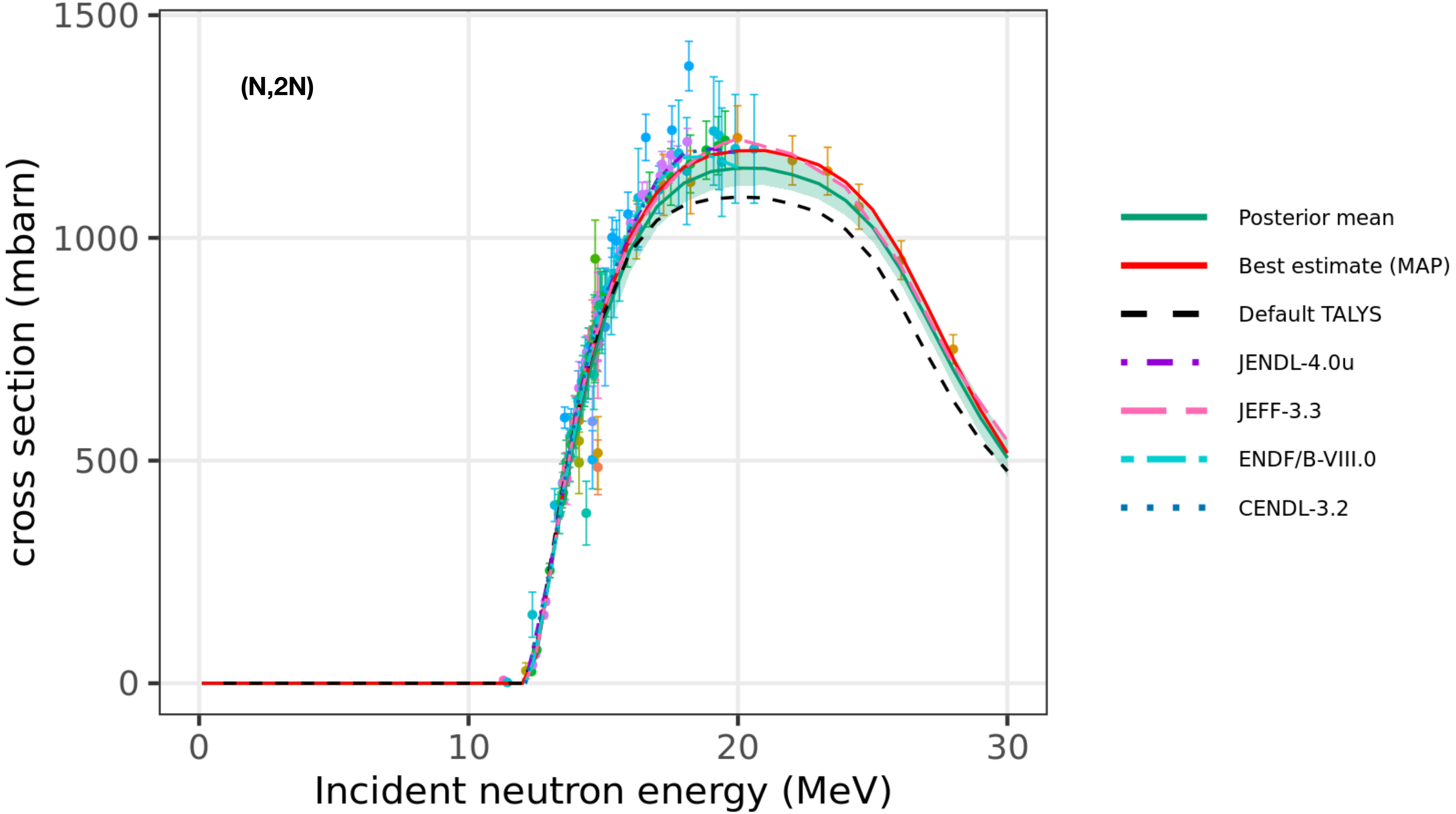
- Outlier uncertainty is actually a representation of disbelief.
- The smooth reference f lacks the resonance structure that the data sees. y>>f, the uncertainty gets underestimated.

PPP renormalization is valid only when the model is a good estimate of the true value. In resonance regions, and for outliers, it may create a problem.

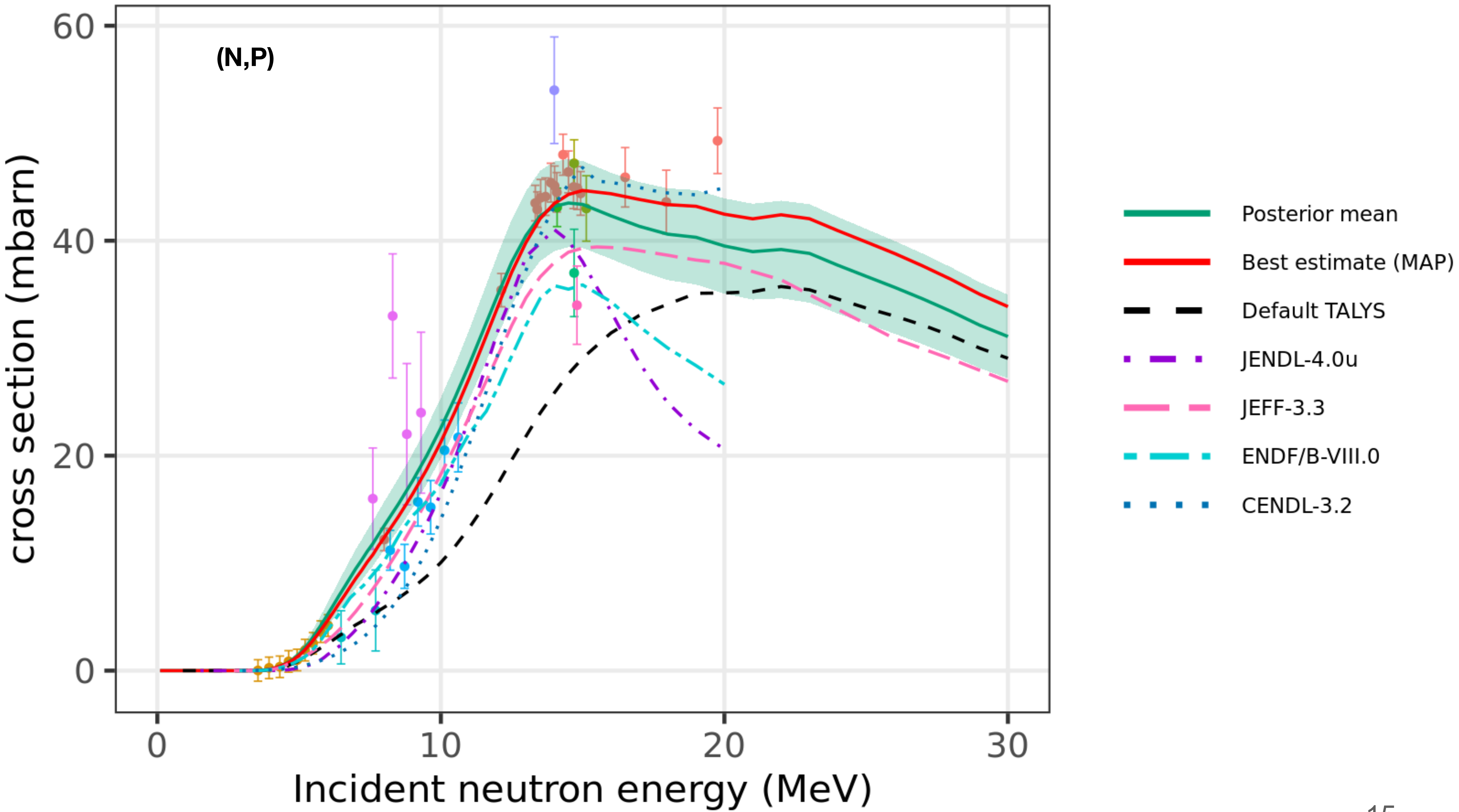
Uncertainty quantification of $\sigma_{(N,TOT)}$ for Zr-90



Uncertainty quantification of $\sigma_{(N,2N)}$ for Zr-90



Uncertainty quantification of $\sigma_{(N,P)}$ for Zr-90



Summary

- Development of Nuclear data Evaluation pipeline of Uppsala (NEPU)

  ✓ Based around the TALYS

  ✓ Treatment of inconsistent experiment

  ✓ Model defects treatment with GP

  ✓ Generalizability and automatization

We present preliminary investigation of uncertainty in Zr-90.

- **The χ^2 paradox**

  When the covariance matrix is dominated by fully correlated systematics, GLS optimizes shape over magnitude. A visually biased fit can be statistically correct given the covariance model assumed.

- **PPP renormalization can introduce new problems when the model does not describe the data.**

NEPU

https://github.com/UU-nuclear

THANK YOU.

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