# Inference of Photonuclear Theory Parameter Covariances Using ML-Enabled MCMC

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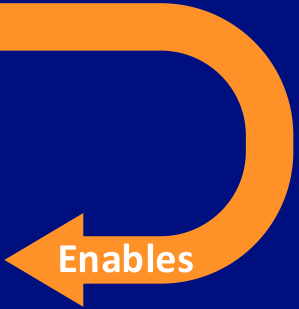
1/8/2026

LA-UR-25-30648

# Outline

1. Global photoreaction emulator
   1. Deep neural network design
   2. Performance tests

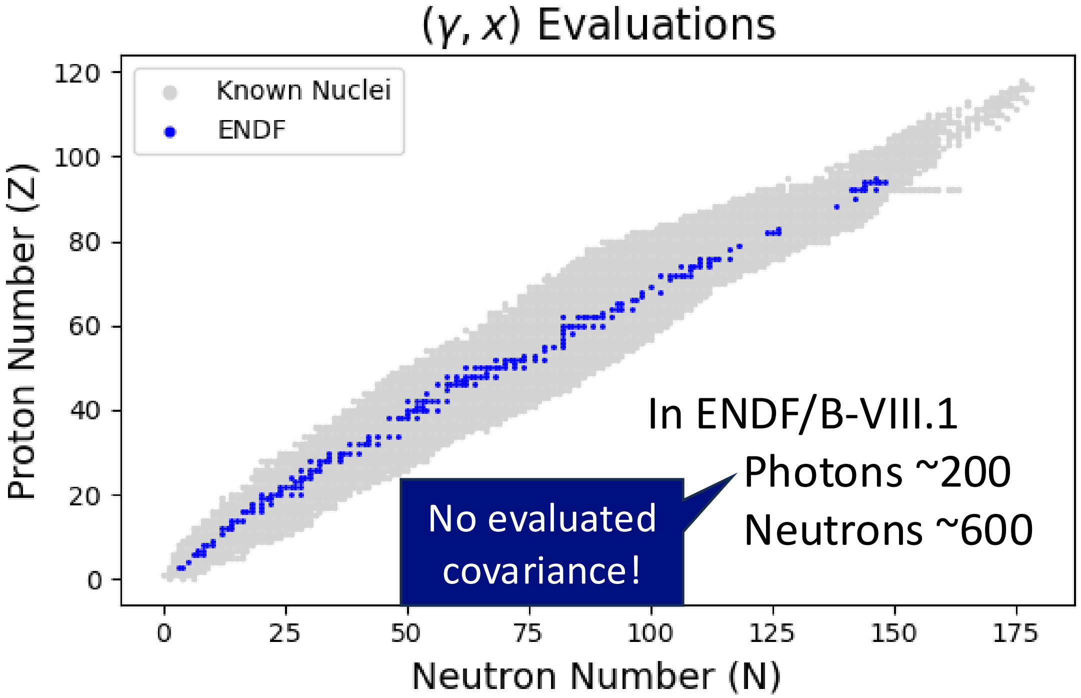



2. Enhanced Bayesian Evaluation (MCMC)
   1. Avoid assumptions in GLS / Kalman
   2. Additional capabilities to handle data limitations

# WHY: photonuclear data are sparse

- Experimental data are less abundant and less reliable
  - Traditional evaluation approaches break down
  - Composite observables (ratios or yield) are often more reliable

- How can we use ML to get better evaluated covariance?
  - Emulate the theory model
  - Plug into MCMC framework



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Enables

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# Deep Neural Network Emulator for CoH3

- Mapping $X \mapsto \sigma_{\mathrm{ZA}}(\gamma, c)(E_\gamma)$
- Features $X \equiv [\mathcal{N}, \Gamma, \mathcal{F}, \beta, \Lambda]$

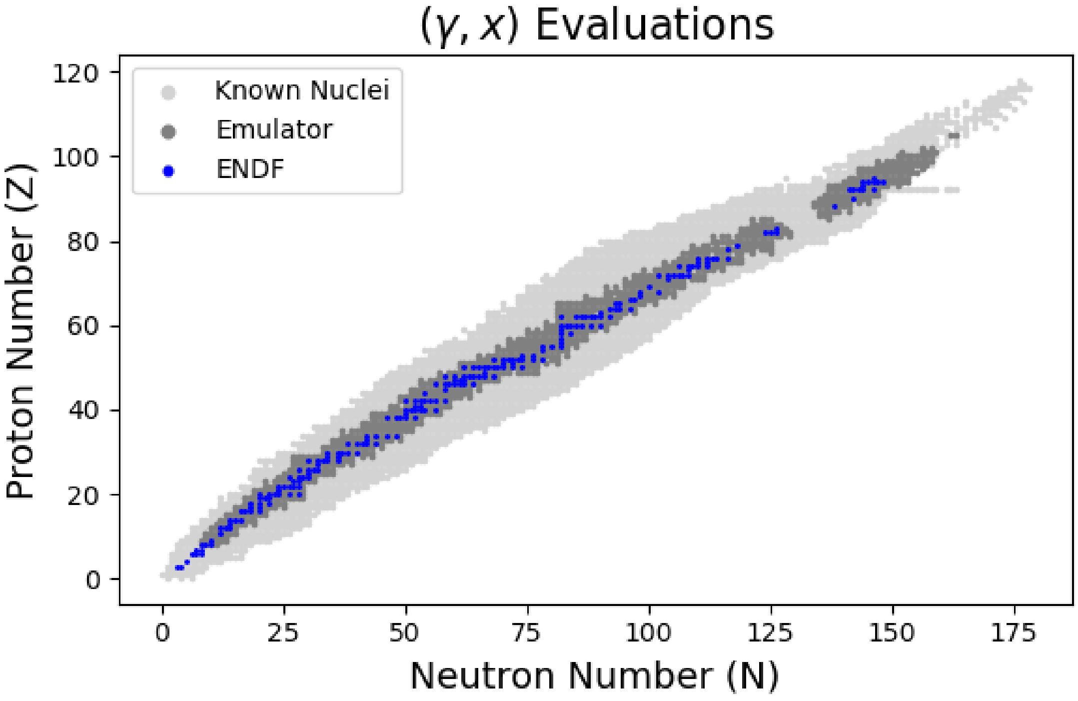
$\mathcal{N}_i \subset \mathbb{R}^{p_\mathcal{N}}$ are fundamental nuclear parameters

$\Gamma_i \subset \mathbb{R}^{p_\Gamma}$ are GDR parameters

$\mathcal{F}_i \subset \mathbb{R}^{p_\mathcal{F}}$ are fission-barrier descriptors (if applicable)

$\beta_i \subset \mathbb{R}^{p_\beta}$ are deformation parameters

$\Lambda_i \subset \mathbb{R}^{p_\Lambda}$ are level density parameters.



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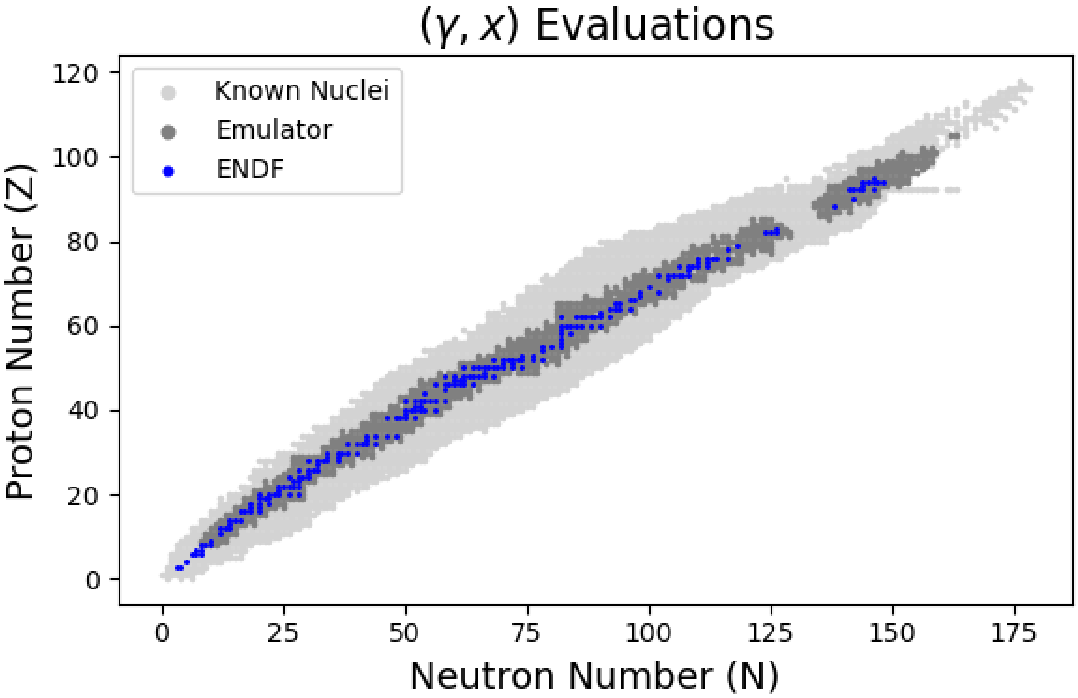
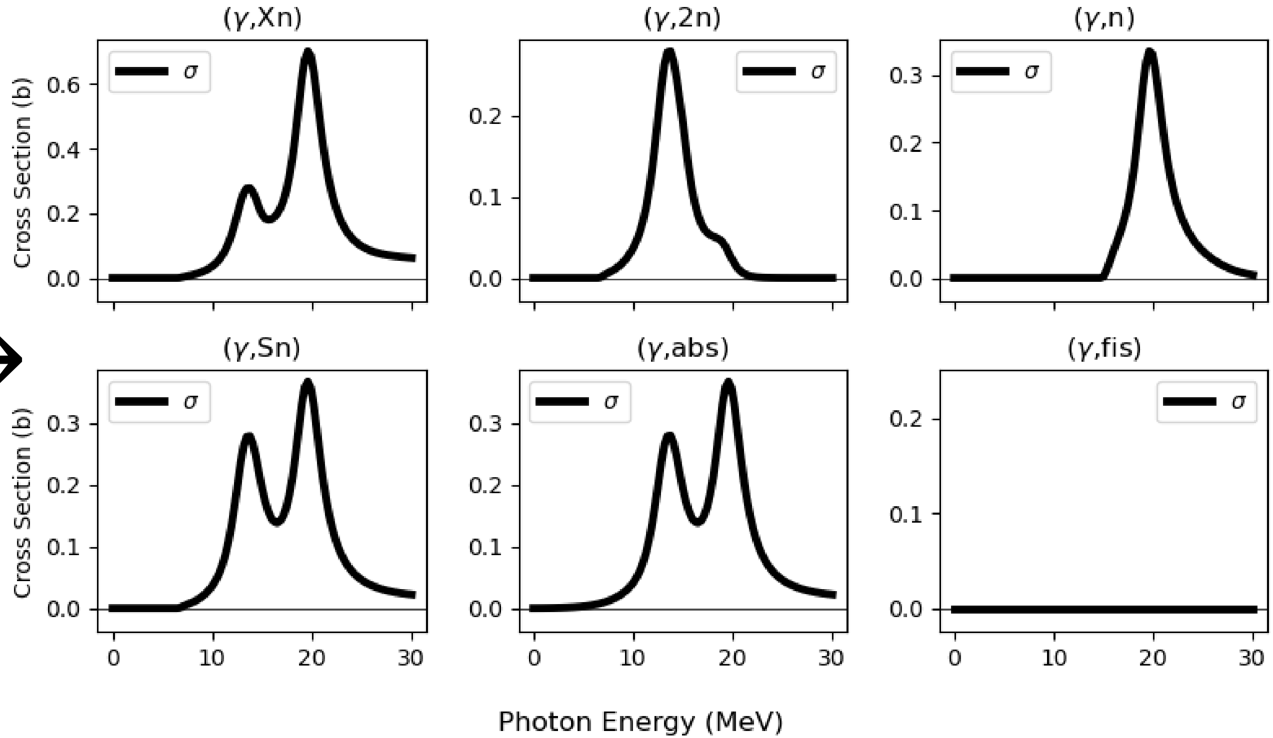


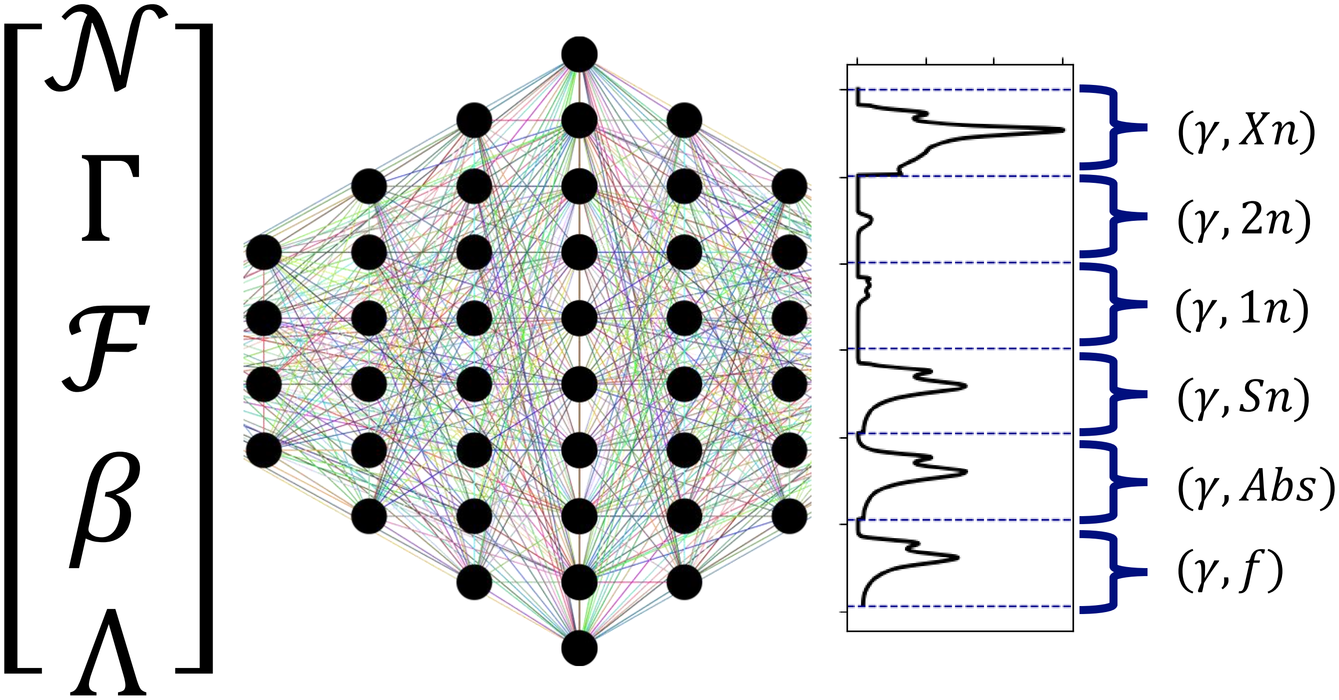
# Deep Neural Network Emulator for CoH3

$$X \quad \mapsto \quad \sigma_{\mathrm{ZA}}(\gamma, c)(E_\gamma)$$

$$\begin{bmatrix} \mathcal{N} \\ \Gamma \\ \mathcal{F} \\ \beta \\ \Lambda \end{bmatrix} \longmapsto$$



# Vectored outputs allow us to apply physics constraints across energies and channels




$$(\gamma, Xn)_i \geq (\gamma, 1n)_i + 2(\gamma, 2n)_i + (\gamma, f)_i$$

$$0 \leq \sigma_{i_{\text{pred}}} \ \forall \ i$$

$$\left[\frac{\partial \sigma_i}{\partial E_i}\right]_{\text{true}} - \left[\frac{\partial \sigma_i}{\partial E_i}\right]_{\text{pred}}$$

# Training Data Generation:

## - Generate global prior vector
## - Sample phase space around prior w/ Latin Hypercube

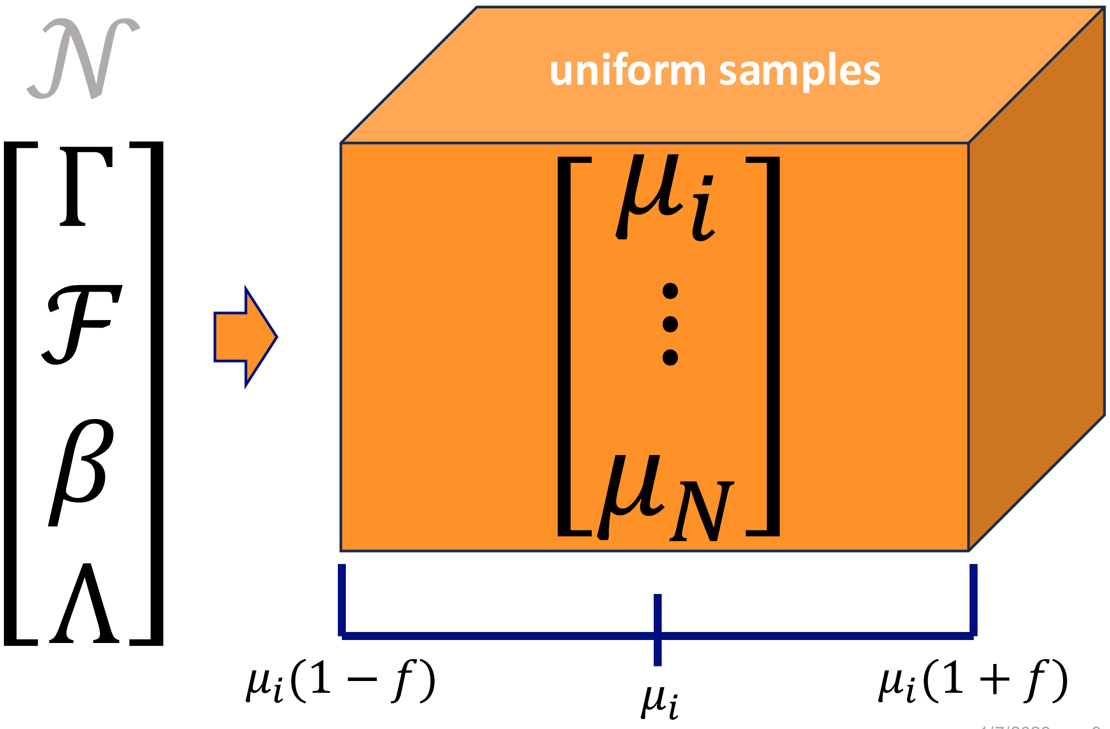
E1 GDRs experimentally determined when available, systematics otherwise
V.A. Plujko, O.M. Gorbachenko, R. Capote, and P. Dimitriou (2018)

M1, E2, M2 GDRs from systematics given in TALYS manual
If bimodal E1, then M1 is also bimodal

Fission barriers from:
O. Iwamoto, T. Nakagawa, et al, (2009).

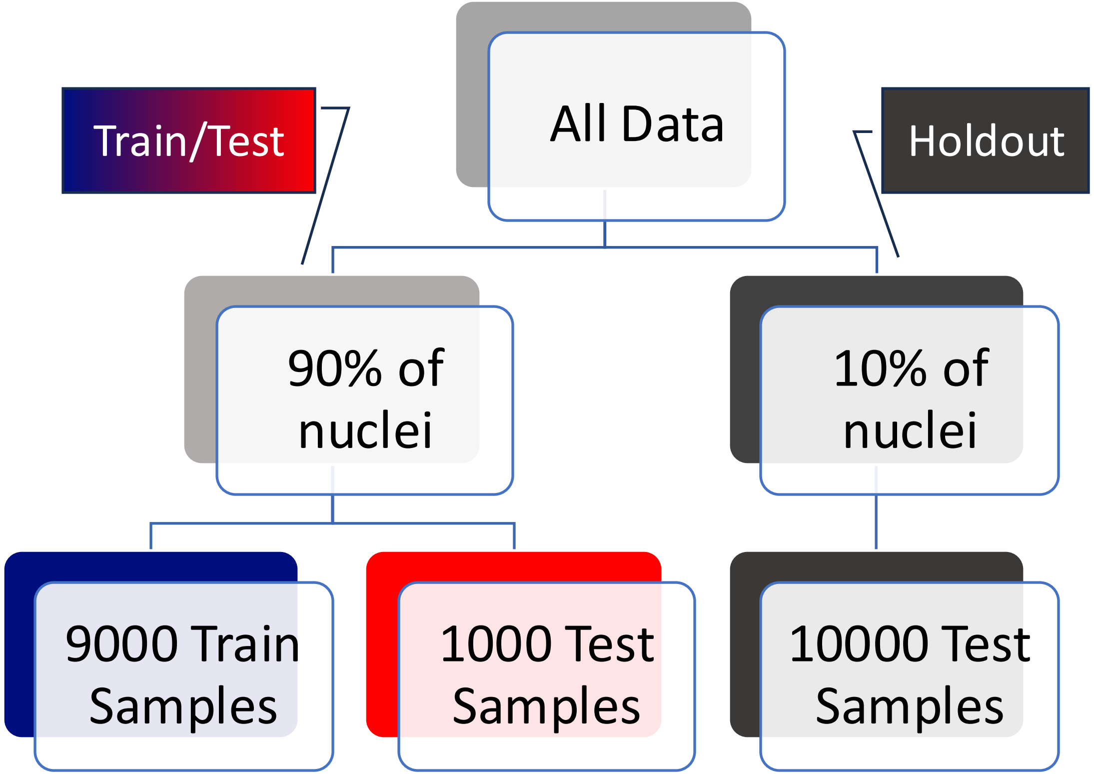
Deformation parameters from:
P. Moller, J.R. Nix, W.D. Myeres, and W.J. Swiatecki (1995)

Level Density parameters from:
Gilbert-Cameron model

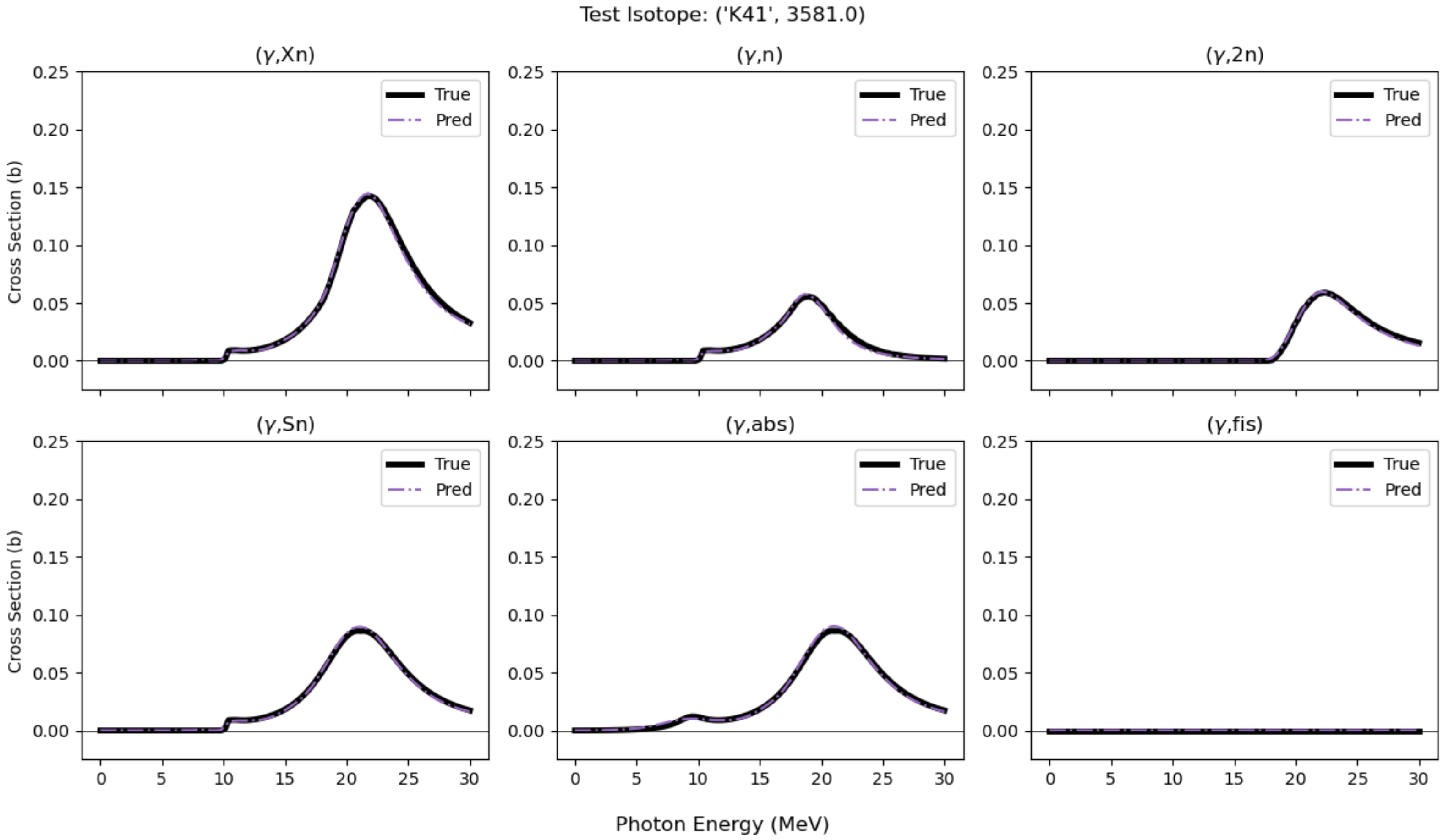


# Training, testing, and holdout sets

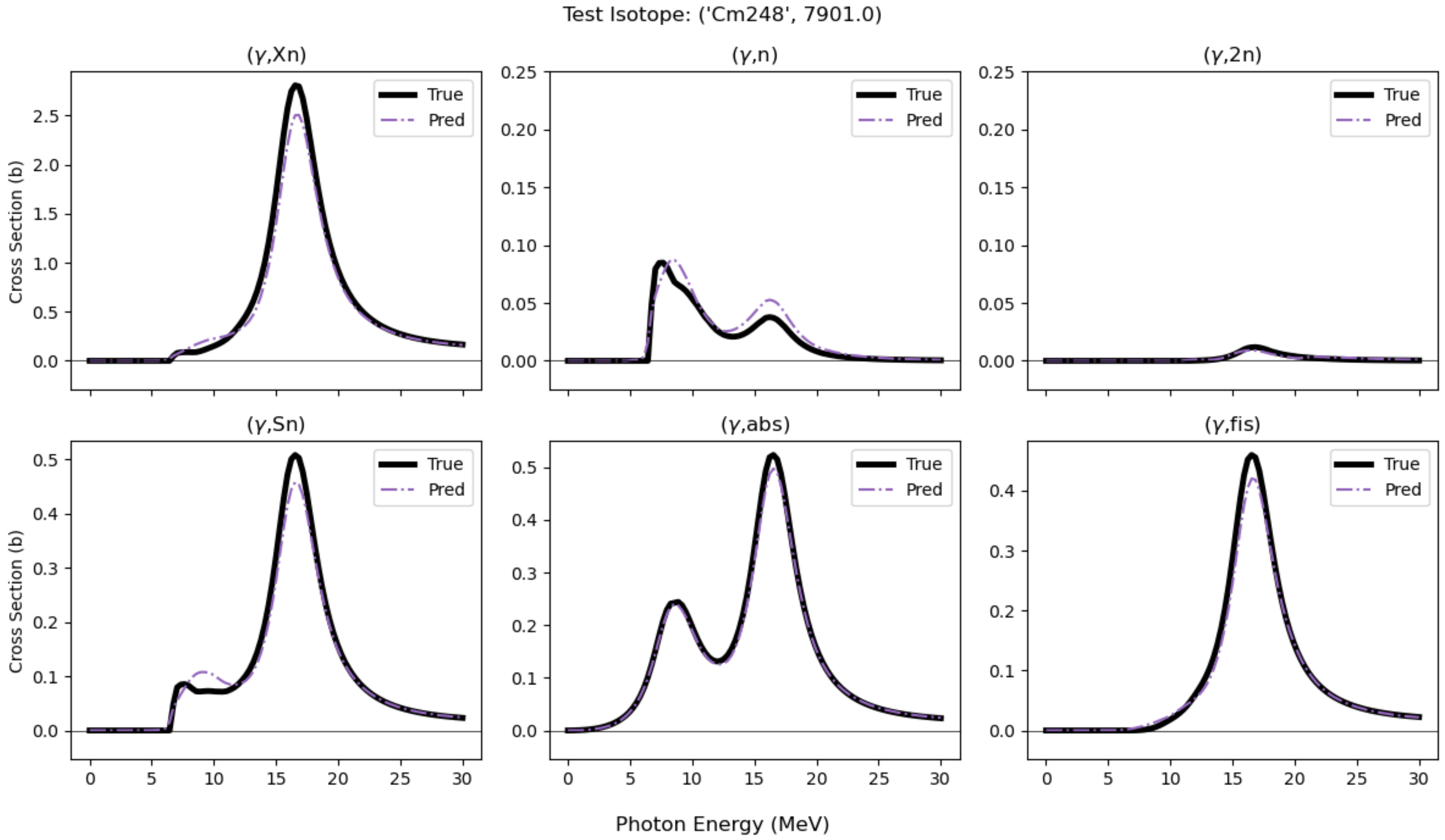
- Network never sees holdout nuclei
- Train and test samples are evenly balanced across nuclei



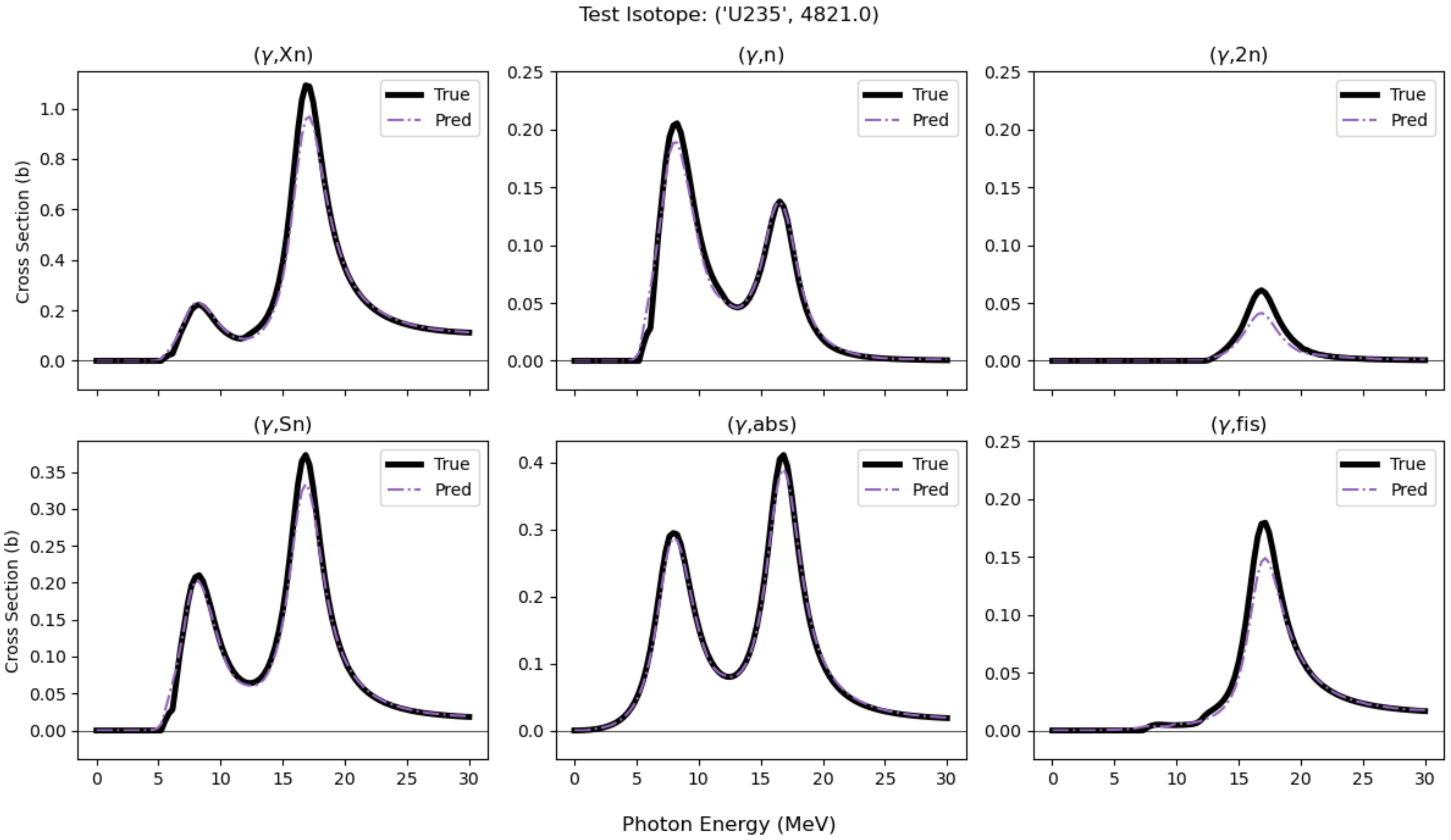
# Median performance overall (49th quantile)



# Worst performance overall (99th quantile)

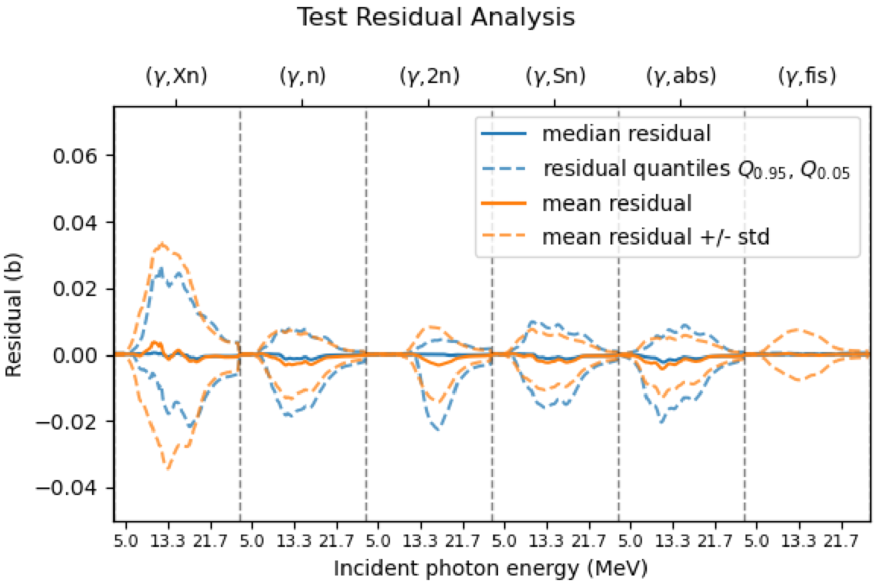


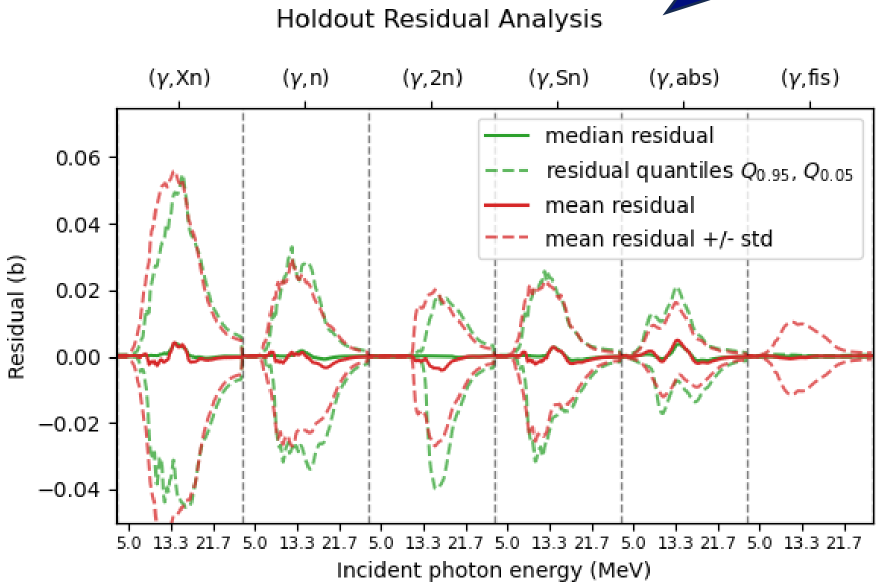
# Median performance for U-235 / Pu-239



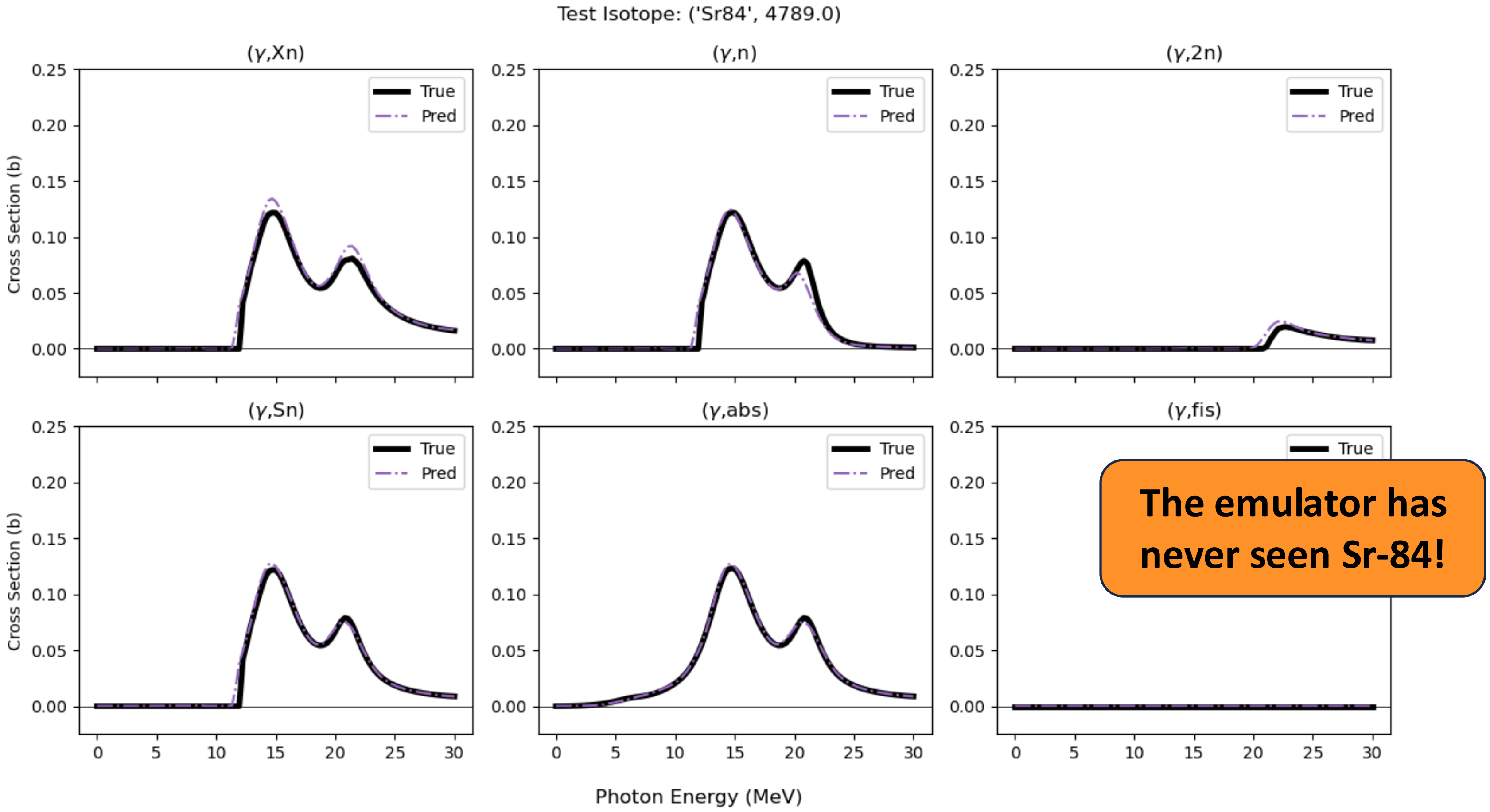
# Residual analysis shows unbiased photo-reaction predictions on test set

Comparable performance on holdout set



# Median performance in holdout (48th quantile)



# Emulator makes traditional Bayesian evaluation faster, enabling better posteriors

2.5 million X speedup

- Speed & ease of use
  - Prior covariance matrix converges with ~5k samples
  - Reproducibility across team

| Model | CoH3 | Emulator |
|---|---|---|
| CPU (s) / 1 sample | 153.90 | 6.33e-05 |
| CPU (s) / 5k samples | 7.7e+05 | 0.32 |

- Plug & play with fancy Bayesian Monte Carlo algorithms
  - More flexible modelling
  - Better tools for physics interpretations

```
from tensorflow import load_model

loaded_model = load_model('path/to/my/saved_emulator.keras')

pred = loaded_model(X)
pred = inverse_transform(pred)
```

Keras/TensorFlow model is differentiable, can be added to graph for Hamiltonian Monte Carlo

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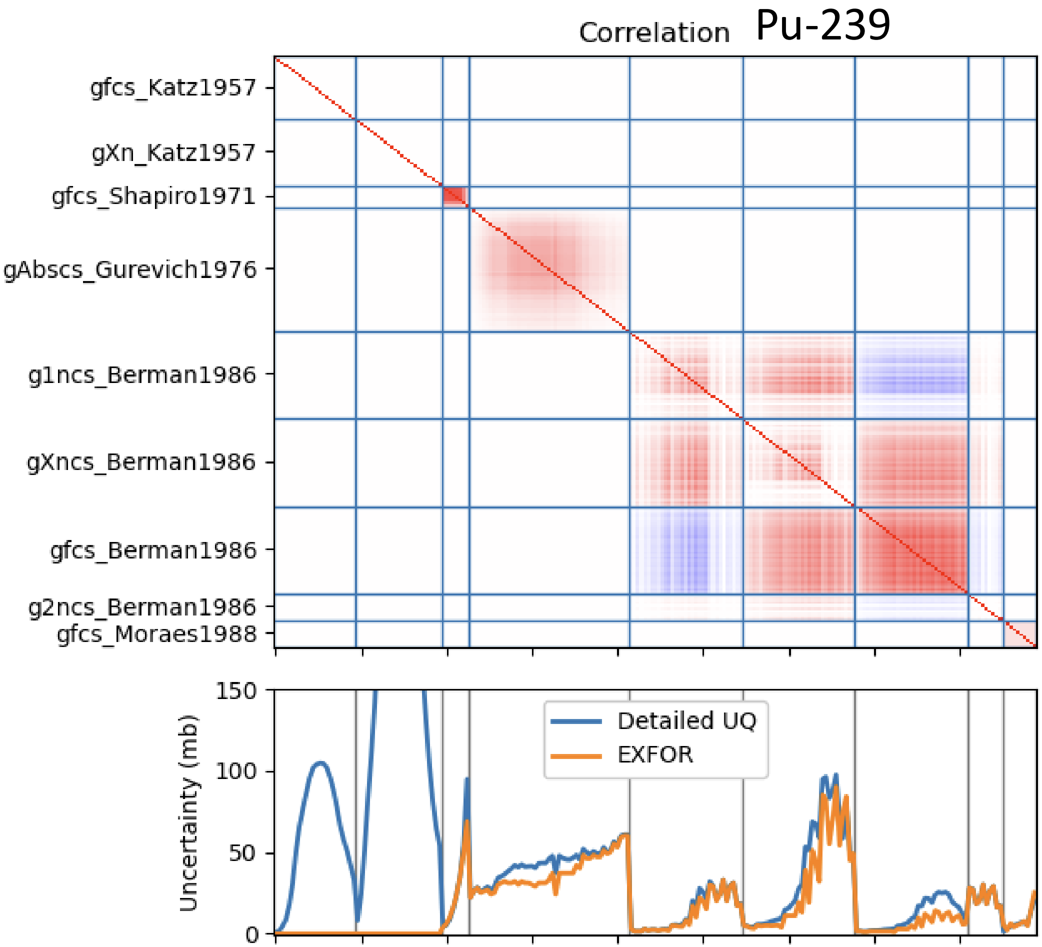
Enables

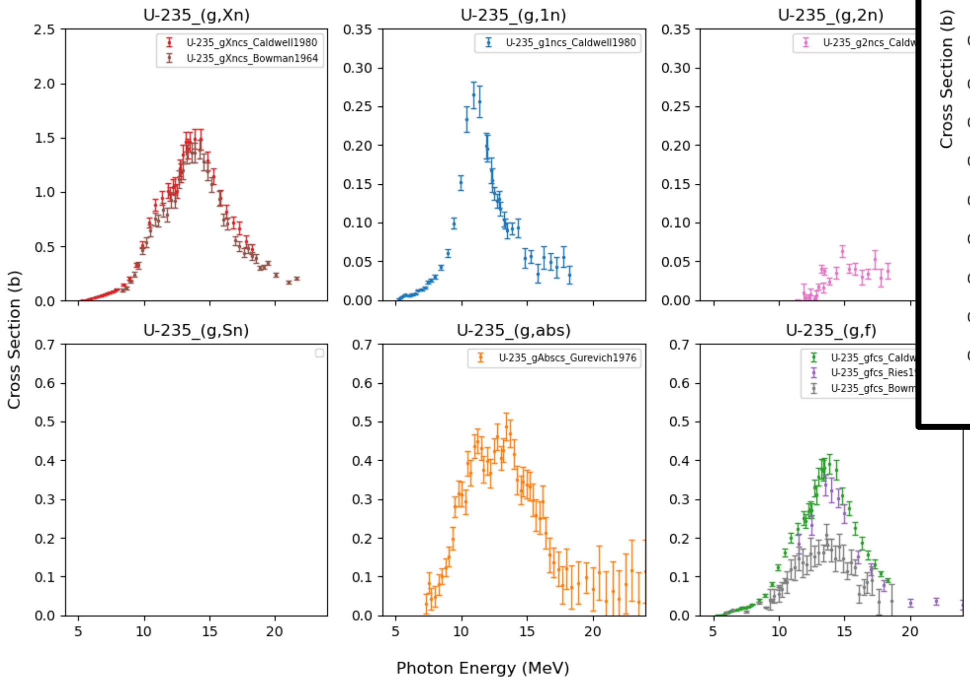
# Preliminary experimental UQ for demonstration

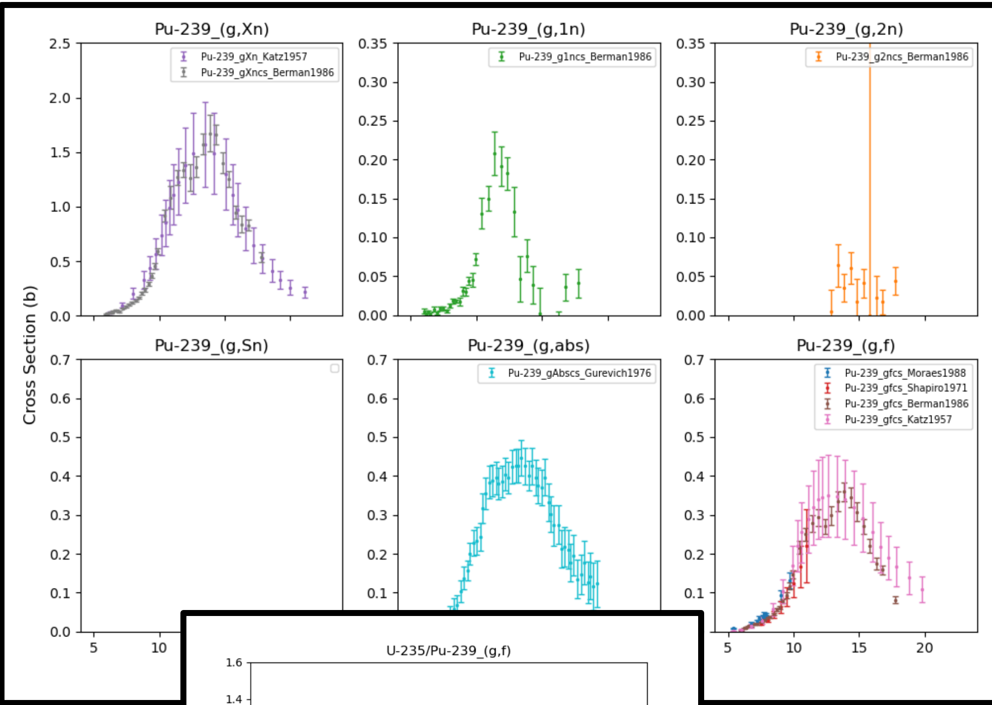
- Photo-reaction data
  - Detailed look at Pu-239
  - Started U-235
  - Planned U-238

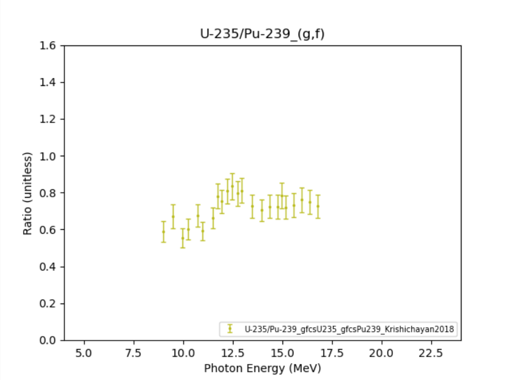
- Fission ratio data exist between all three of these nuclei



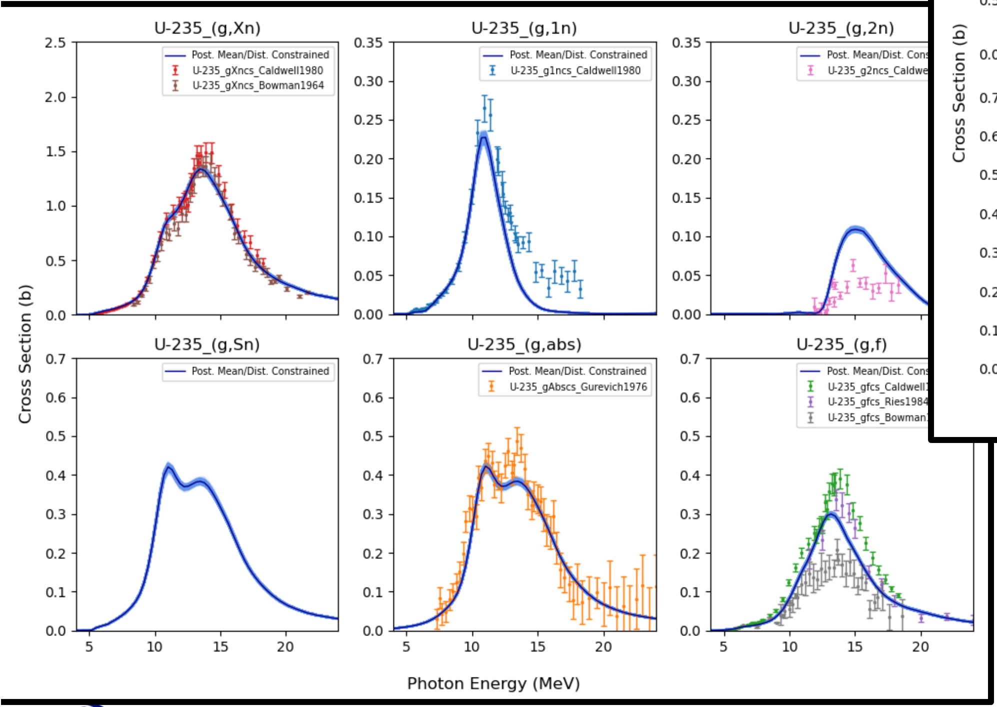
# MCMC framework allows clean simultaneous evaluation across channels and isotopes

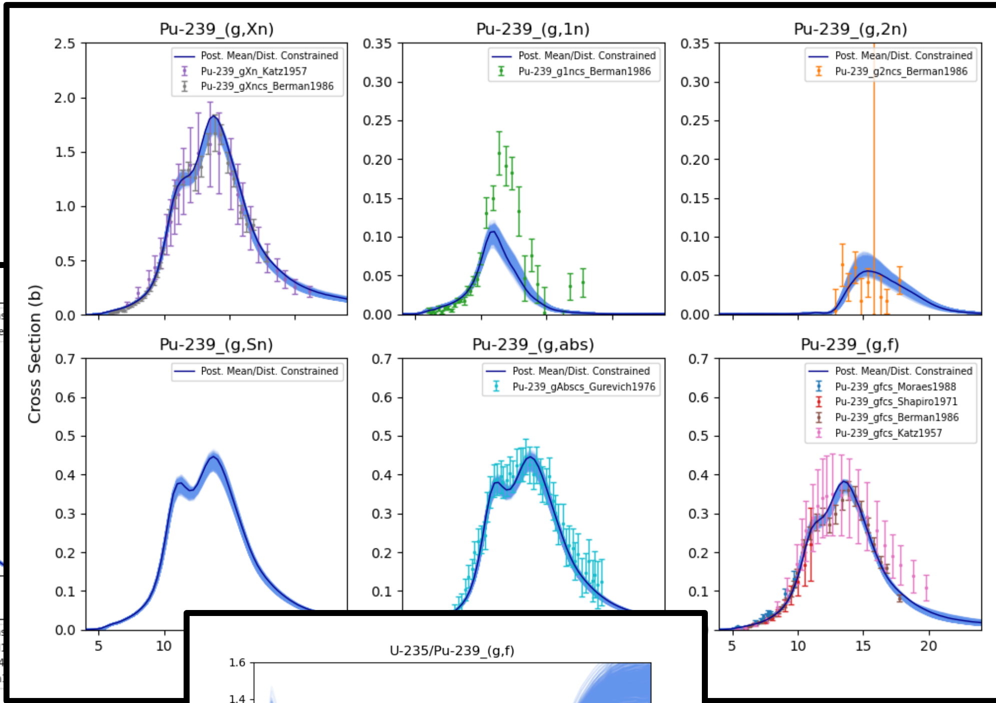


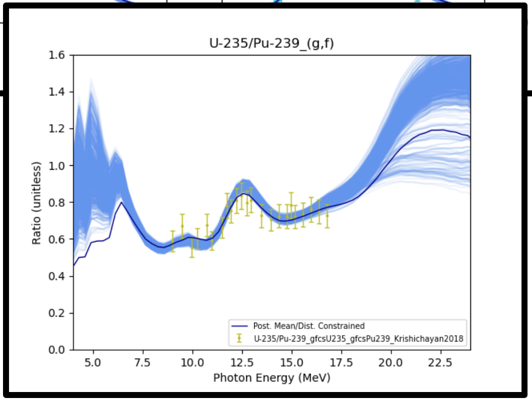



# MCMC framework give posterior parameter samples – very flexible output

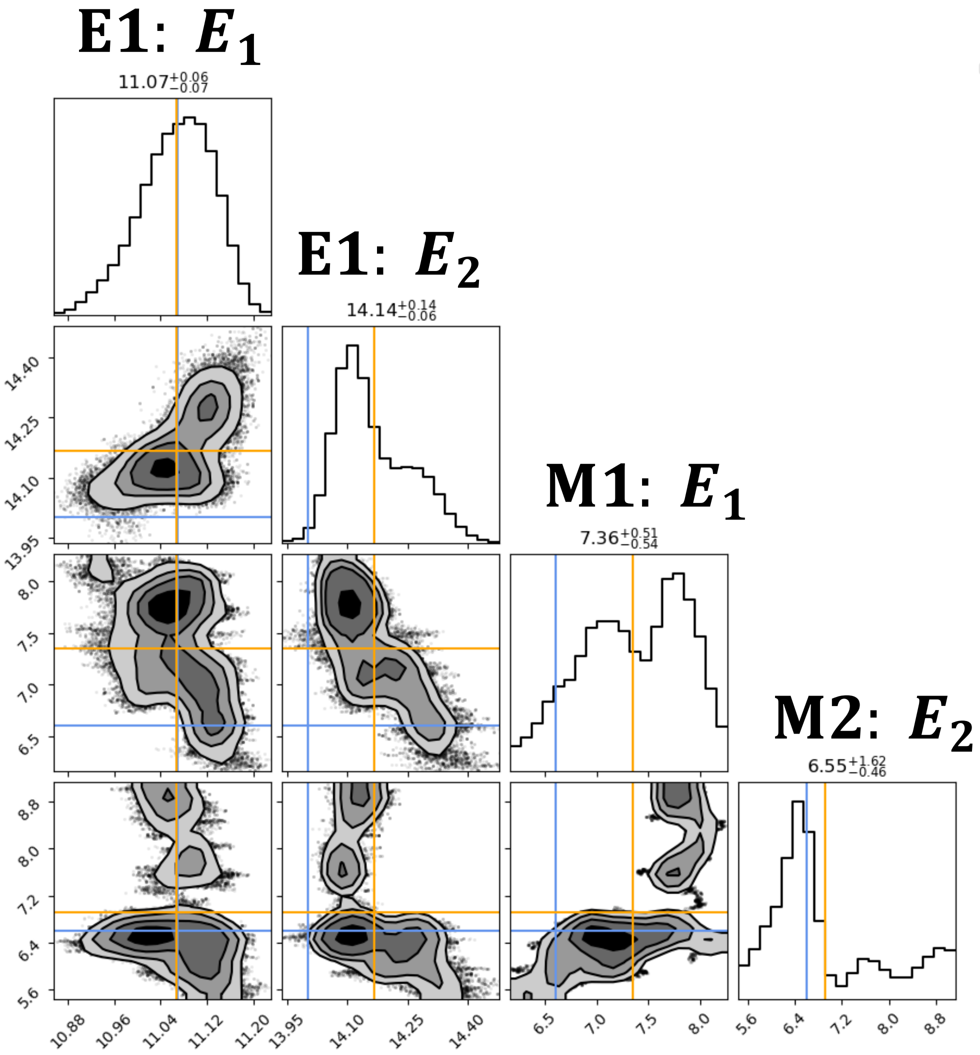


# MCMC gives parameter posteriors

- Can put back into CoH3 to get all physics data
- Some parameters have bimodality
  - Important physics interpretation
- Prior and posterior are far from one another



# Conclusions

1. Global photoreaction emulator
   1. Deep neural network design
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- **Fast, accurate, easy to use**
- **Performance on holdout nuclei is interesting… alludes to future work**

2. Enhanced Bayesian Evaluation (MCMC)
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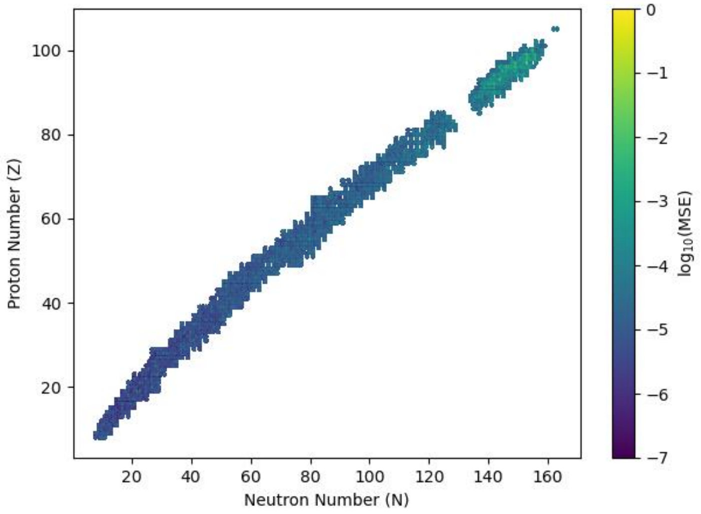
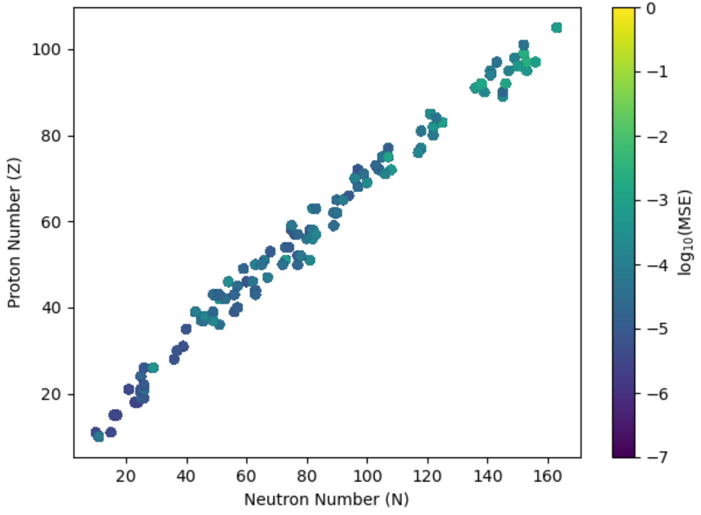
- **Main result so far is to enable MCMC evaluation**
  - **No assumptions (linearity/Gaussianity)**
  - **More complex analysis**
- **Still rigorous/interpretable… just made feasible with ML**

# Acknowledgements

Research reported in this presentation was in part supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory under project number(s) 20240878PRD4, 20250691ECR


Proton Number (Z)
Neutron Number (N)
log$_{10}$(MSE)
20
40
60
80
100
120
140
160
0
−1
−2
−3
−4
−5
−6
−7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20
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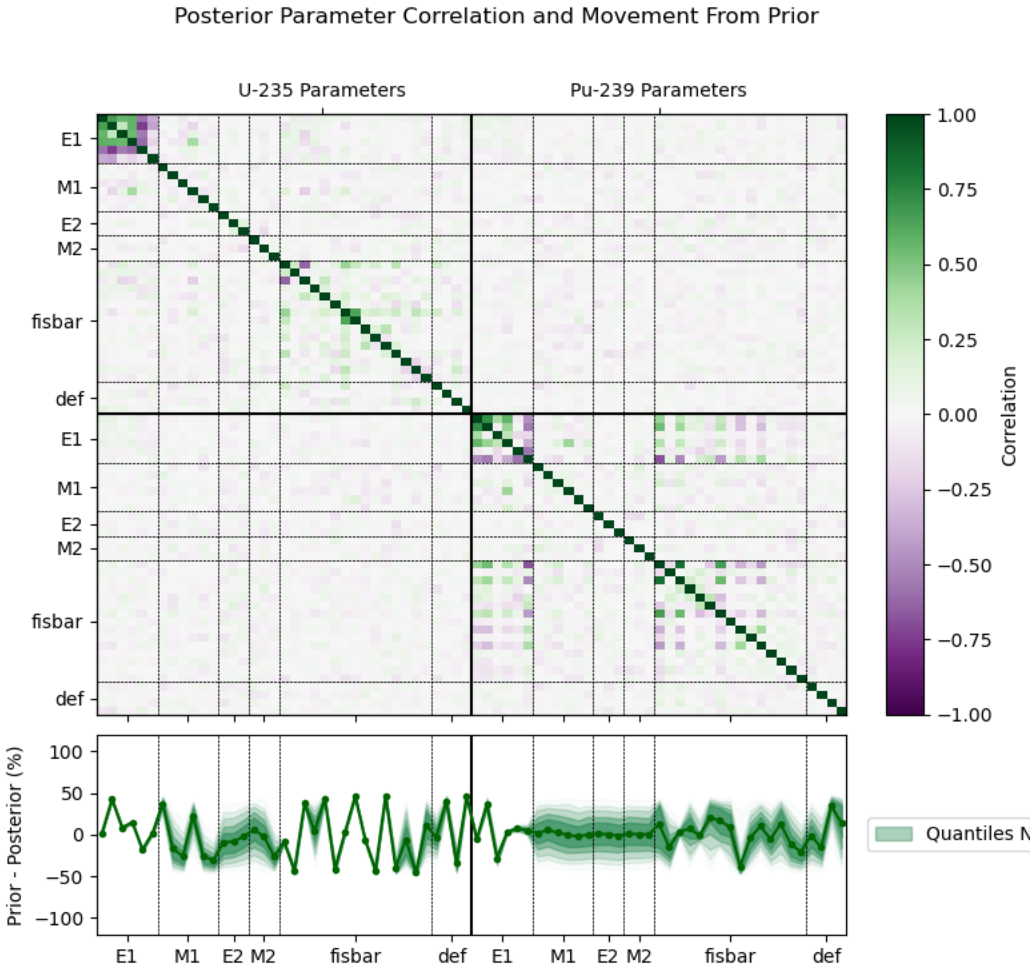
Posterior Parameter Correlation and Movement From Prior
U-235 Parameters
Pu-239 Parameters
E1
M1
E2
M2
fisbar
def
Correlation
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Prior - Posterior (%)
100
50
0
−50
−100
Quantiles N