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Development of an Automated Uncertainty Quantification Pipeline in Nuclear Data Evaluation

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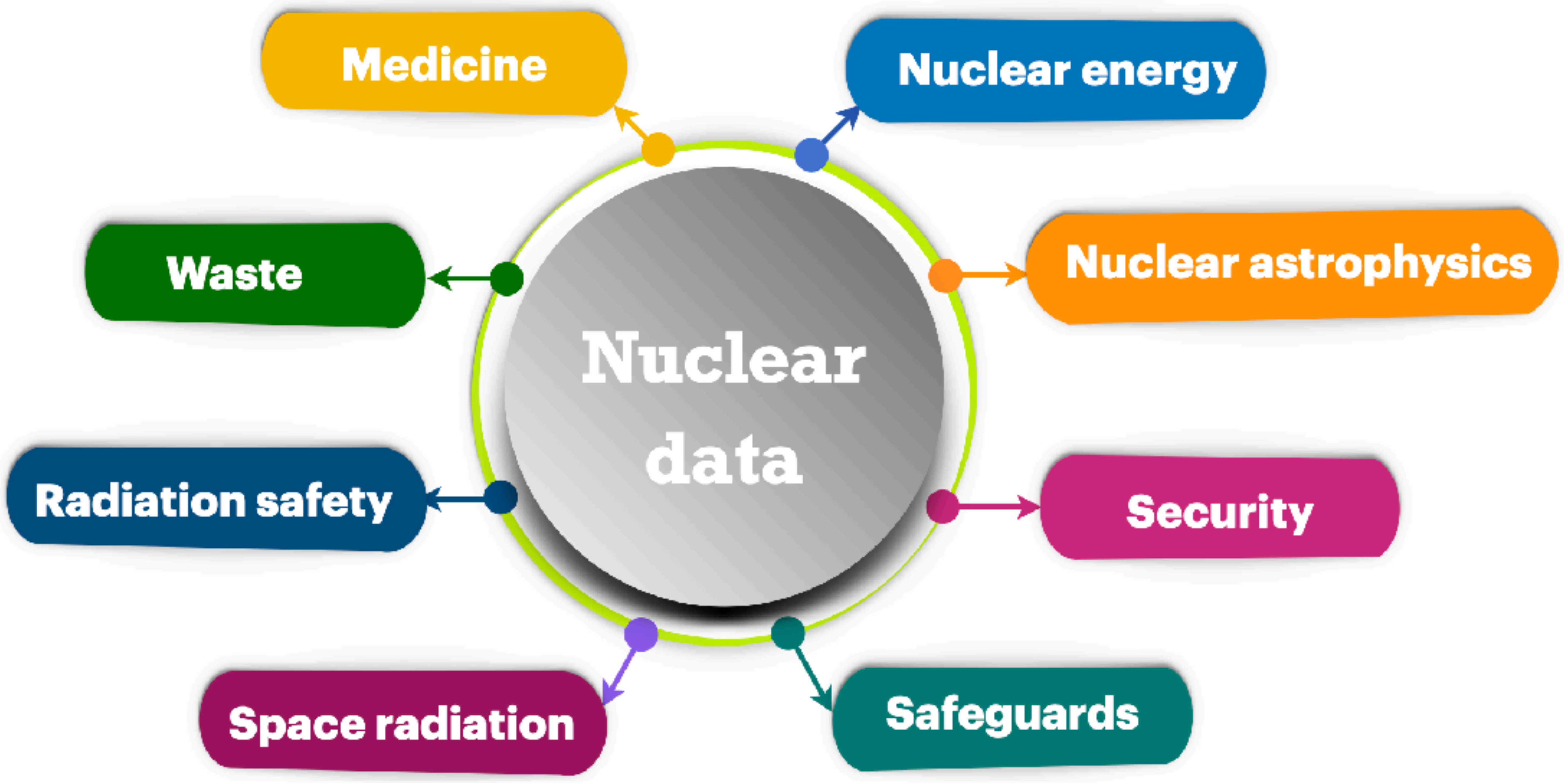
Swedish Energy Agency

Nuclear Data Evaluation



Nuclear data for Generation IV reactors

Challenges

Inadequate experimental data and nuclear theories

Nuclear data evaluation

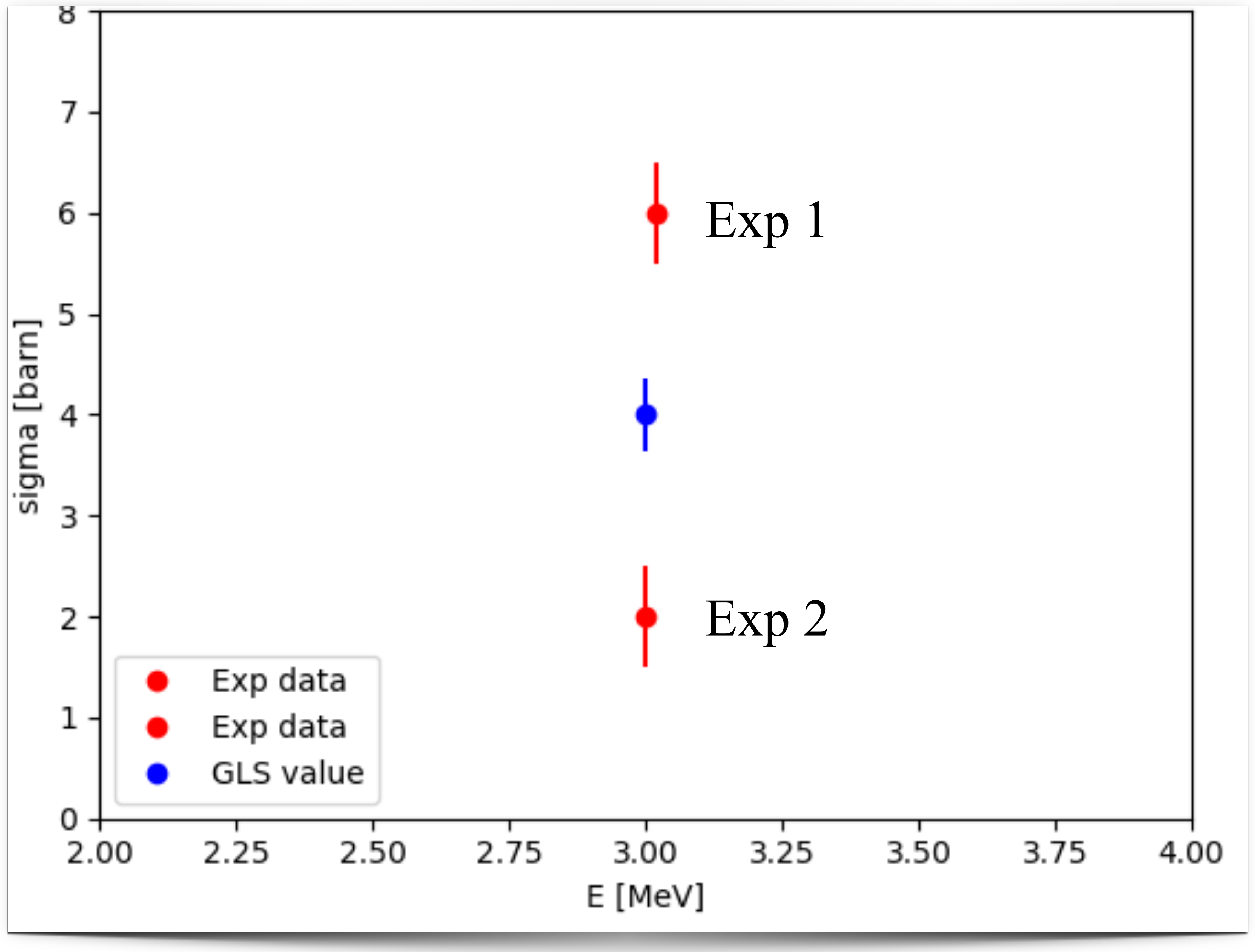
- Data from different experiments
- Use nuclear models
- Quantify uncetainties
- Estimate cross-section and associated uncertainties

Why do we get uncertainties wrong?

Uncertainties in cross-section

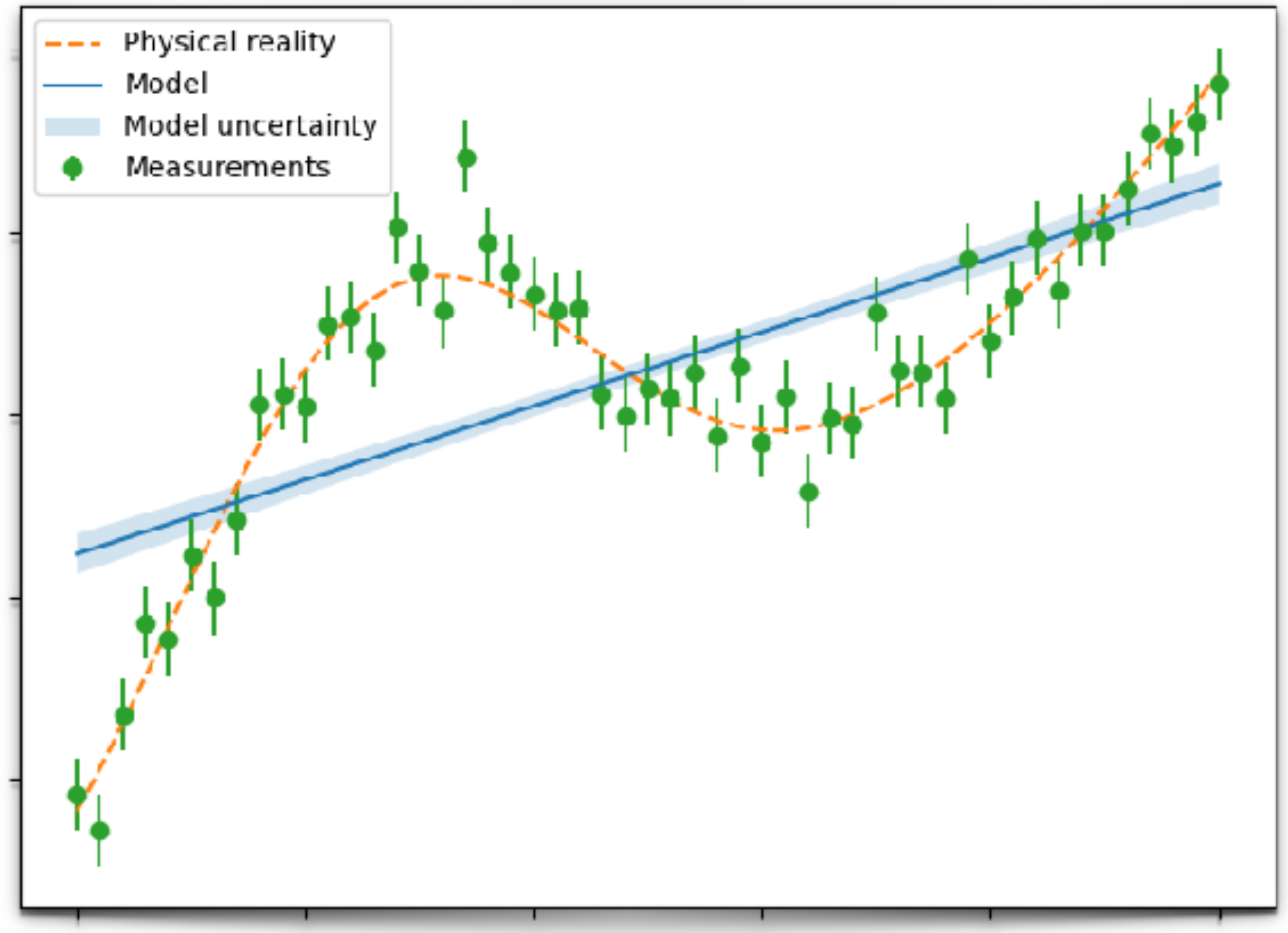
Inconsistent experiments

- Different measurements disagree beyond quoted uncertainties
- Underestimated systematic errors
- Outlier experiments can bias the evaluation



Imperfect models

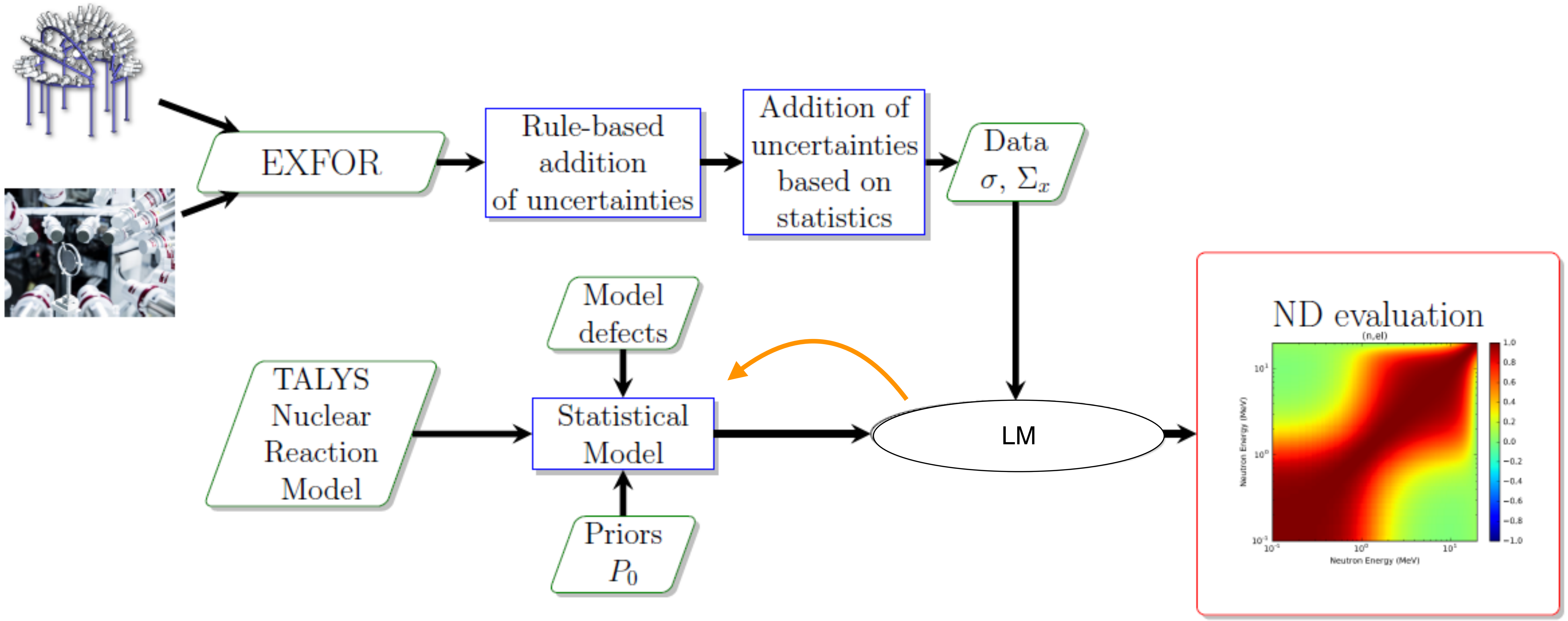
- Nuclear models are approximations
- Residual model discrepancies remain even after parameter optimization
- Neglecting model defects causes underestimated uncertainties



NEPU: Nuclear Data Evaluation Pipeline of Uppsala

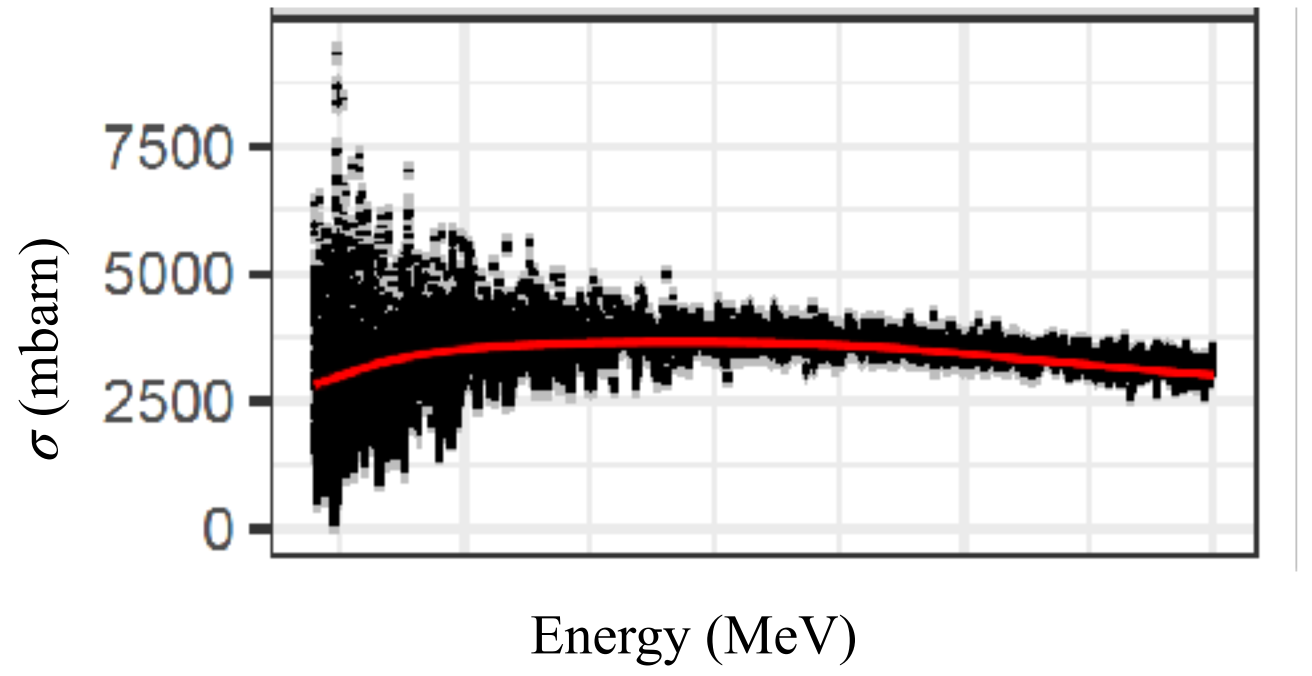
A pipeline for nuclear data evaluation that implements (and further develops) methodology to treat model defects and inconsistent experimental data that has originated in research activities at UU.
Goal: Automatization, Reproducible.

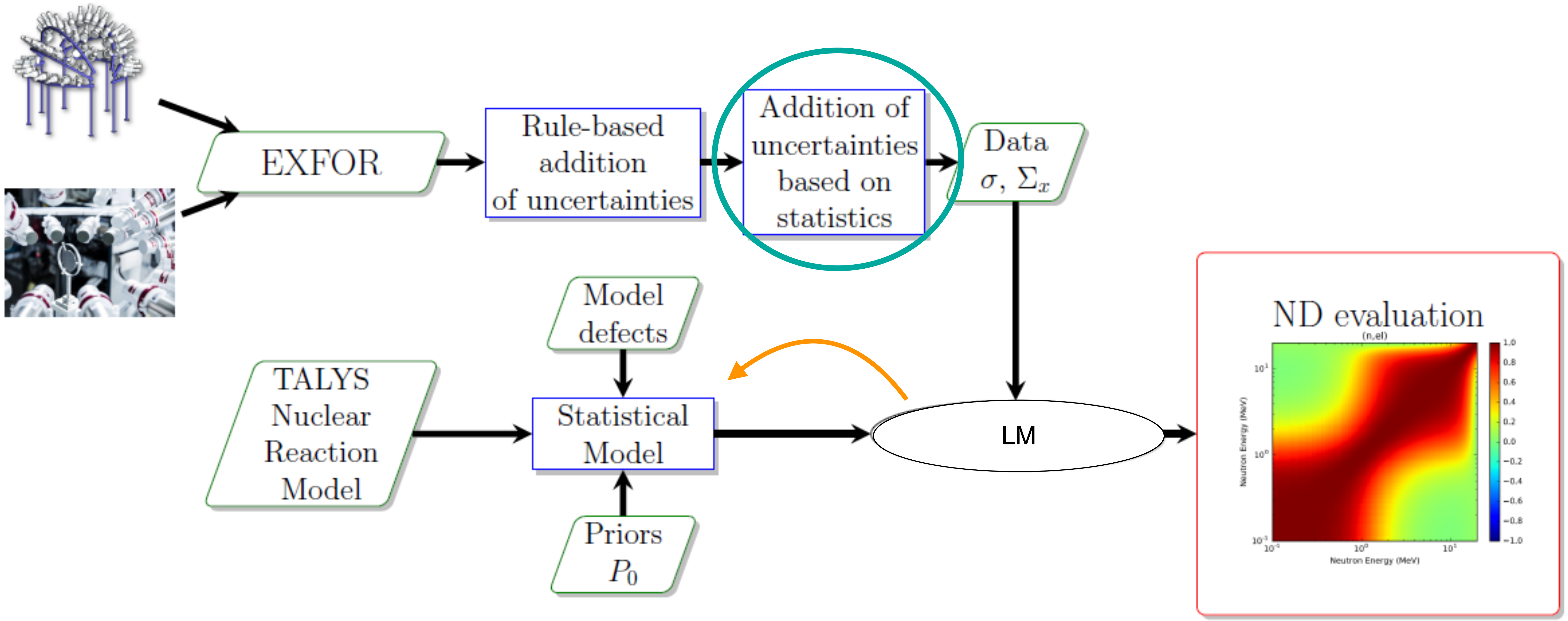
G. Schnabel, H. Sjöstrand, J. Hansson, D. Rochman, A. Koning, R. Capote Nucl. Data Sheets 173, 239 (2021)
A.Göök, E. Andersson-Sundén, J. Hansson, and H. Sjöstrand, EPJ Web of Conf. 294, 04005 (2024)

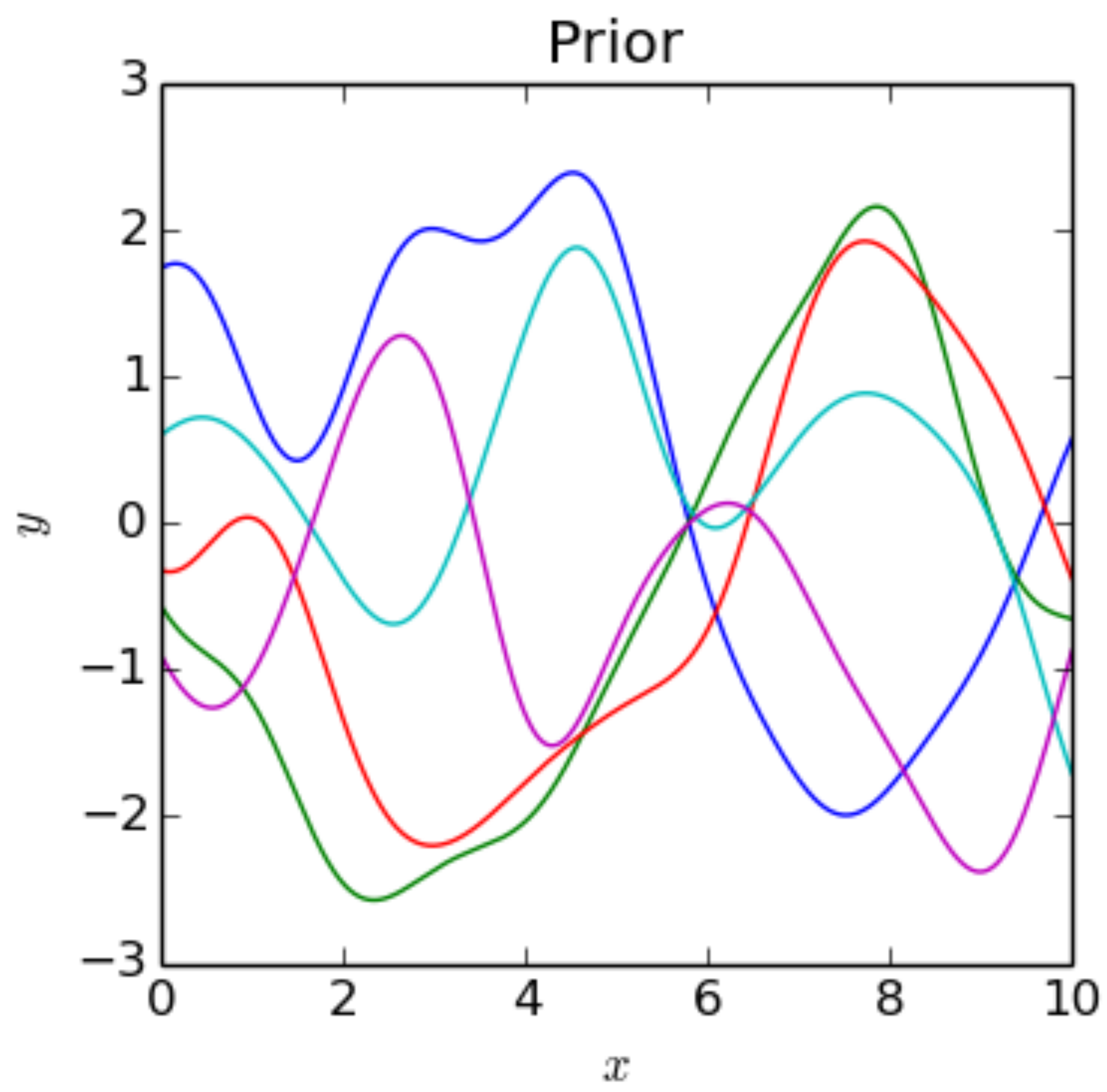


Treatment on random uncertainties

- TALYS produces a smooth curve, missing resonance structures in the data
- The mismatch creates residuals larger than the reported uncertainties
- NEPU handles it with a heteroscedastic GP that learns the energy-dependent noise directly from the data
- It is treated as an additional random uncertainty in the regression







A Gaussian process is

- A probability distribution over functions.
- Defined by a mean function (prior expectation) and a covariance function (kernel) to describe correlation of function at different energies

Squared exponential kernel

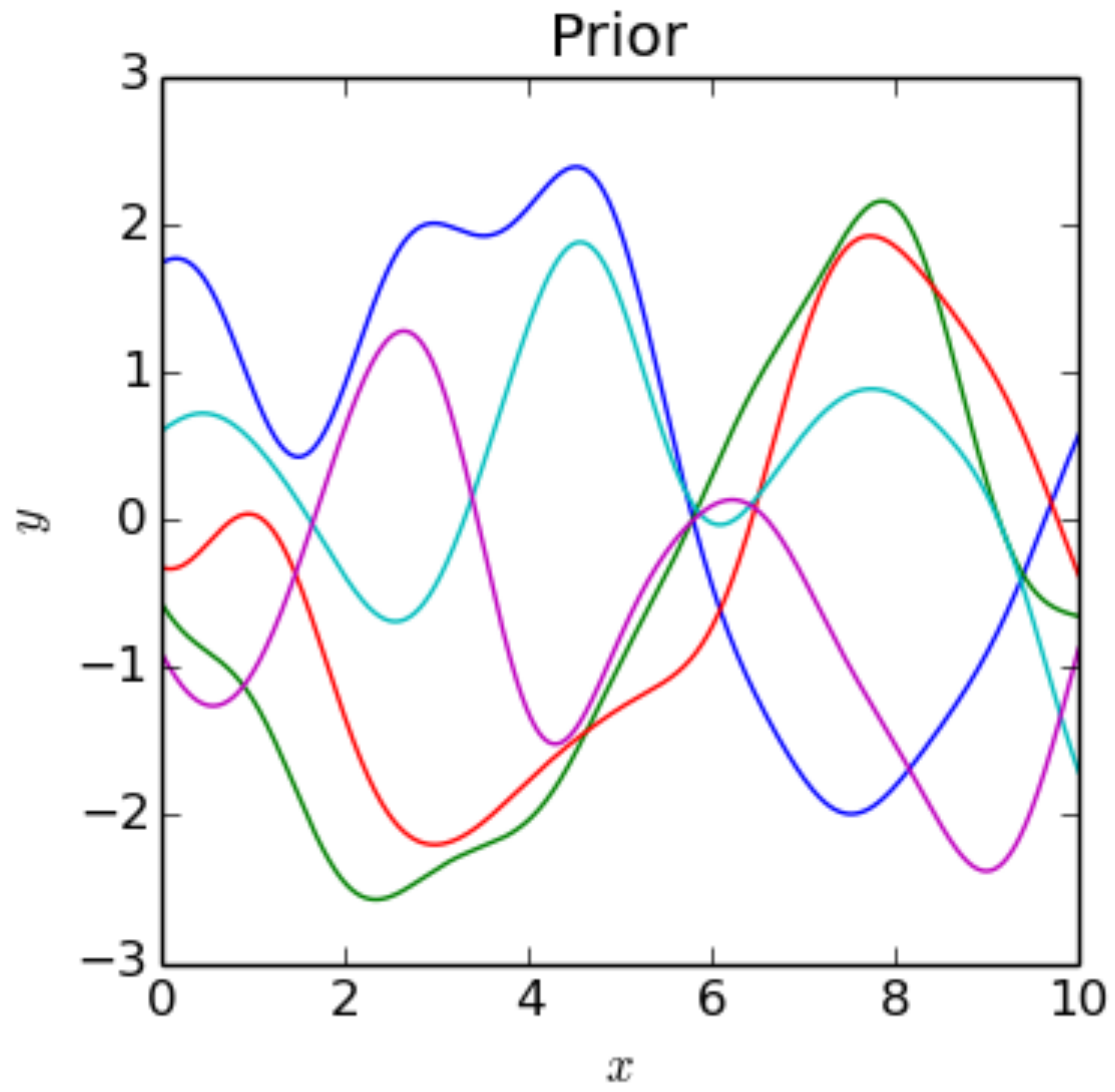
$$k(E_i, E_j) = \delta^2 \exp\left(-\frac{E_i - E_j}{\lambda}\right)^2 + \tau^2 A_{ij}$$

Length scale, λ : determines how smooth the solutions are.

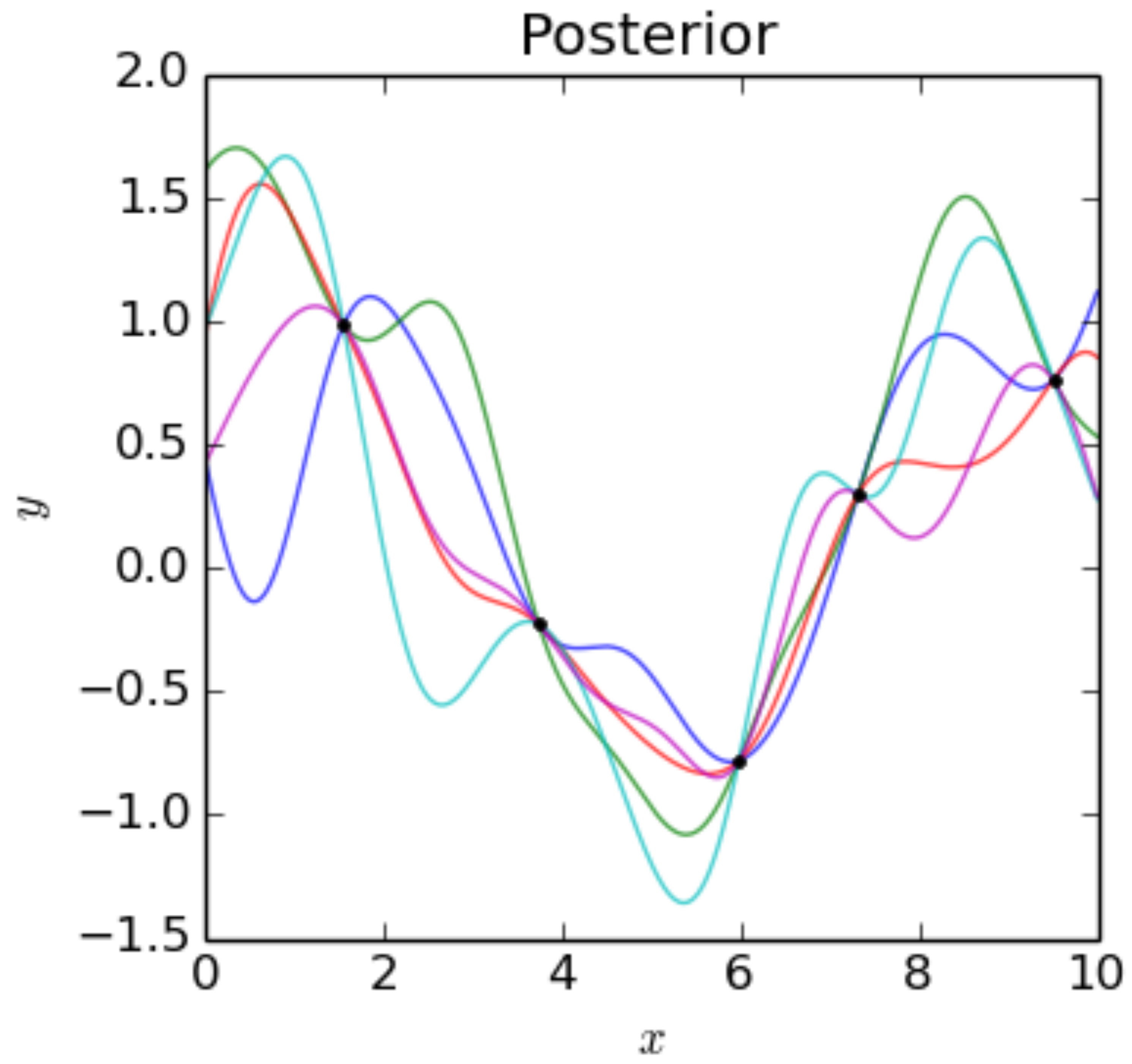
Amplitude, δ: determines how big variations the solutions can have.

Nugget parameter, τ: models measurement noise.

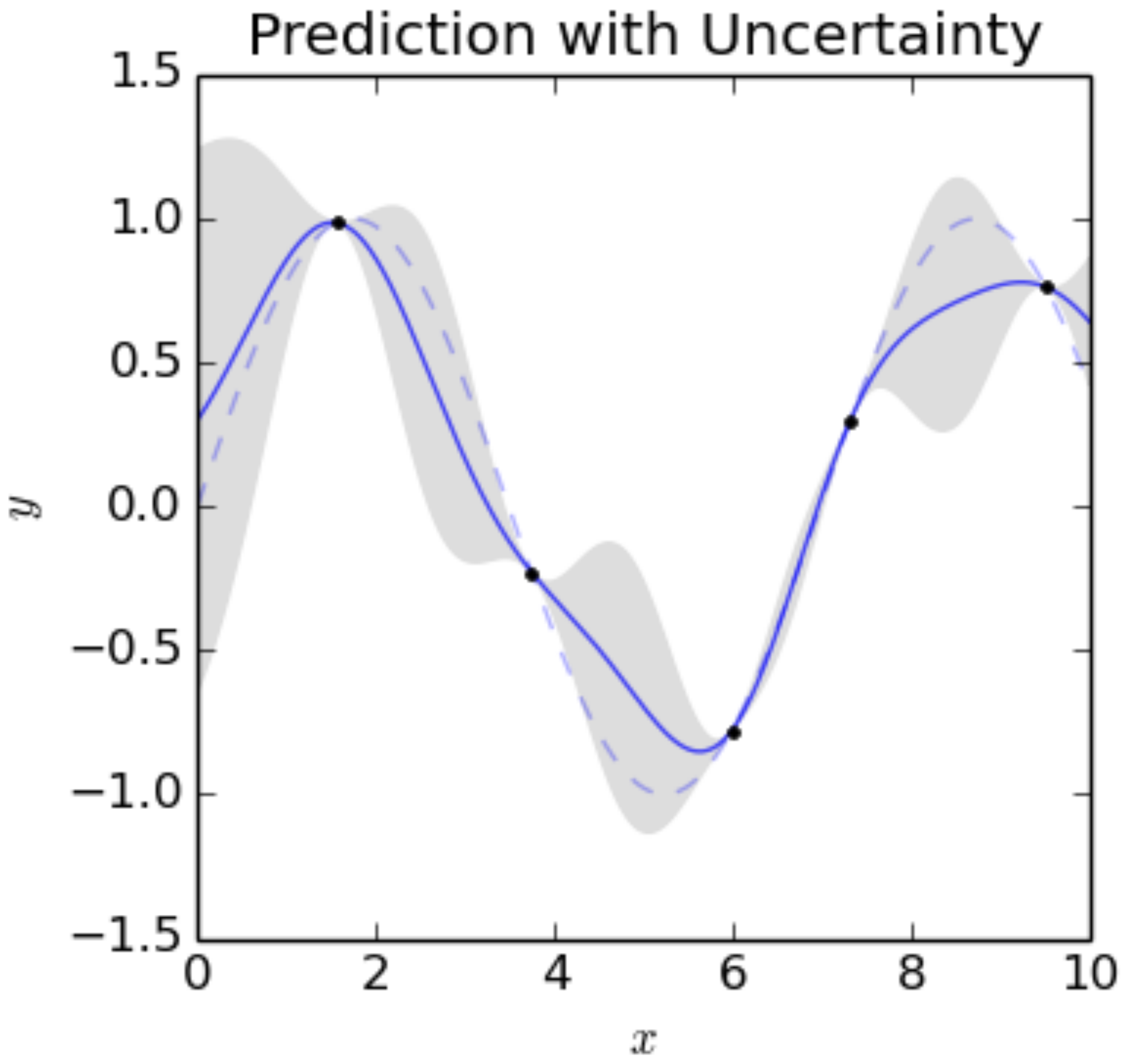
Figure credit: https://commons.wikimedia.org/wiki/File:Gaussian_Process_Regression.png#/



Draws from the prior distribution show smooth random functions consistent with the kernel

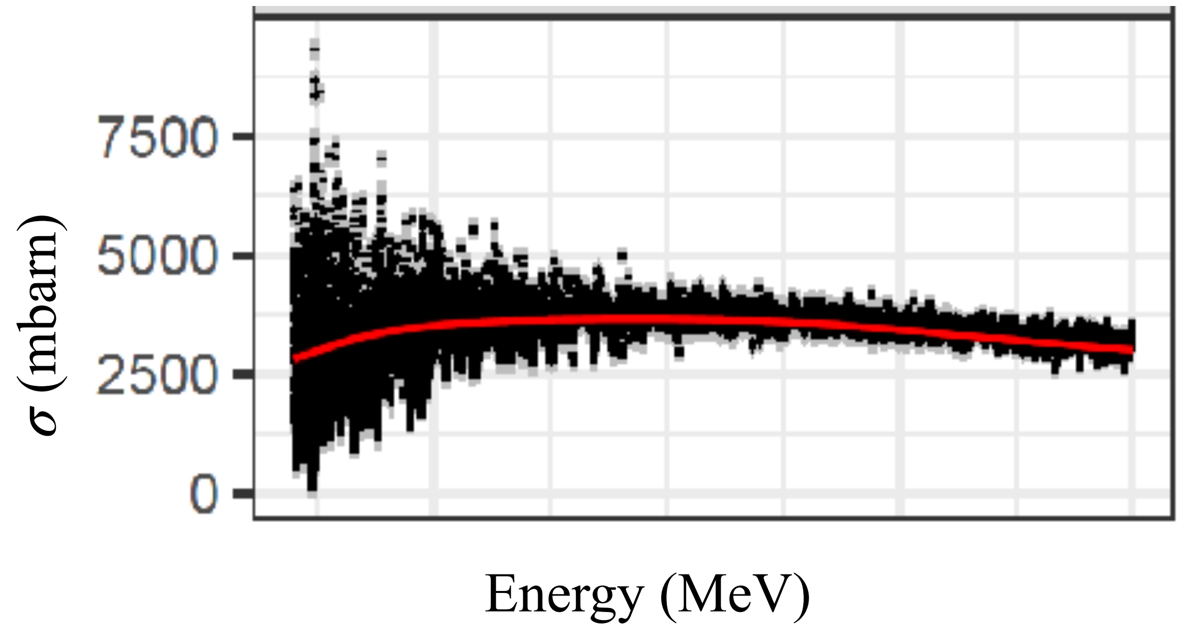


After conditioning on observations, posterior samples are pulled toward the data points



The posterior mean gives the best estimate of the function at every energy. The shaded region shows uncertainty.

Figure credit: https://commons.wikimedia.org/wiki/File:Gaussian_Process_Regression.png#/

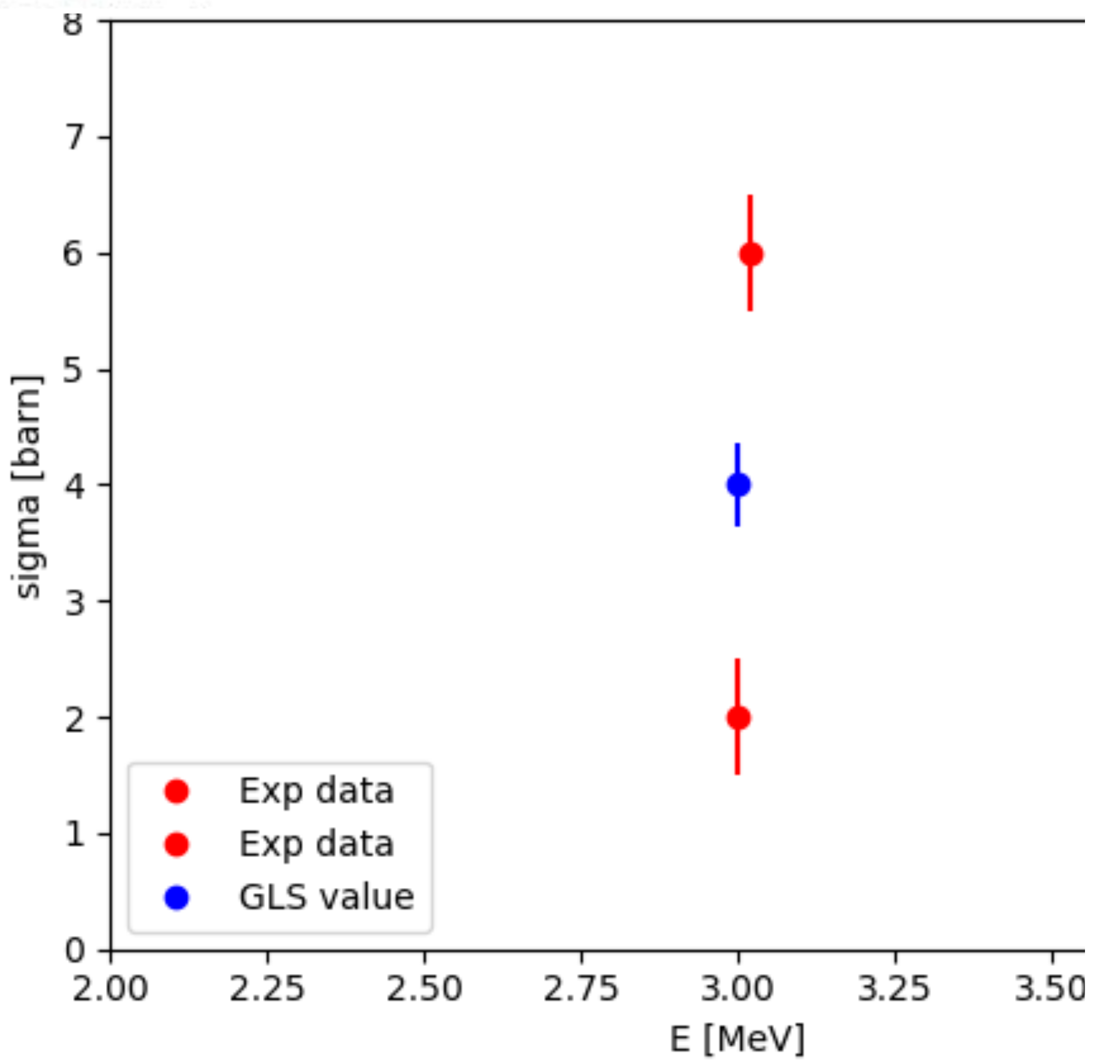


$$k(E_i, E_j) = \delta^2 \exp\left(-\frac{E_i - E_j}{\lambda}\right)^2 + \tau^2 A_{ij}$$

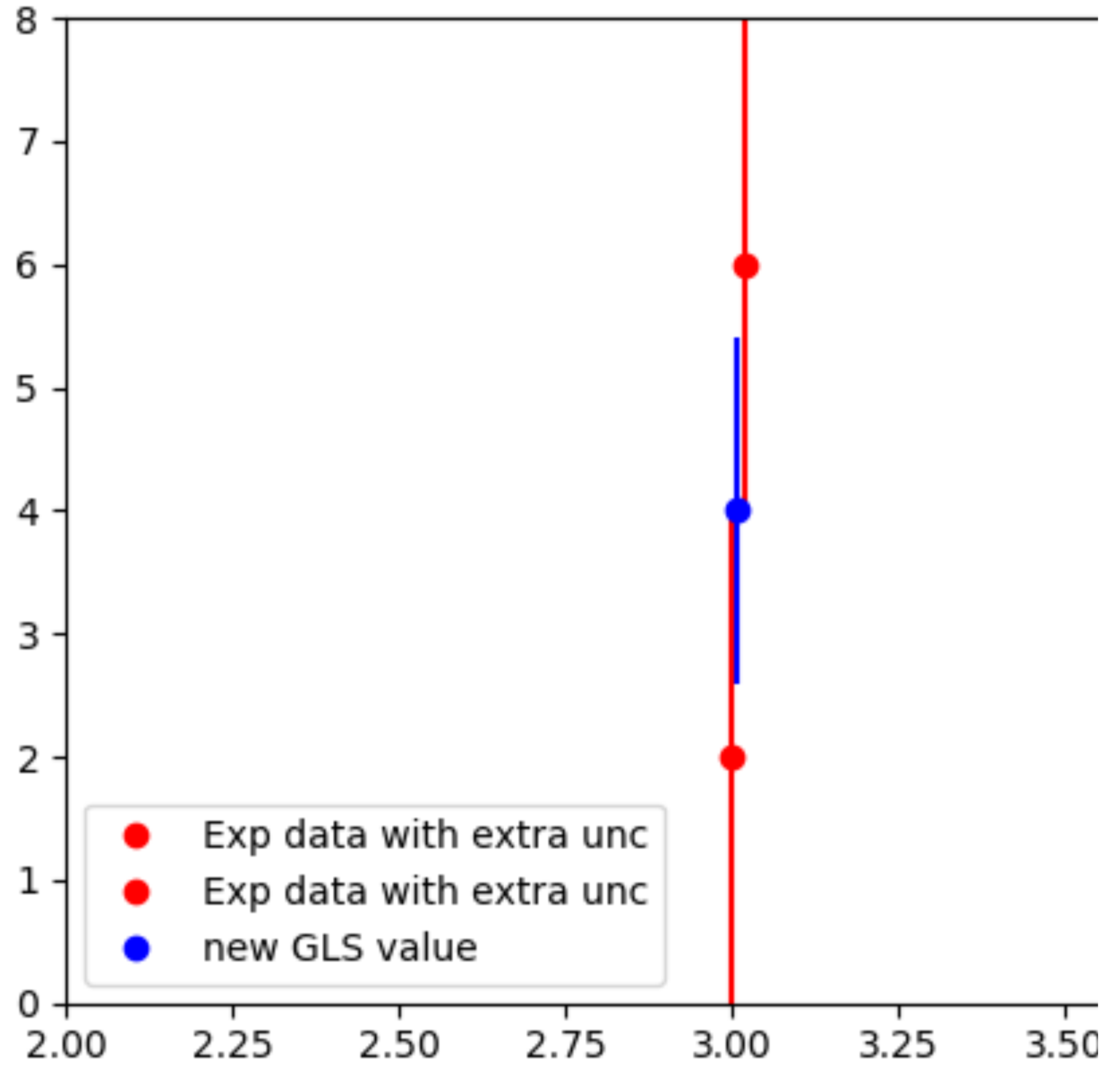
Heteroscedastic GP:

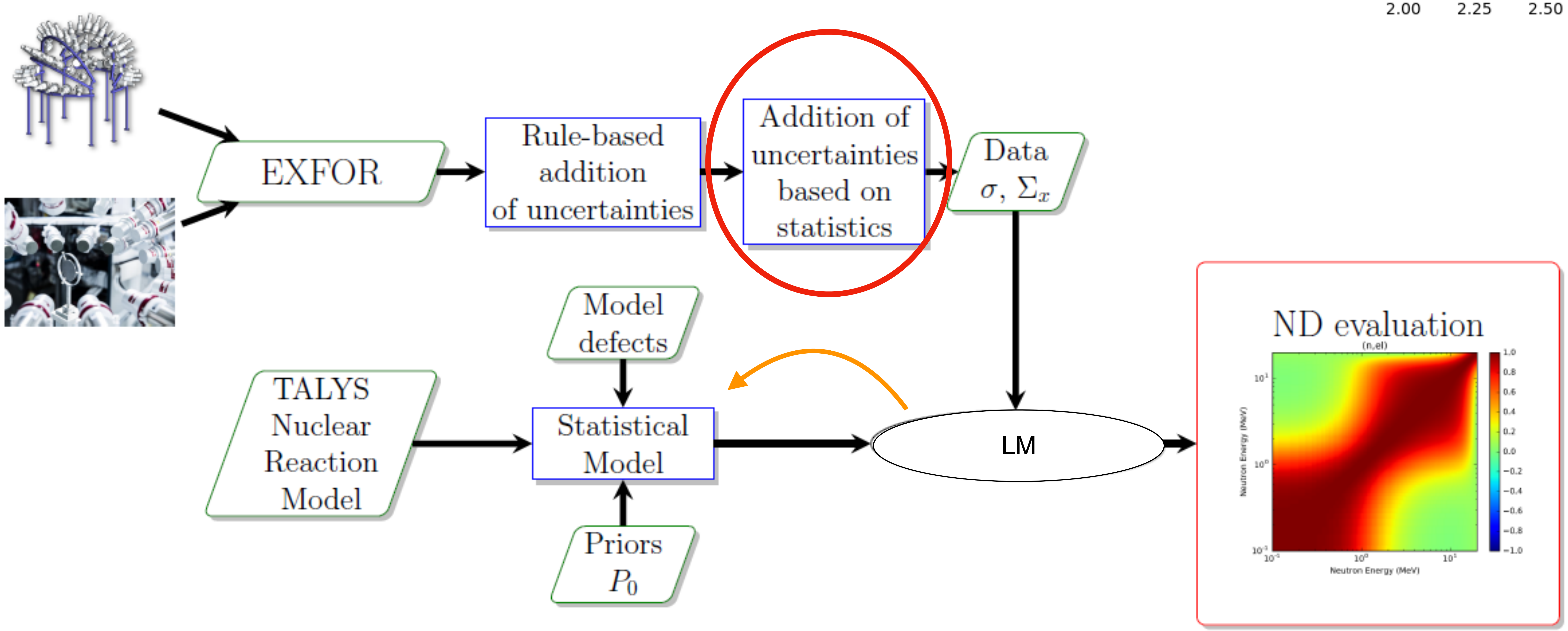
- Heteroscedasticity means different variation of data
- Heteroscedastic GP allows the nugget parameter to vary.

Treatment on systematic uncertainties

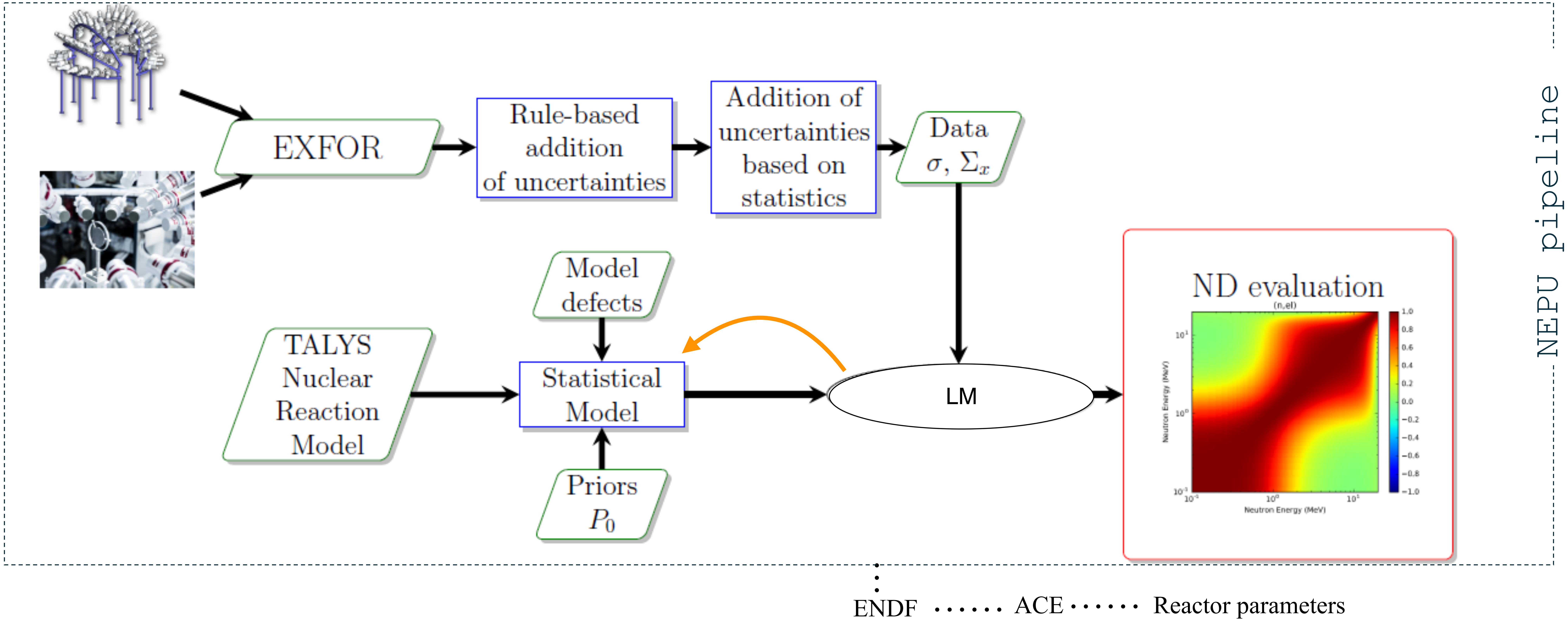


- Datasets often disagree at the normalization level
- Marginal likelihood optimization detects inconsistencies automatically
- Additional uncertainty components are added where the data require them





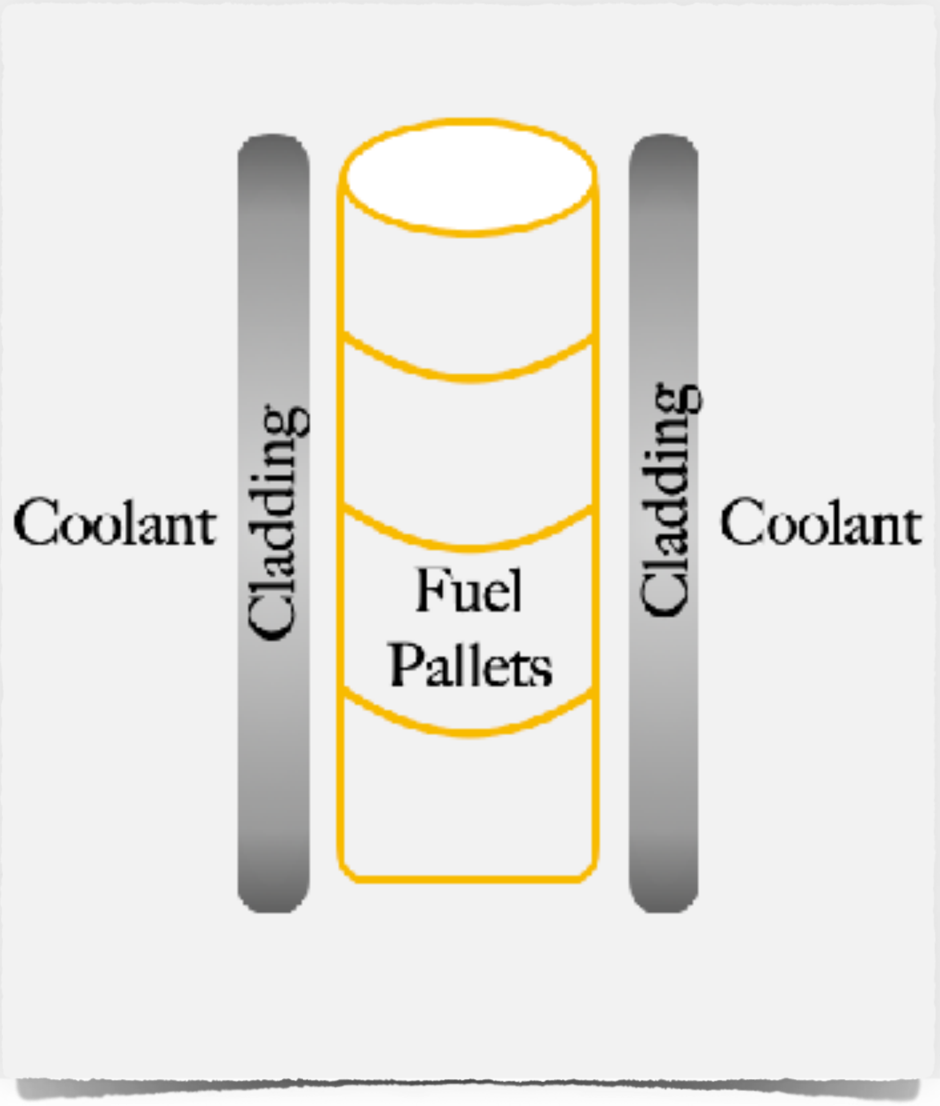
- Evaluate TALYS parameter sensitivity
- Fit a GP over the energy-dependent parameters
- Optimize parameters with the Levenberg-Marquardt algorithm
- Add a GP in the observable domain for extra uncertainty
- Re-optimization



Zr-90 on NEPU

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.

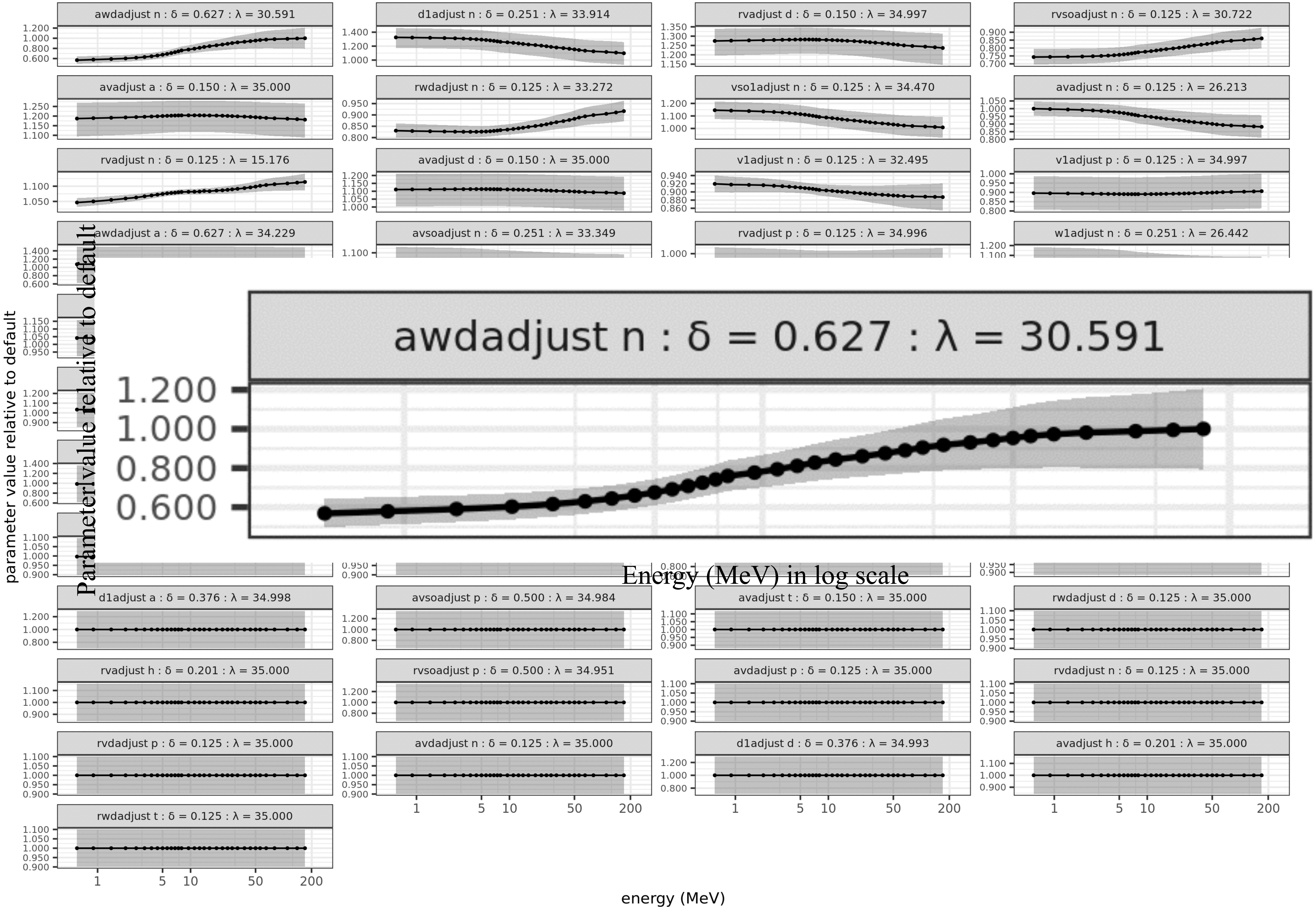
We plan to use latest TENDL input with TALYS-2.2

Total exp data 1727 (1-150 MeV)

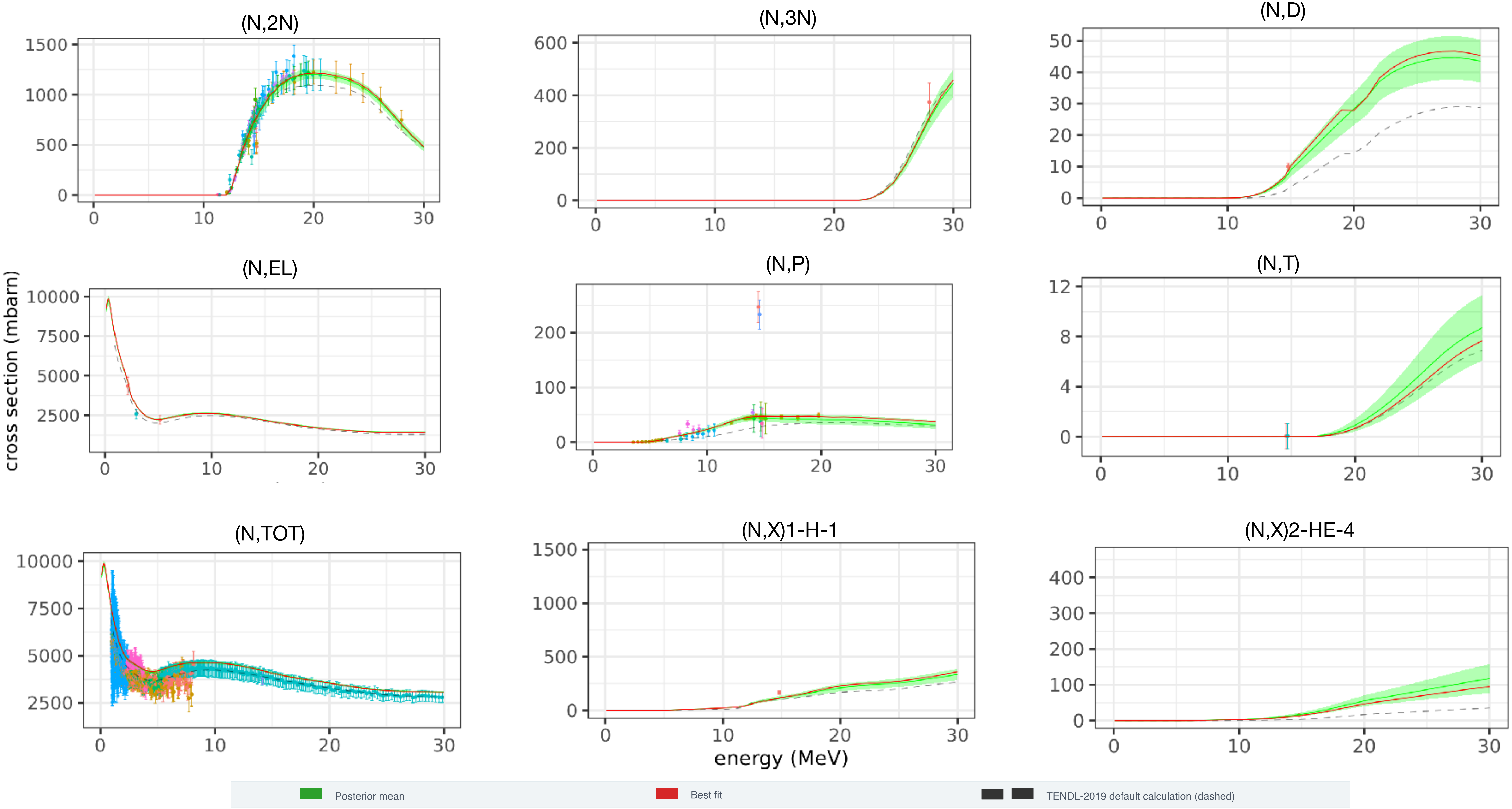
Number of TALYS free parameters 3834 (with energy dependence)

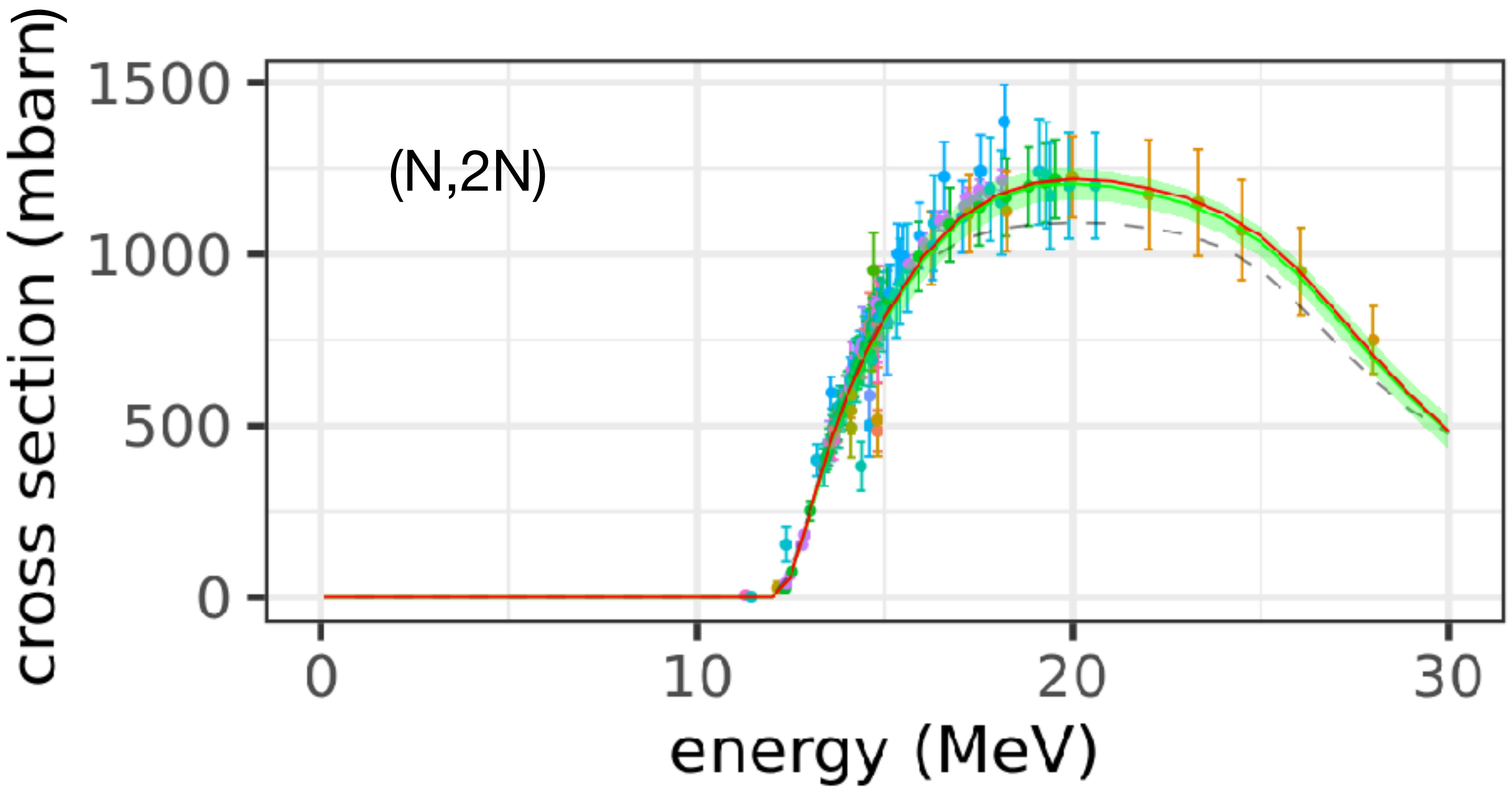
number of adjustable selected parameters: 1614 / 3834

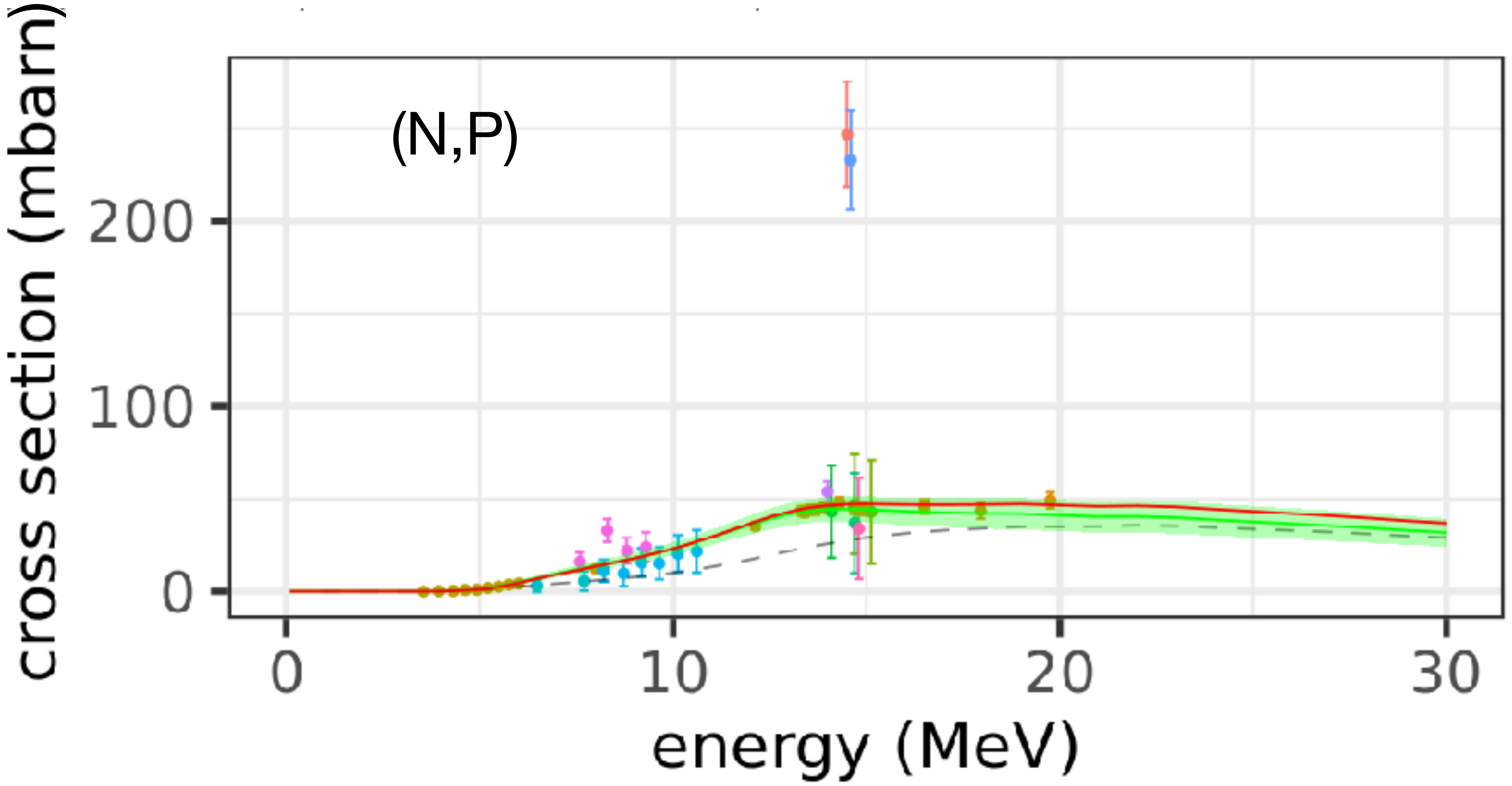
GP treatment on energy dependent model parameters



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







TALYS defaul tcalculation with TENDL2019 input

Posterior mean

Best fit

Summary

- Nuclear data underpins all of nuclear science and engineering
- Uncertainties are critical for safety analysis but difficult to quantify
- 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.

https://github.com/UU-nuclear

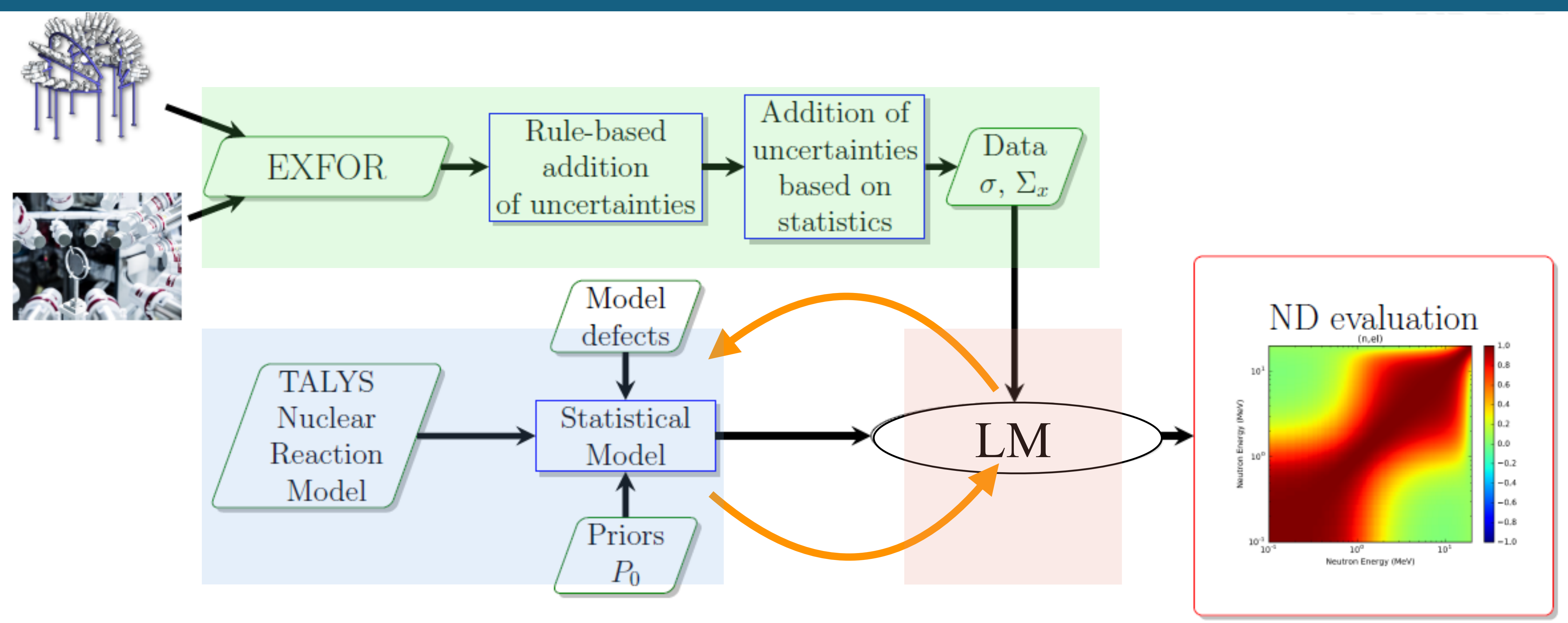
Acknowledgements

Swedish Energy Agency for financial support, Dardel by NAISS for computing resources.

We are glad to collaborate & share.

THANK YOU.

Pipeline Architecture



https://github.com/UU-nuclear

Script 01 – EXFOR experimental data retrieval

Script 02 – TALYS reference calculation (prior) with TENDL input

Script 03 – Rule based addition of uncertainties. e.g. Avoid Peelle's pertinent puzzle

Script 04a – HetGP: random unc. correction, inflate resonance σ

Script 04b – MLO: systematic unc. tuning

Script 05a – Jacobian Sesitivity matrix with $\frac{\partial \sigma}{\partial p}$

Script 05b – Parameter selection

Script 06 – GP hyperparameter (energy dependent) optimization

Script 07 – 1st Levenberg Marquardt

Script 7.5 – GP model defect Fit GP to residuals, add to covariance

Script 10 – 2nd LM optimization + defect

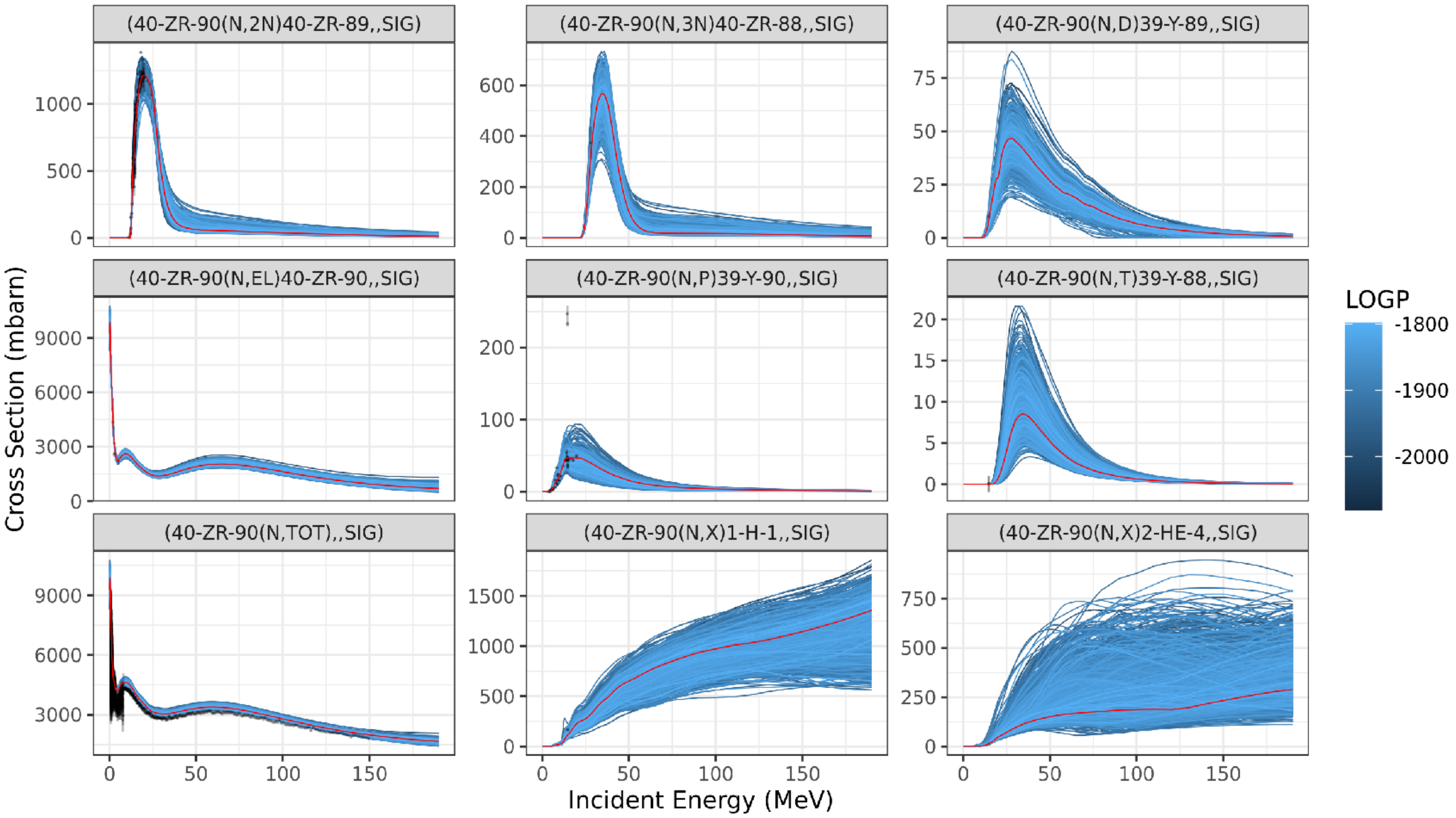
Script 11 – Posterior approximation with GLS

Script 12 – Random TALYS files 2000 posterior samples + 1 best estimate

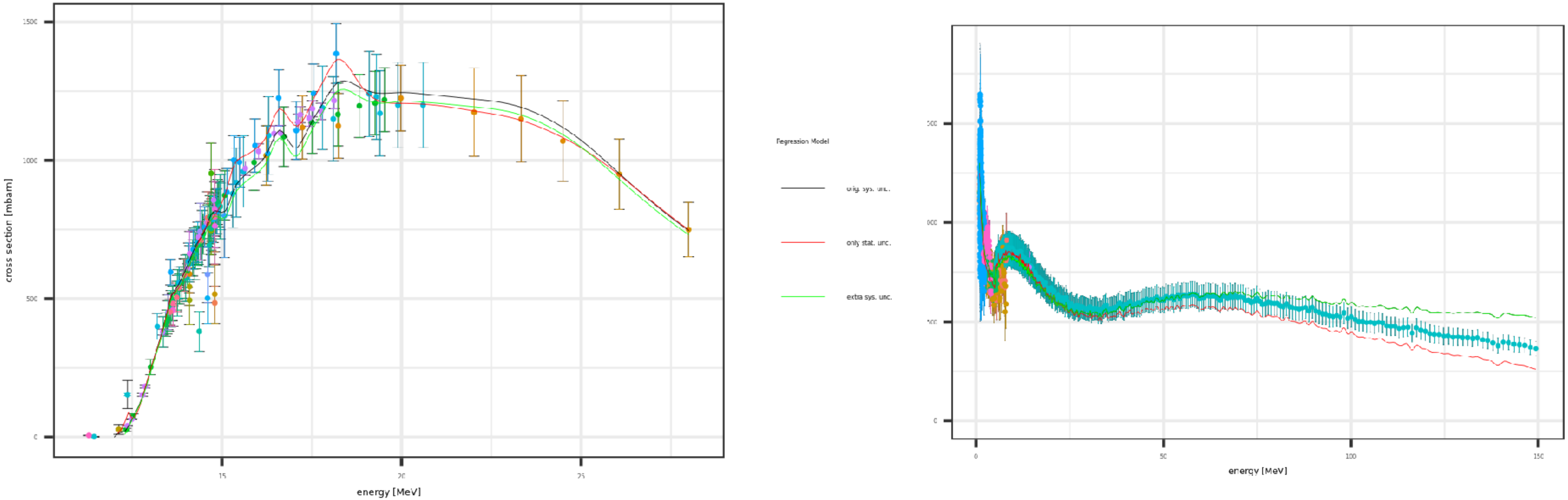
NEPU pipeline

ENDF ······ ACE ······ Reactor parameters

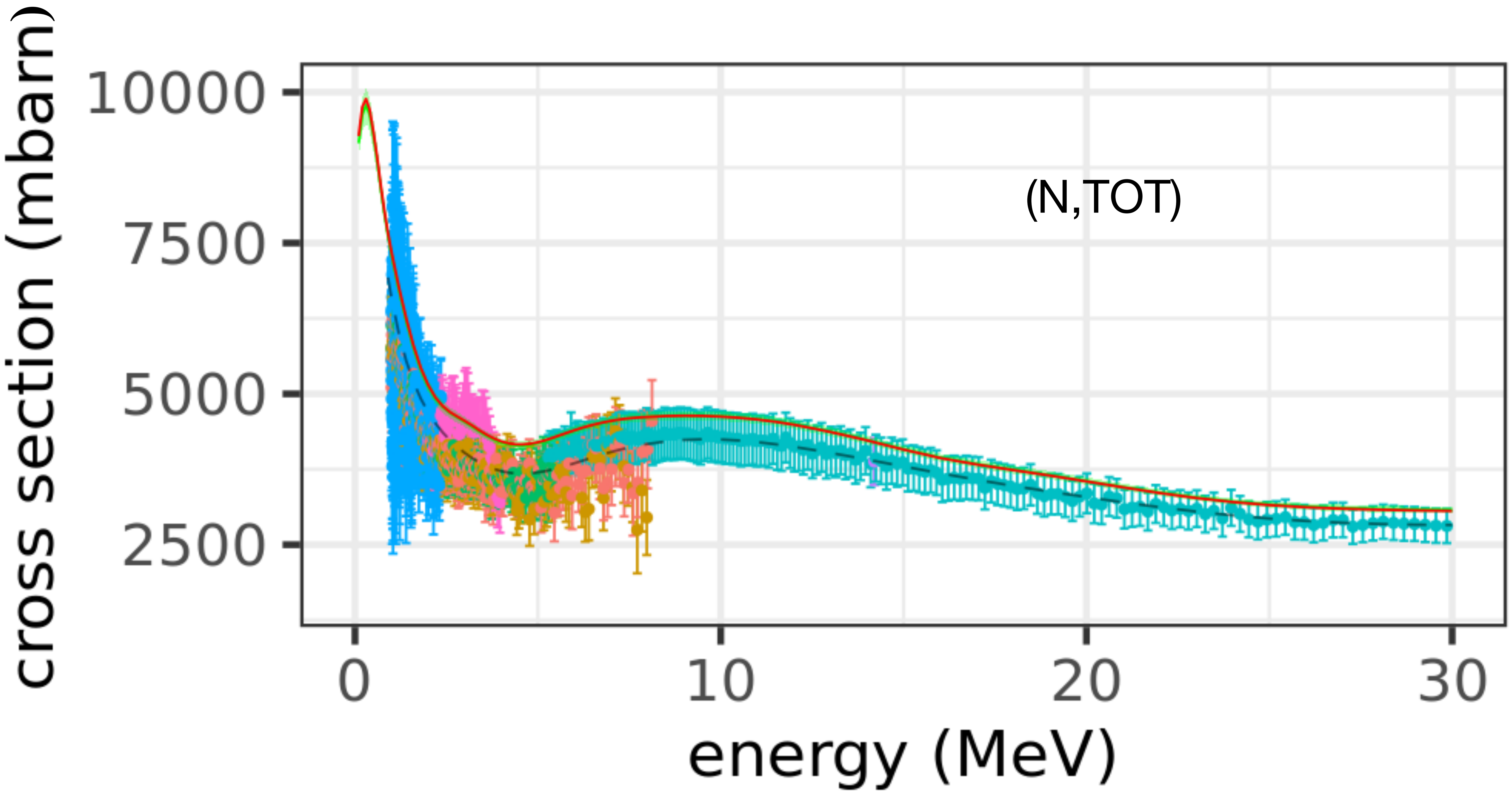
2000 random samples for cross-section



MLO uncertainty



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



- - - - - - - TALYS defaul tcalculation with TENDL2019 input

Posterior mean

Best fit