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# Pu9(n,f) cross section covariances including USU components

**Georg Schnabel**

**Nuclear Data Section**
**Division of Physical and Chemical Sciences NAPC**
**Department for Nuclear Sciences and Applications**
**IAEA, Vienna**

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# Outline

- From GMAP to probabilistic programming
- Evaluation with USU components
- Updating covariance matrices consistently

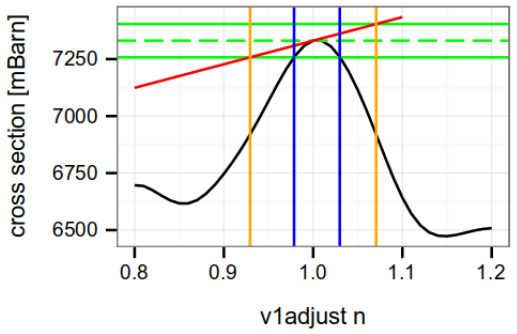
# GMAP

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

Experimental info: multivariate normal

Linear "model"

Prior: multivariate normal

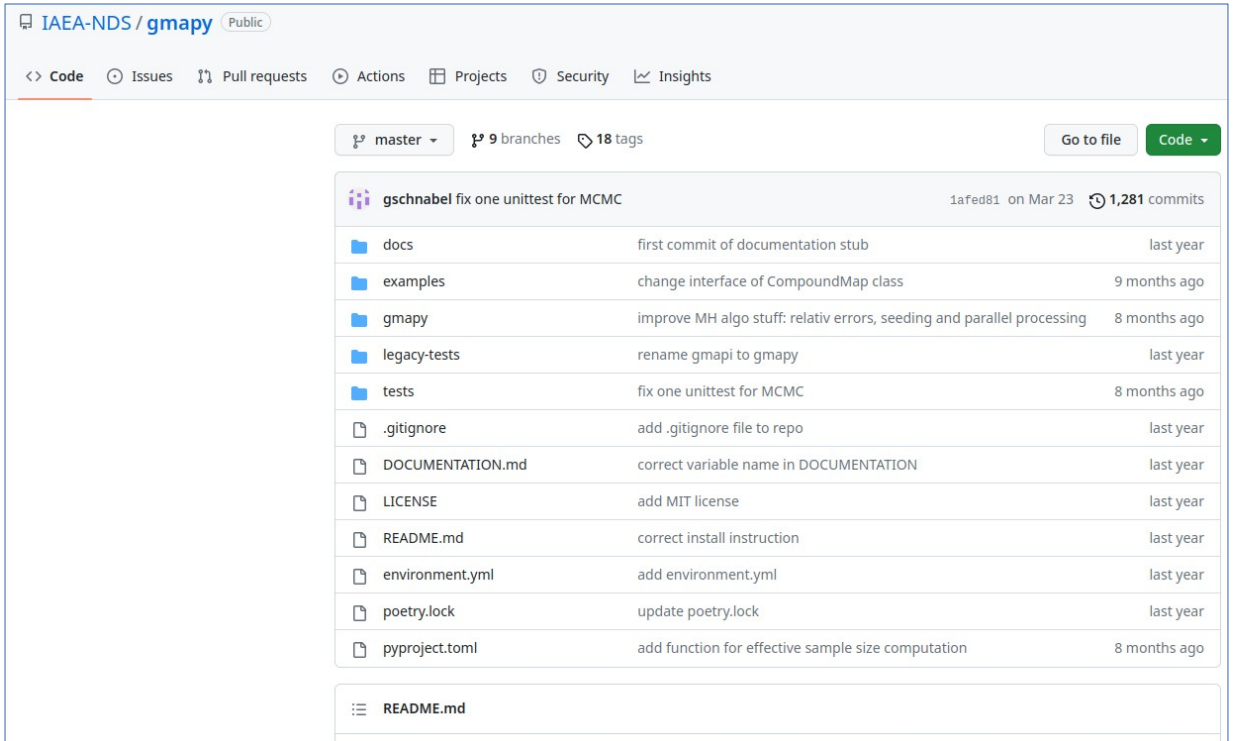



**Optimization (Iterative GLS)**

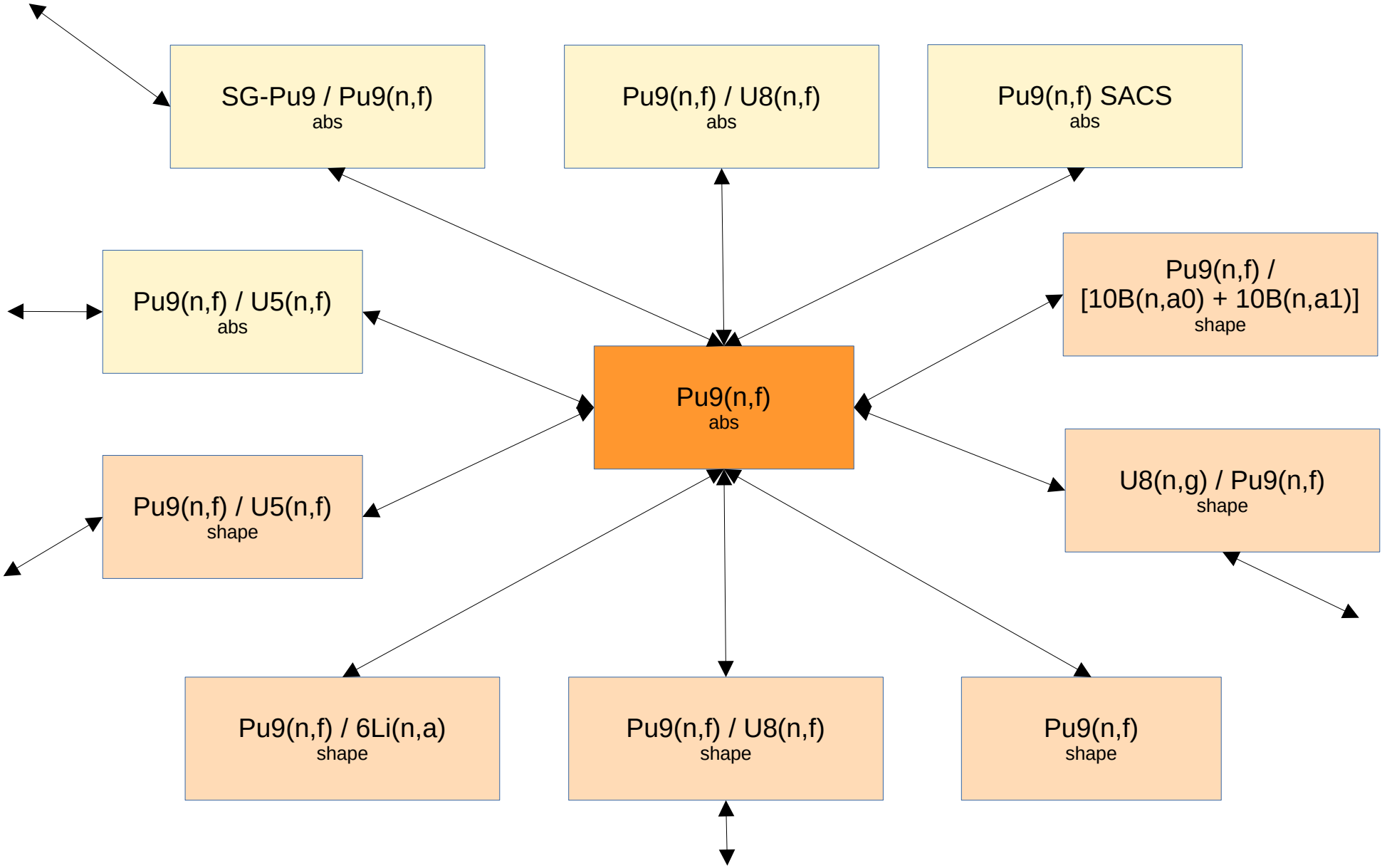
Ref: W.P. Poenitz, "Data interpretation, objective evaluation procedures and mathematical techniques for the evaluation of energy-dependent ratio, shape and cross section data", Proc. of the Conf. on Nuclear Data Evaluation and Procedures (1981)

# Probabilistic programming

- **GMAP** translated to Python and modernized
- **gmapy** is a package/framework for nuclear data evaluation:
  - Leverages Tensorflow probability
  - Nuclear data evaluation scenarios can be formulated as probabilistic programs

# Links between observables (GMA database)



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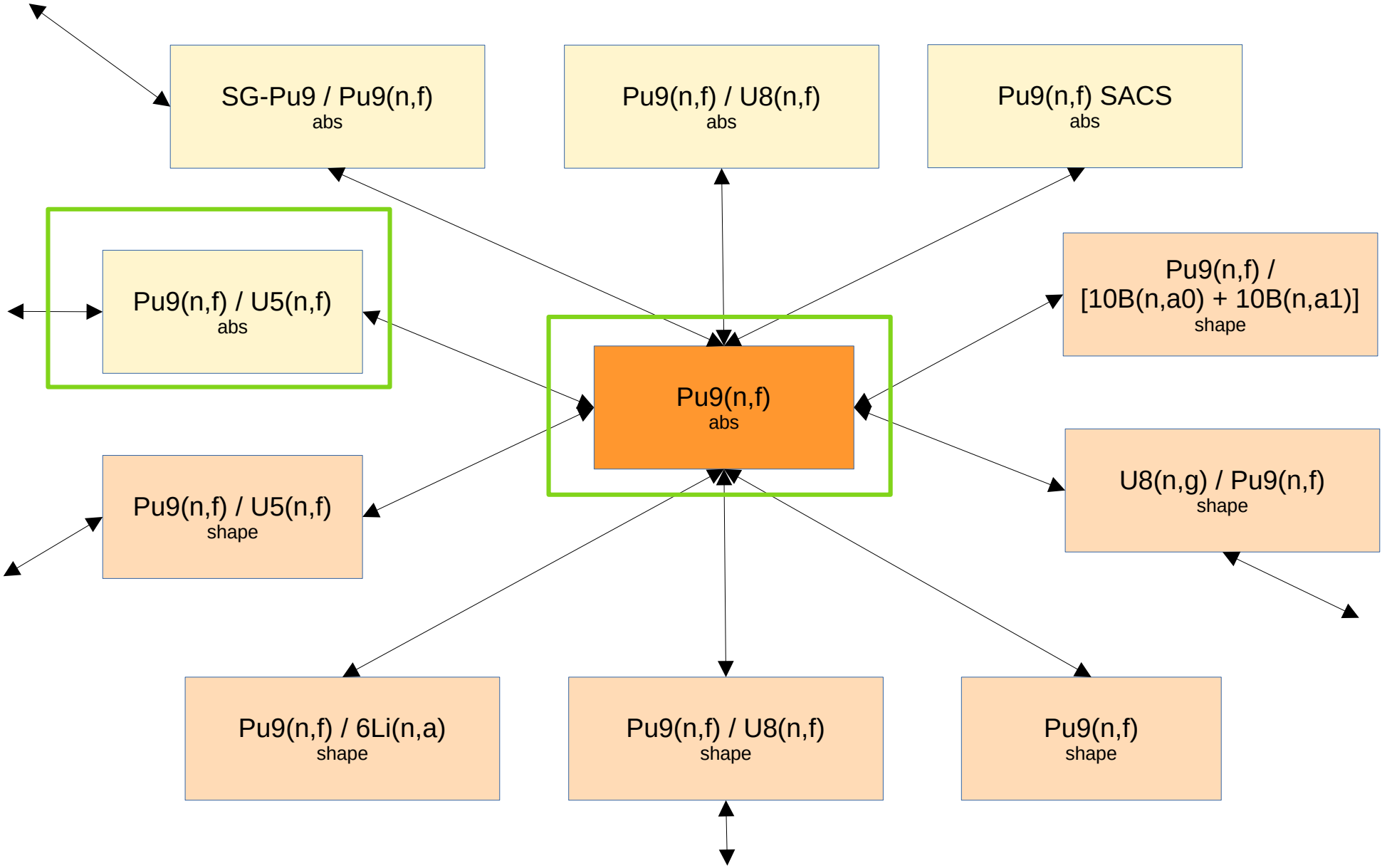
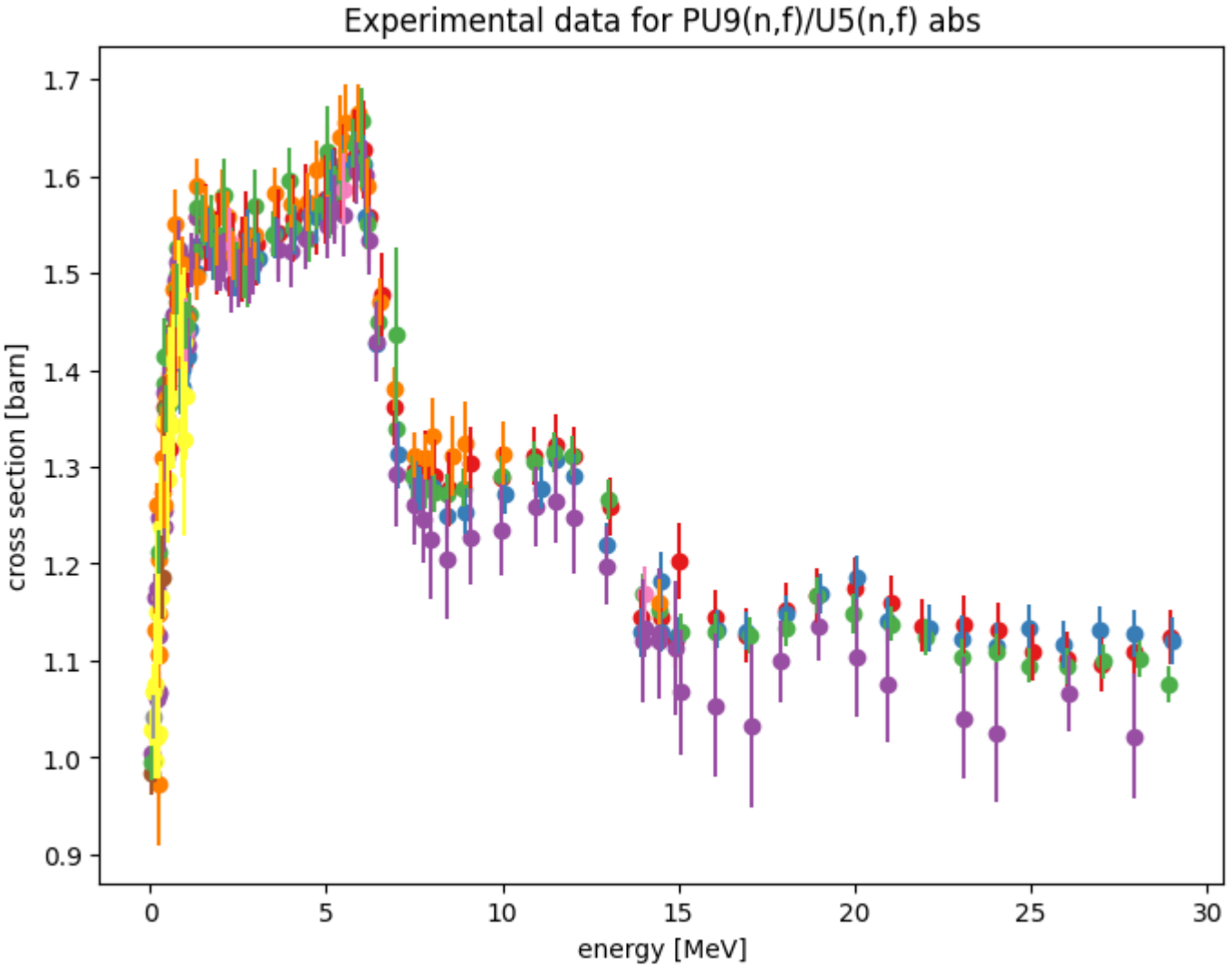


# Experiments in GMA database



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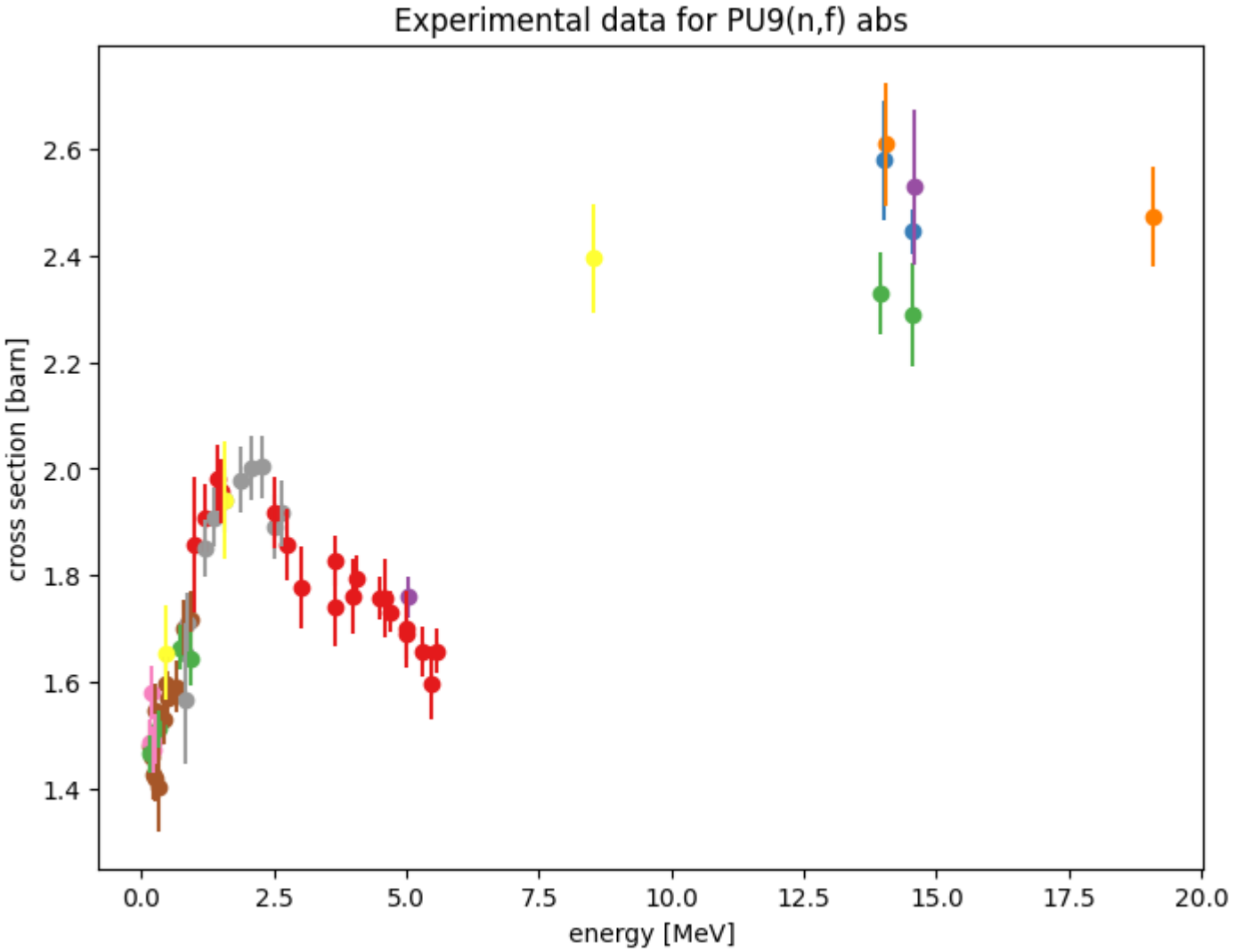

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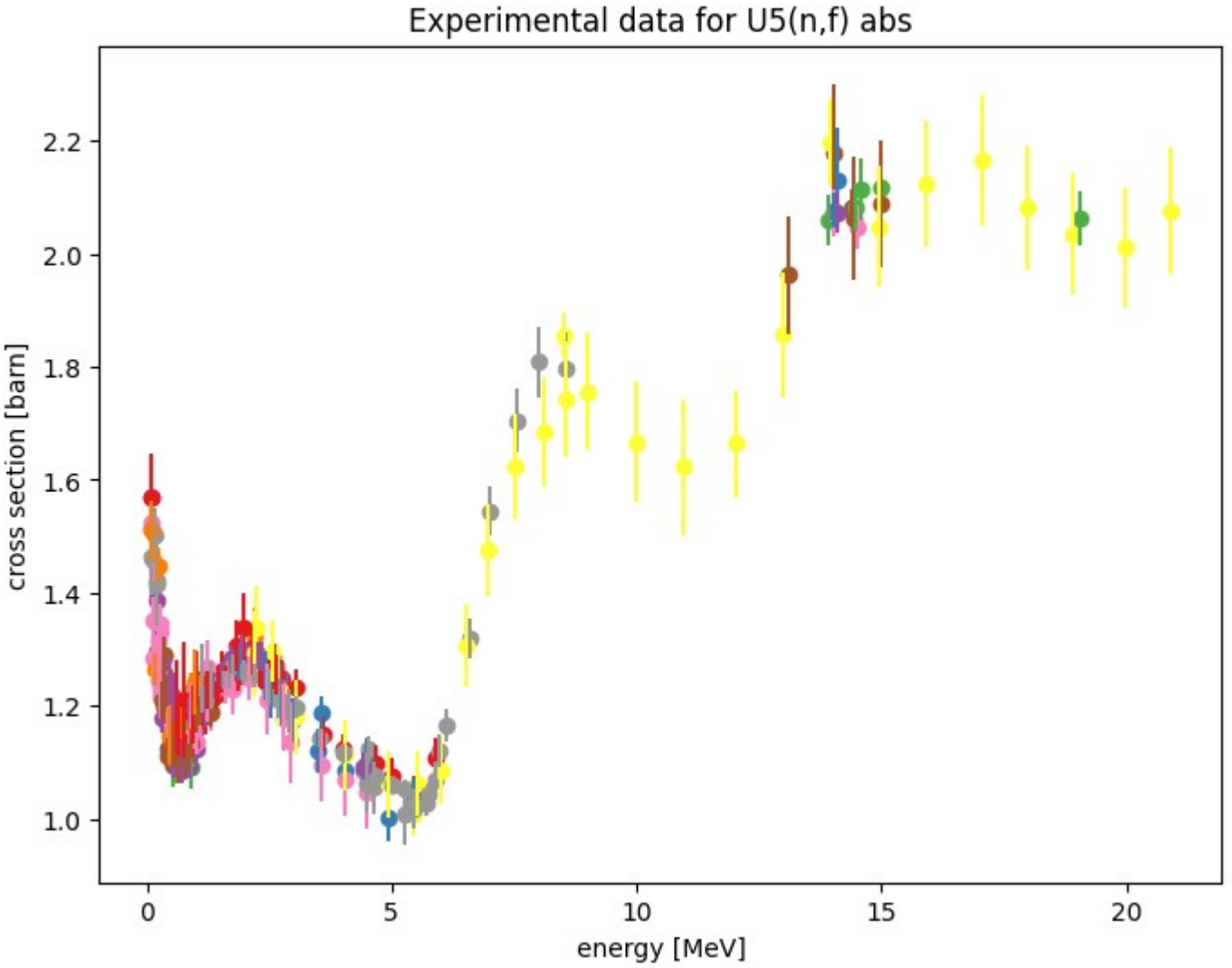
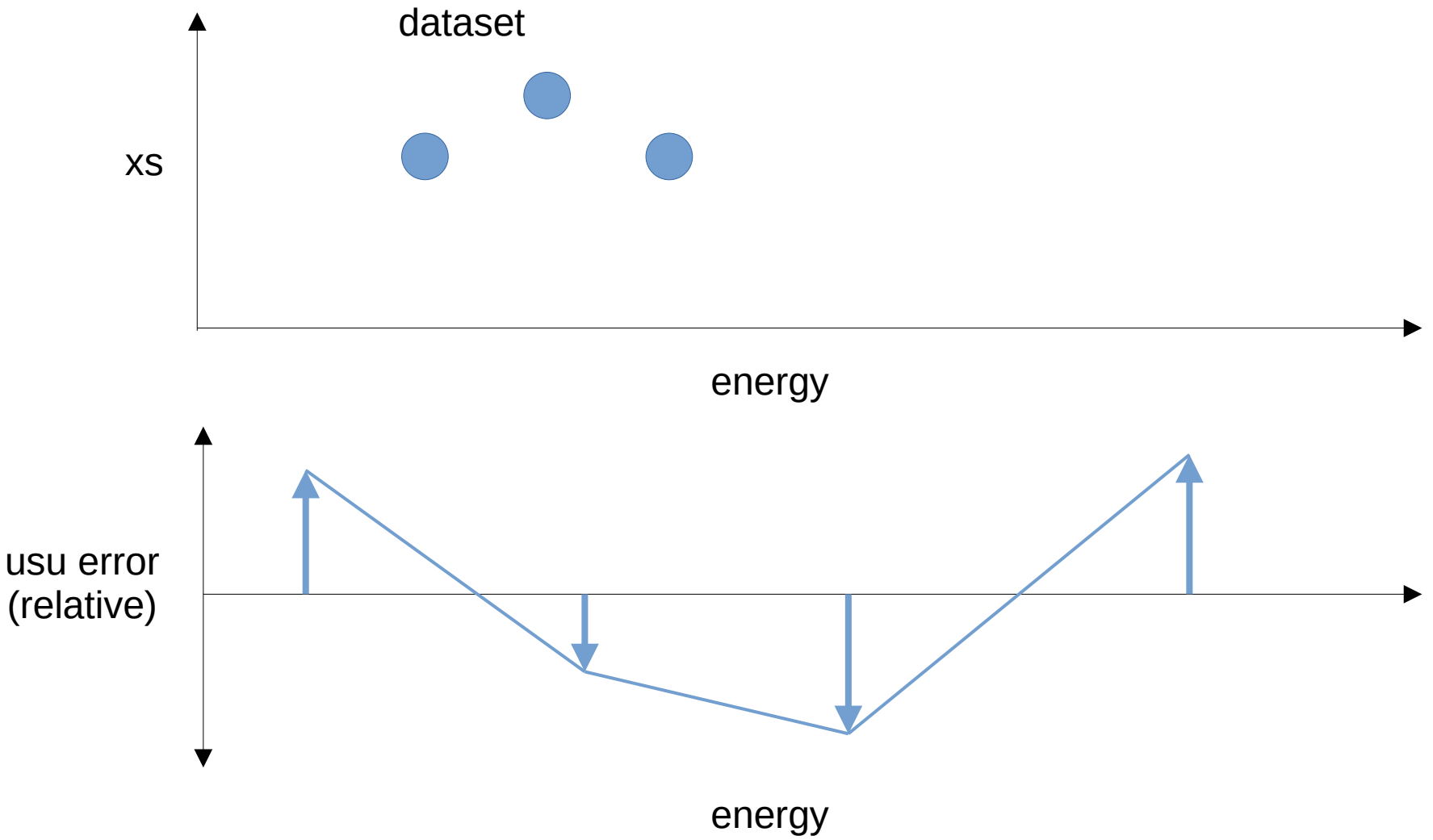


# Definition of energy dependent USU (in a nutshell)



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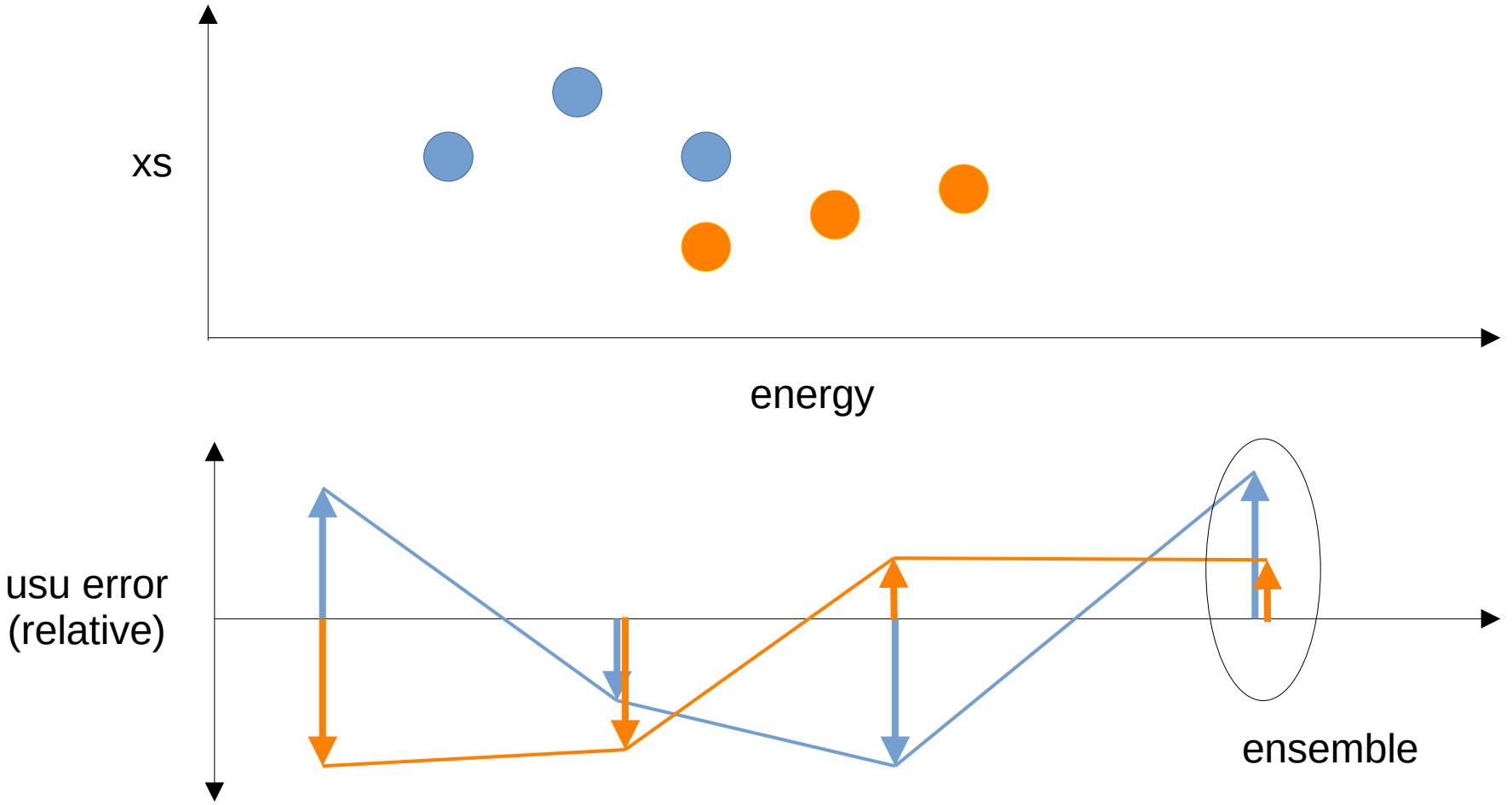



Per energy USU uncertainty can be estimated
by considering ensembles of USU errors
associated with different datasets

# Statistical model with USU

uniform prior

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

*π(USU uncertainties)*

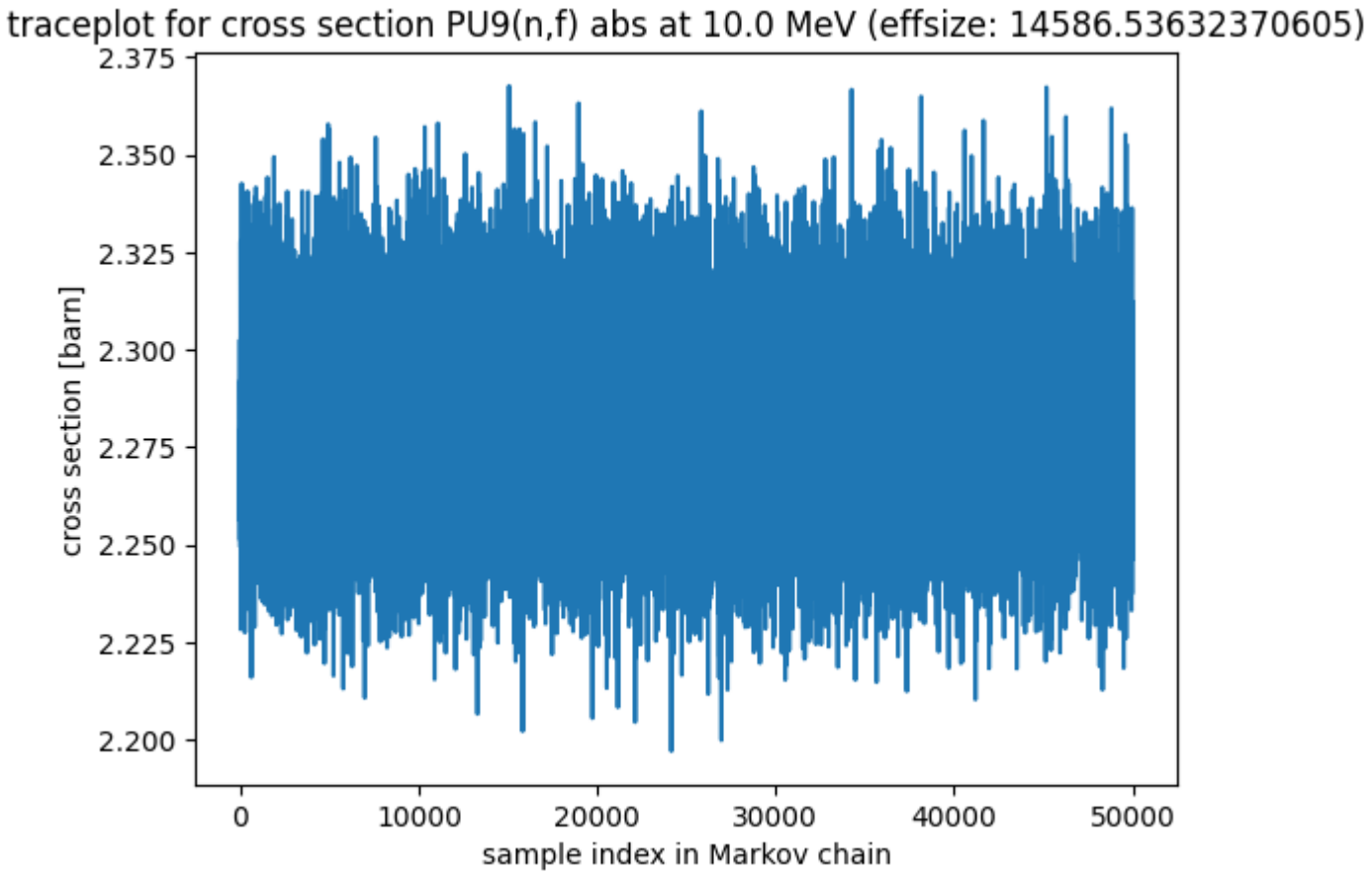
Experimental info:
multivariate normal

*Exact* (non-linear) "model"
(e.g. ratios)

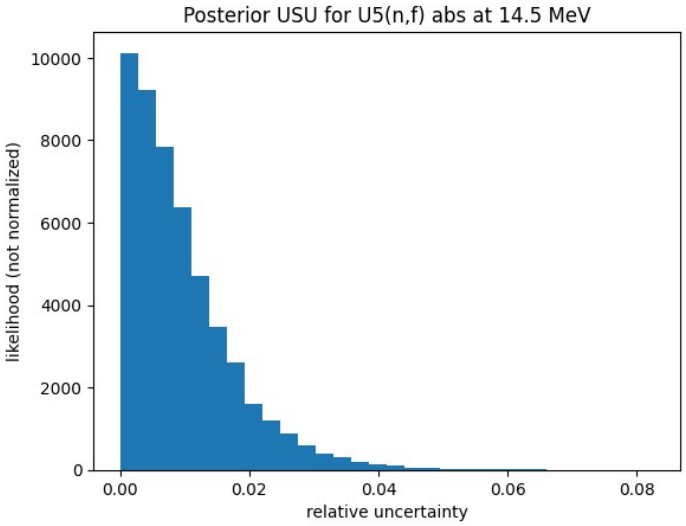
Prior:
multivariate normal

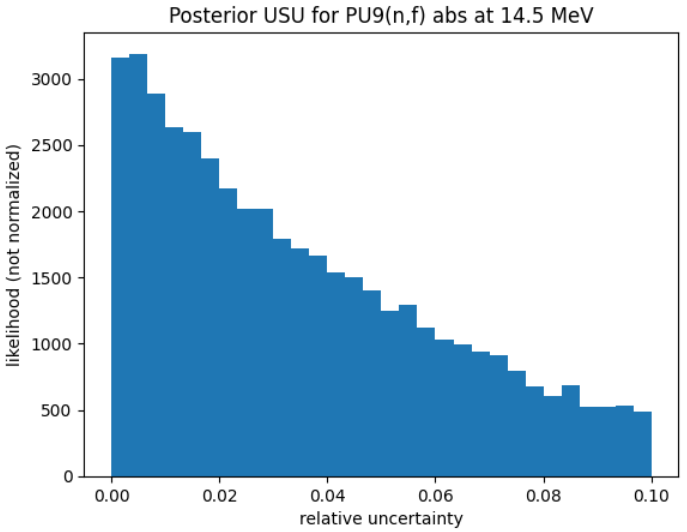
Samples from posterior by Hamilton Monte Carlo

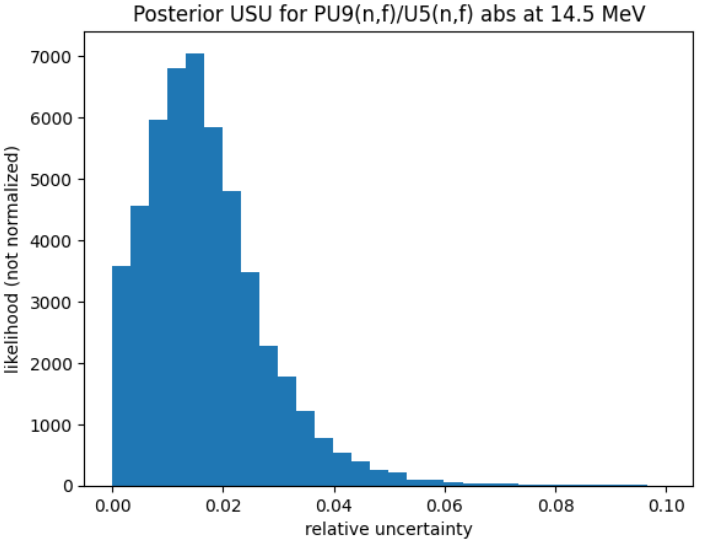
# Convergence of Markov chain



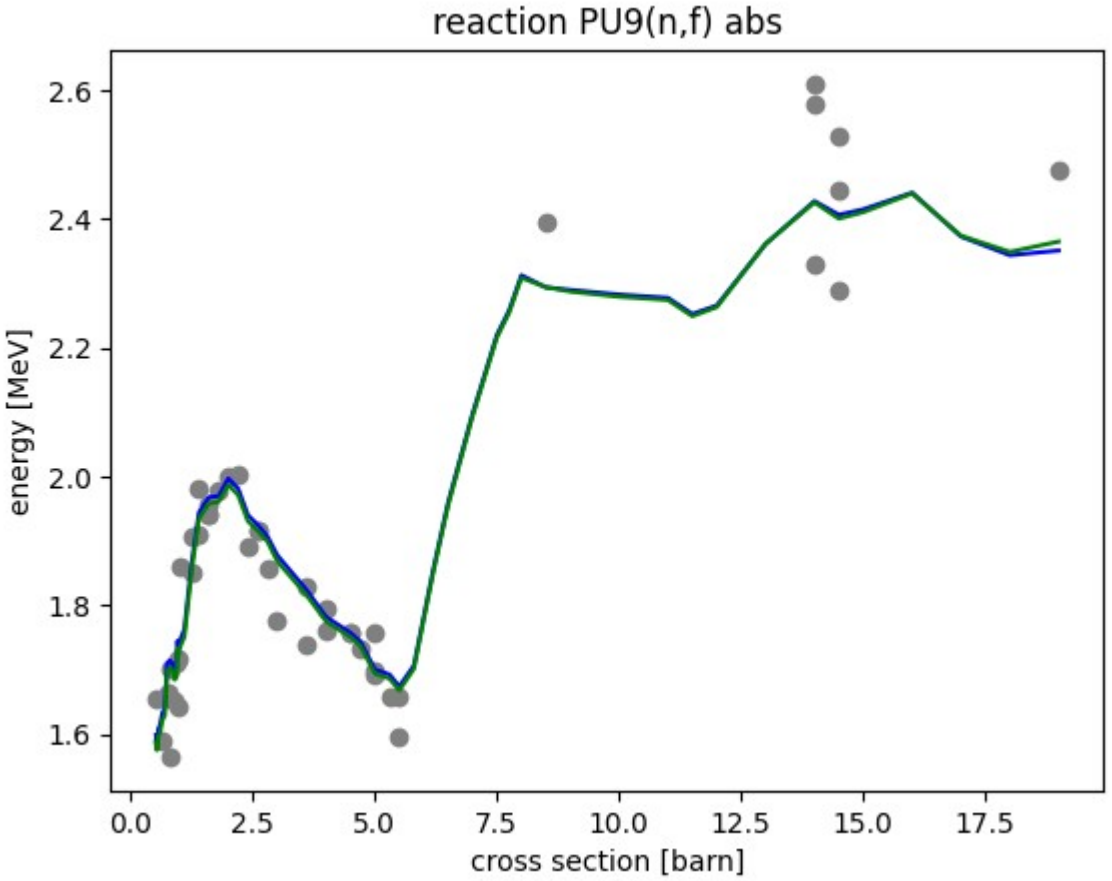
# Is USU present?



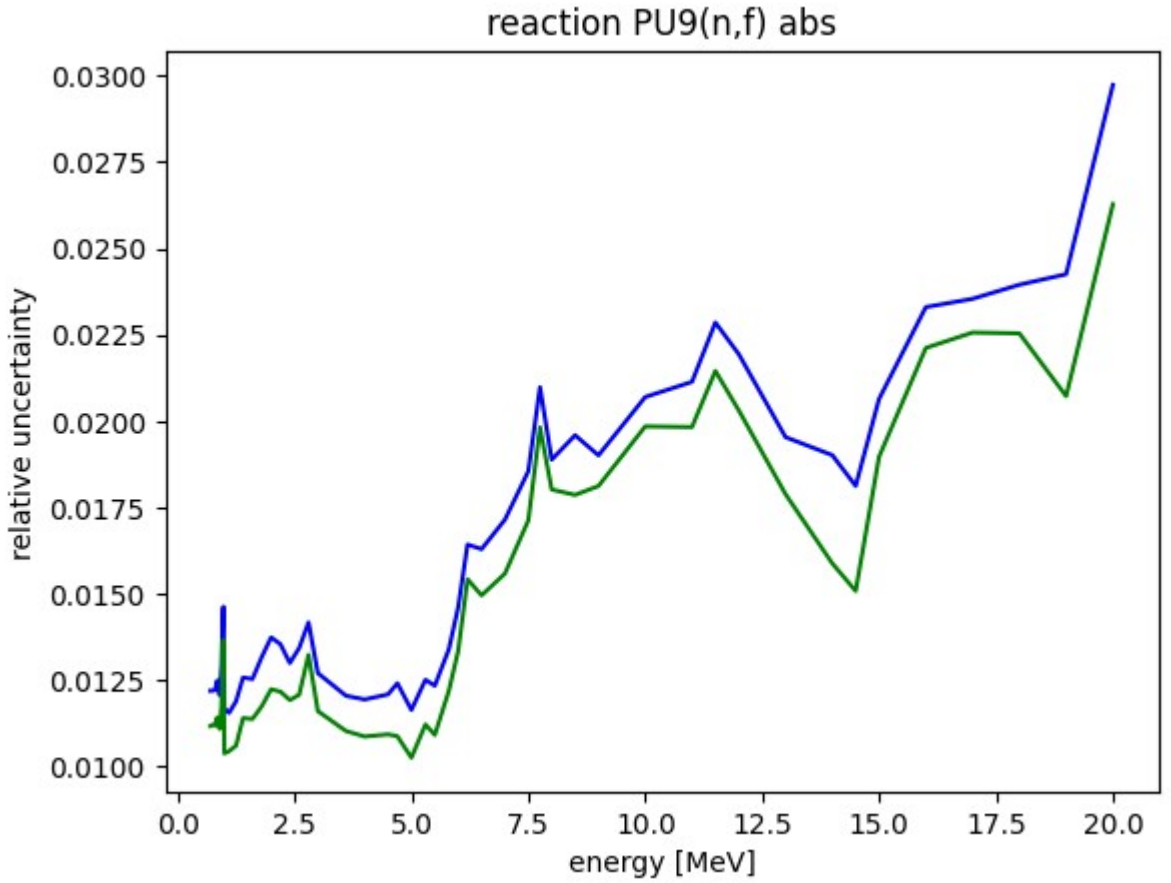



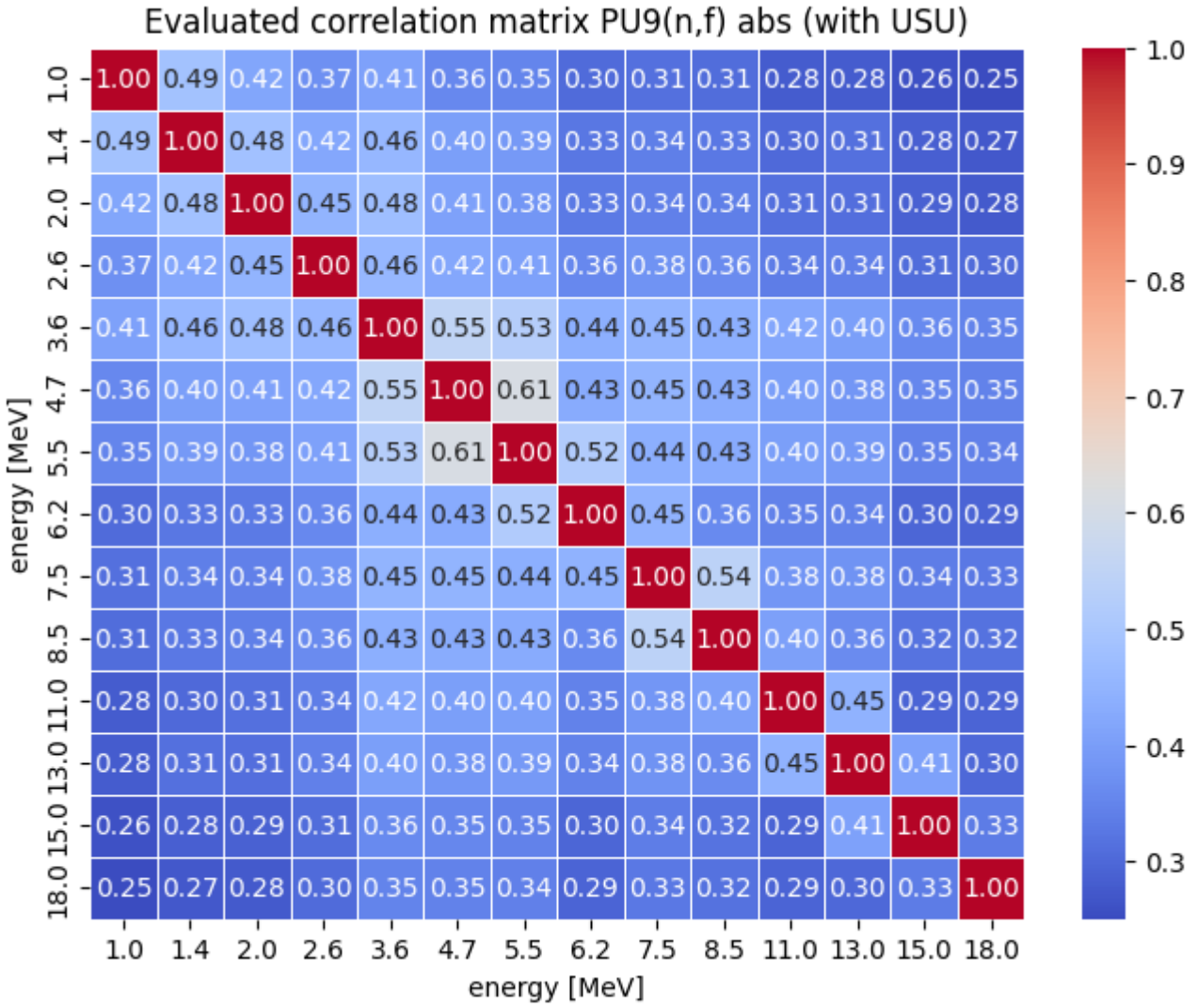
# Impact of USU on cross section evaluation



# Impact of USU on evaluated cross section uncertainty



# Correlation matrix



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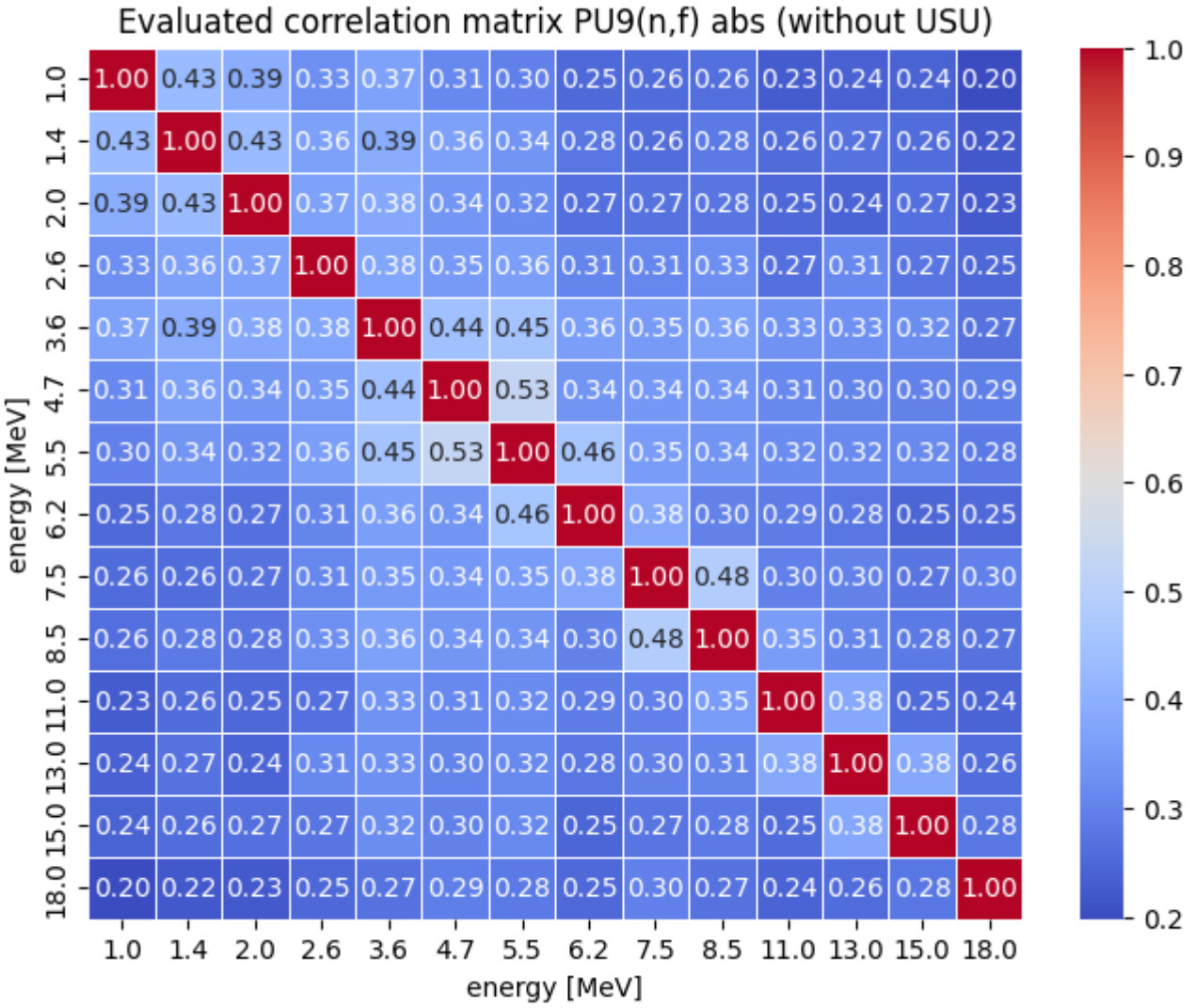


# How to update the covariance matrix of existing evaluation?

# Multivariate normal distribution (MVN)

$$\rho(\vec{x}) = \frac{1}{\sqrt{(2\pi)^N |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T \boldsymbol{\Sigma}^{-1}(\vec{x}-\vec{\mu})\right)$$

**center vector**
(evaluated cross sections)

**covariance matrix**

Evaluation process gives us consistent **μ** and **Σ**

# Multivariate normal distribution (MVN)

$$\rho(\vec{x}) = \frac{1}{\sqrt{(2\pi)^N |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T \boldsymbol{\Sigma}^{-1}(\vec{x}-\vec{\mu})\right)$$

**center vector**
(evaluated cross sections)

**covariance matrix**

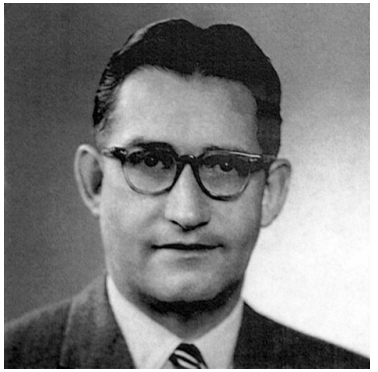
How to change **Σ** if we want our evaluation be based on different **μ'**?

# Kullback-Leibler Divergence

Solomon Kullback

KL divergence for continuous distributions:

$$D_{\mathrm{KL}}(P \parallel Q) = \int_{\mathcal{X}} \log\left(\frac{P(dx)}{Q(dx)}\right) P(dx),$$



Richard Leibler

"Distance" between two distributions

KL divergence = 0: distributions are identical

Specialized to case of two MVN distributions:

$$D_{\mathrm{KL}}(\mathcal{N}_0 \parallel \mathcal{N}_1) = \frac{1}{2}\left\{\operatorname{tr}\left(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0\right) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^{\mathrm{T}}\boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \ln\frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}\right\},$$

# Nuclear data case

$$\mathcal{N}\left(\vec{\mu}_{eval}, \boldsymbol{\Sigma}_{eval}\right)$$

$$\mathcal{N}\left(\vec{\mu}_{lib}, \boldsymbol{\Sigma}_{lib}\right)$$

Adjust $\boldsymbol{\Sigma}_{lib}$ to make distributions as similar as possible measured by KL divergence

# Nuclear data case

$$\mathcal{N}\left(\vec{\mu}_{eval}, \boldsymbol{\Sigma}_{eval}\right)$$

$$\mathcal{N}\left(\vec{\mu}_{lib}, \boldsymbol{\Sigma}_{lib}\right)$$

Adjust $\boldsymbol{\Sigma}_{lib}$ to make distributions as similar as possible measured by KL divergence

$$\boldsymbol{\Sigma}_{lib} = \boldsymbol{\Sigma}_{eval} + \vec{\mu}_{eval}\vec{\mu}_{eval}^{T} - \vec{\mu}_{eval}\vec{\mu}_{lib}^{T} - \vec{\mu}_{lib}\vec{\mu}_{eval}^{T} + \vec{\mu}_{lib}\vec{\mu}_{lib}^{T}$$

# Summary and outlook

- Estimation of Pu9(n,f) covariance matrix using MCMC and incorporating the assumption of unknown energy-dependent USU uncertainties
- Evaluation performed with Python package gmapy
- (Very near-term) Plan: Adjust obtained covariance matrix using KL divergence and evaluated cross section from STD2017