



IAEA

60 Years

Atoms for Peace and Development

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

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CSEWG Meeting

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Outline

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

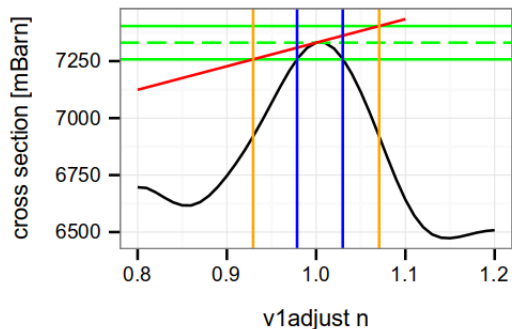
GMAP

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

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)

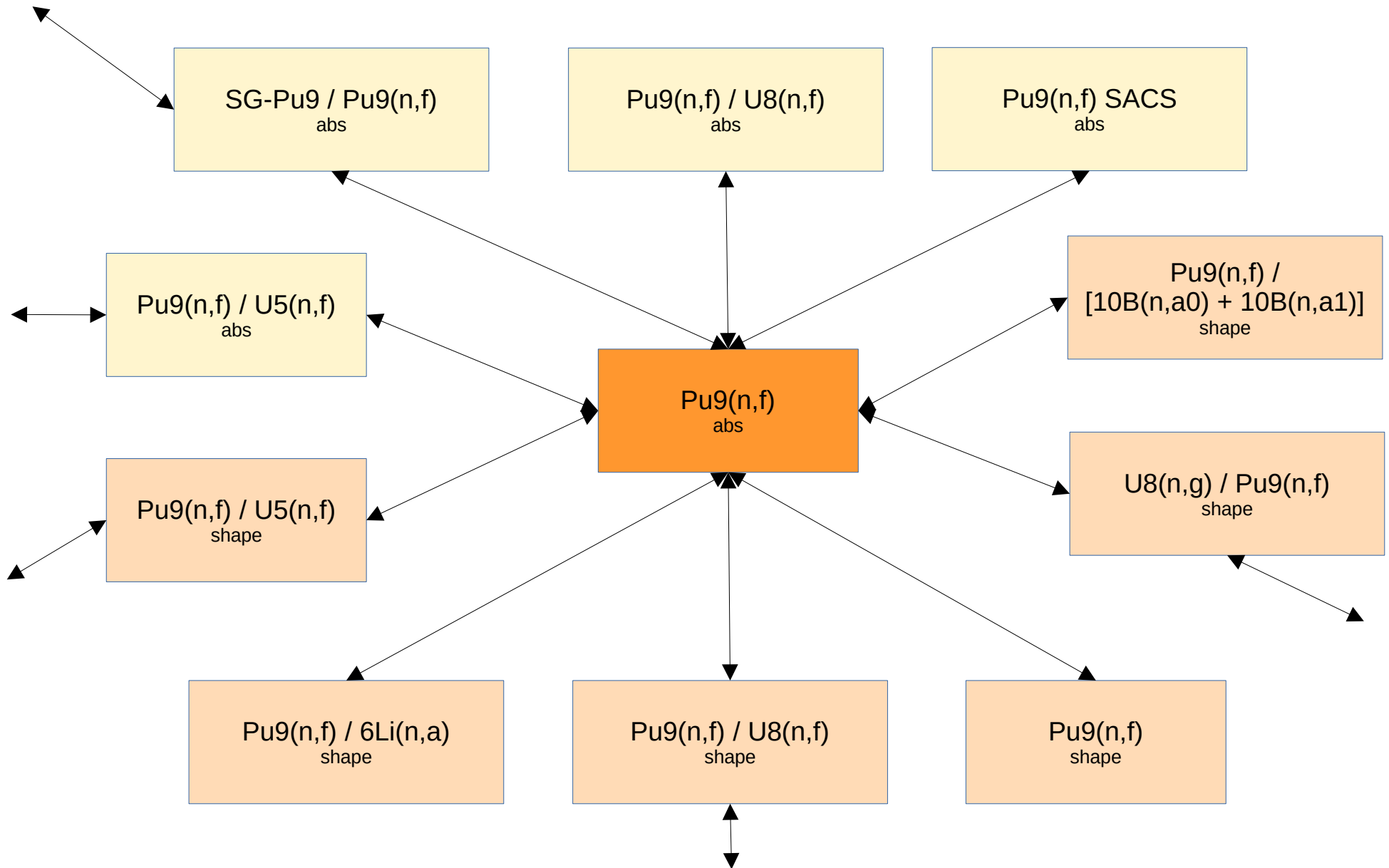
Probabilistic programming

- **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

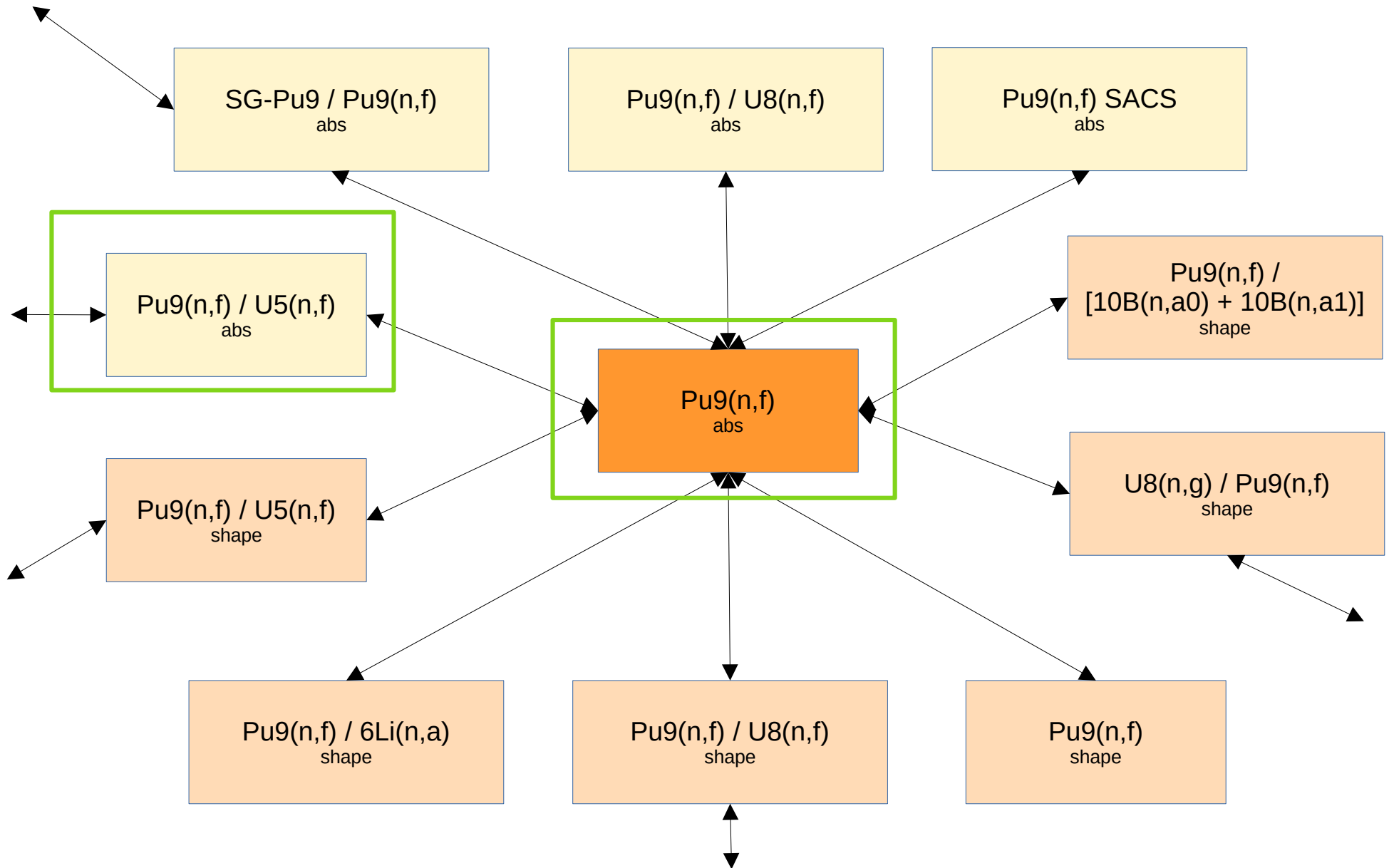
A screenshot of the GitHub repository page for 'IAEA-NDS/gmapy'. The page shows the repository name, a 'Public' badge, and navigation tabs for Code, Issues, Pull requests, Actions, Projects, Security, and Insights. Below the navigation, there are buttons for 'Go to file' and 'Code'. The main content area displays a commit history table with columns for commit message, commit ID, date, and number of commits. The most recent commit is by 'gschnabel' with the message 'fix one unittest for MCMC', commit ID '1afed81', dated 'Mar 23', and '1,281 commits'. Below the commit history, there is a list of files and folders in the repository, including 'docs', 'examples', 'gmapy', 'legacy-tests', 'tests', '.gitignore', 'DOCUMENTATION.md', 'LICENSE', 'README.md', 'environment.yml', 'poetry.lock', and 'pyproject.toml'. Each file entry includes a brief description of the file's content and the date of its last commit.

Commit Message	Commit ID	Date	Commits
gschnabel fix one unittest for MCMC	1afed81	Mar 23	1,281
docs			last year
examples			9 months ago
gmapy			8 months ago
legacy-tests			last year
tests			8 months ago
.gitignore			last year
DOCUMENTATION.md			last year
LICENSE			last year
README.md			last year
environment.yml			last year
poetry.lock			last year
pyproject.toml			8 months ago

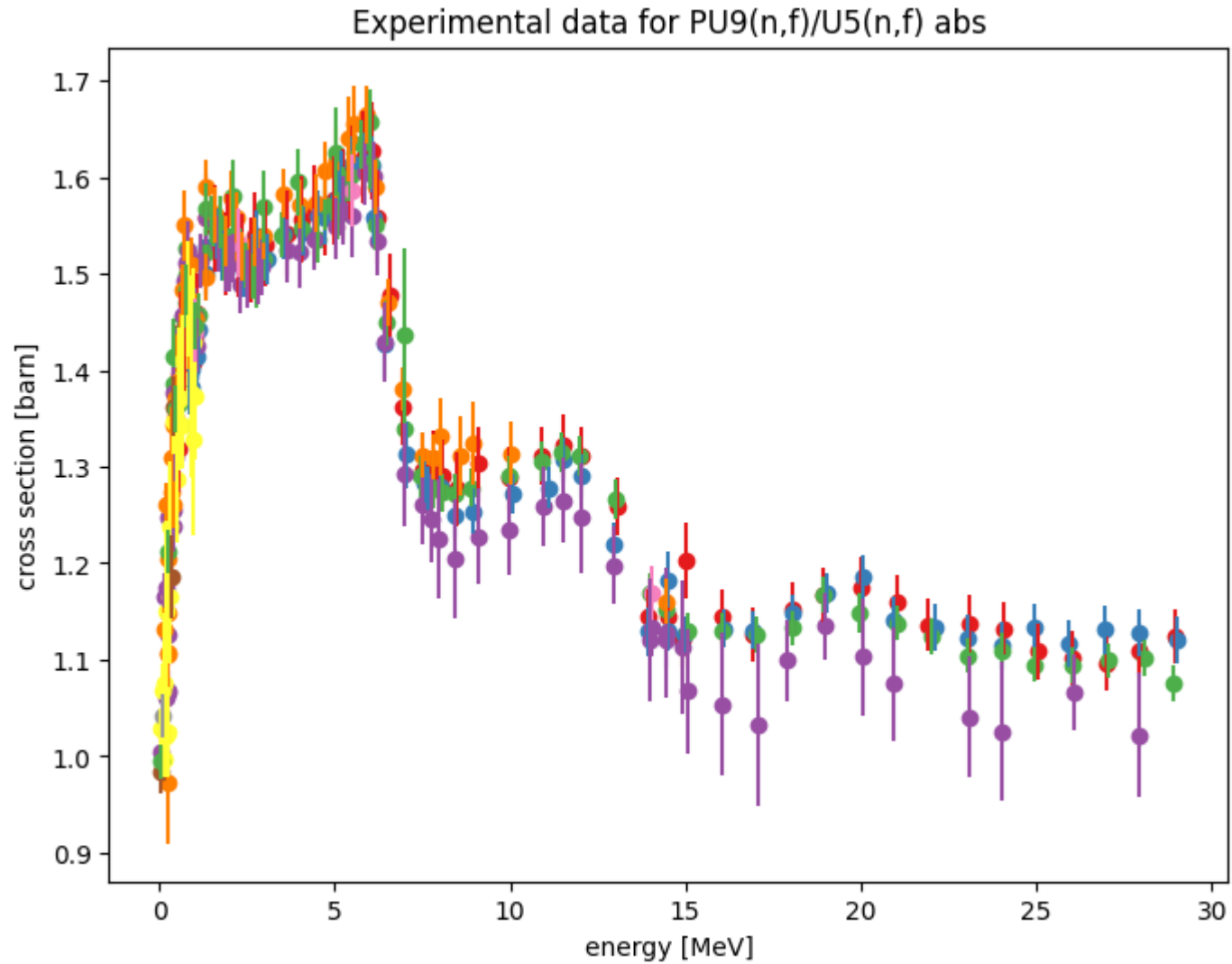
Links between observables (GMA database)



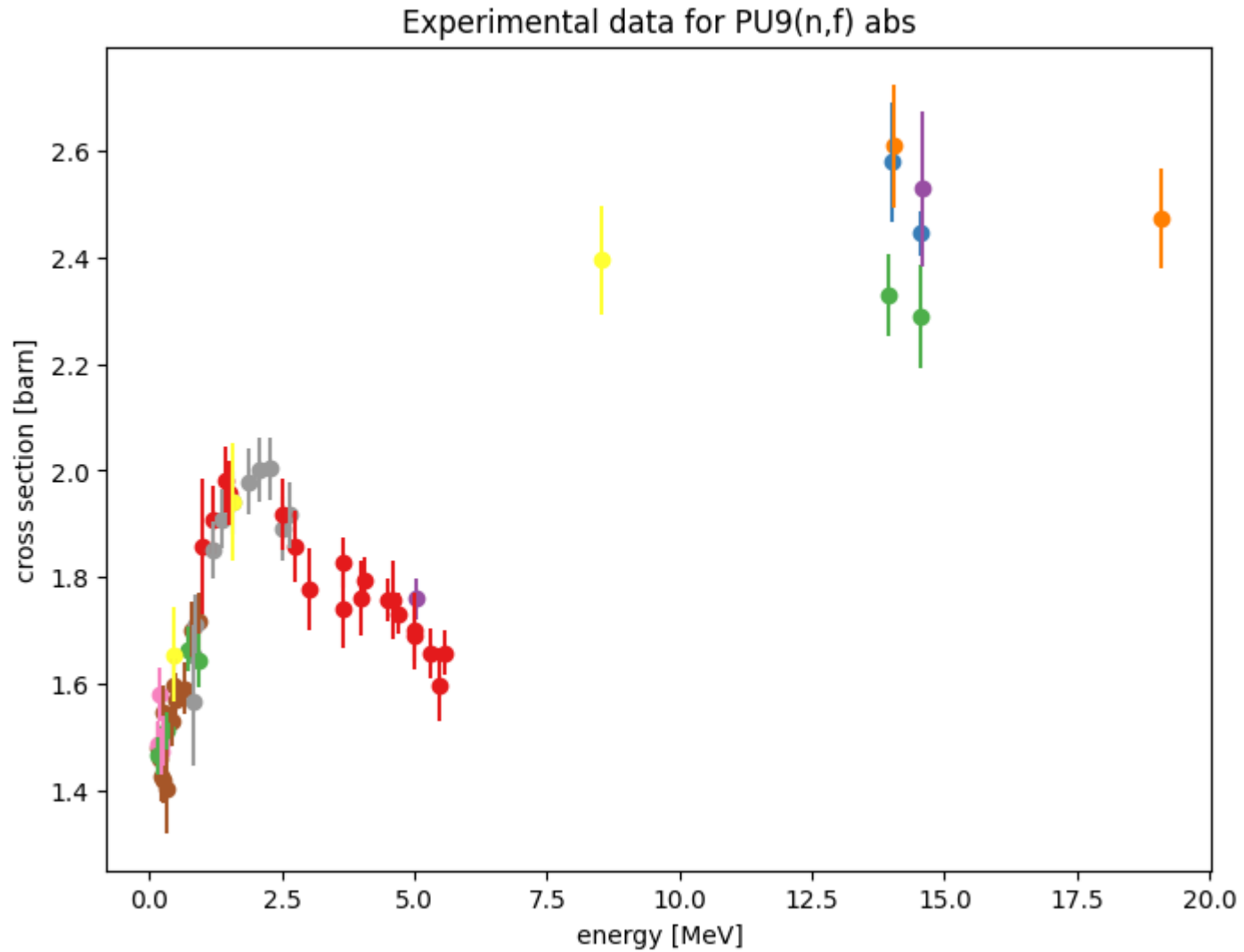
Links between observables (GMA database)



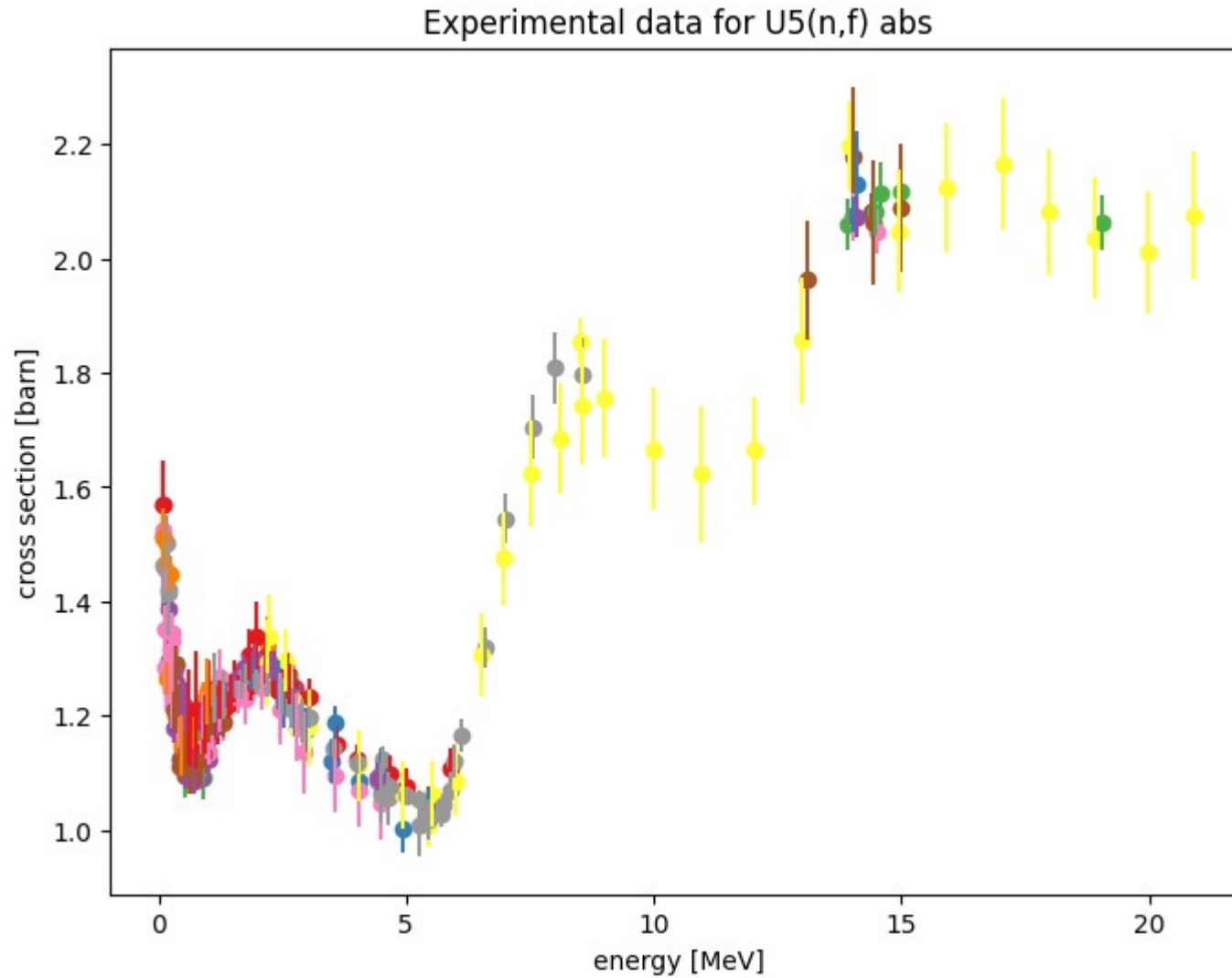
Experiments in GMA database



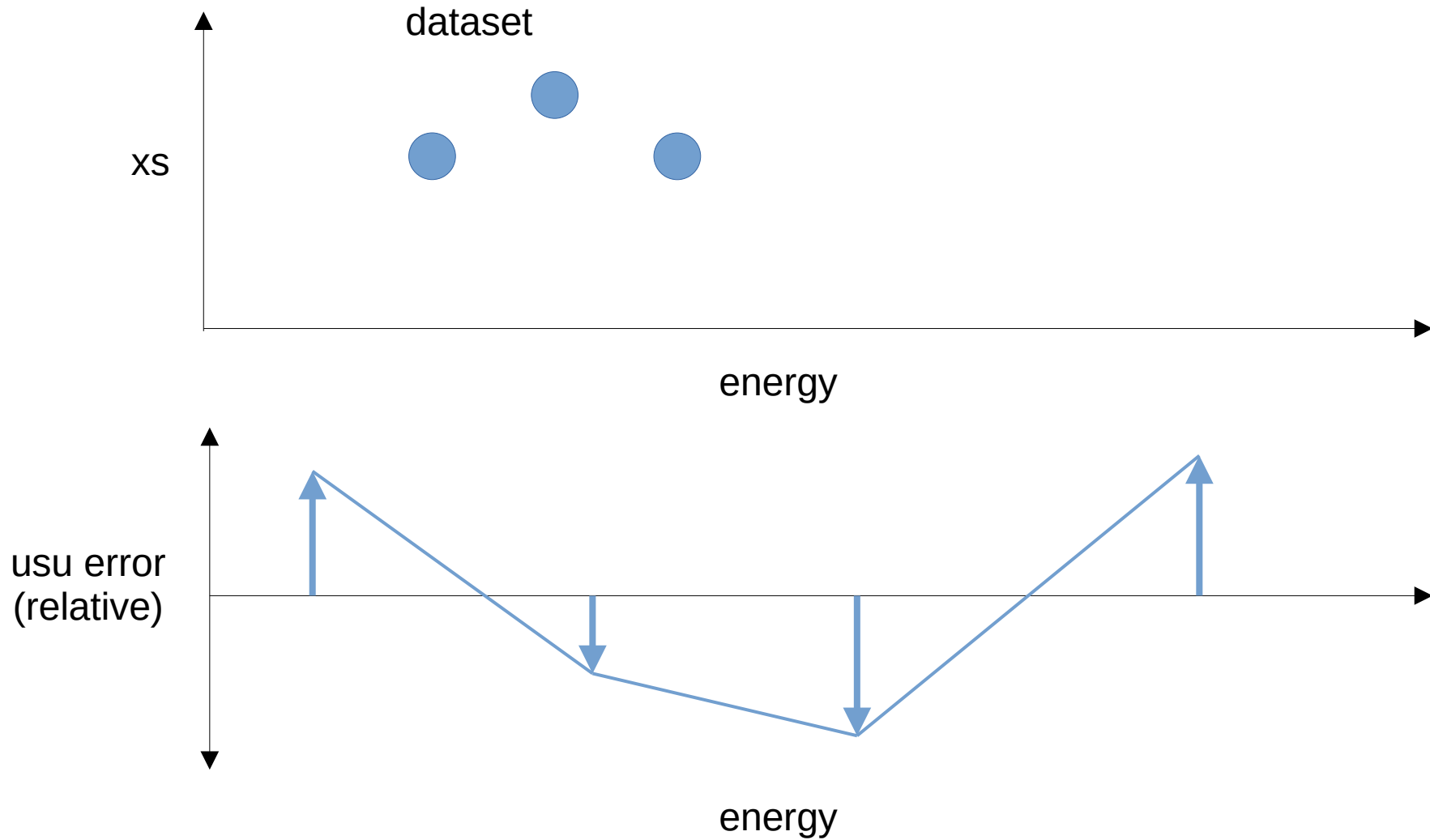
Experiments in GMA database



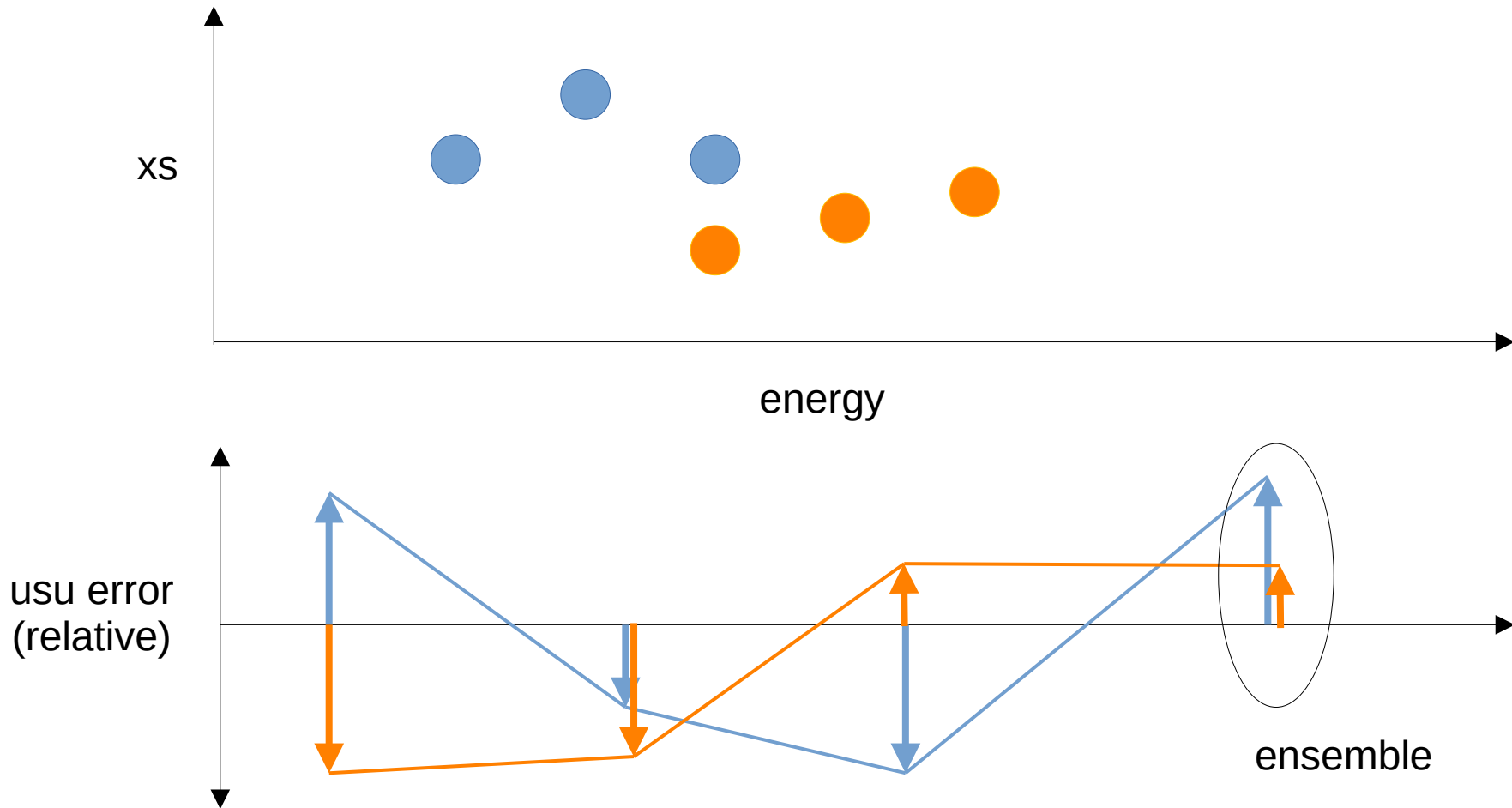
Experiments in GMA database



Definition of energy dependent USU (in a nutshell)



Definition of energy dependent USU (in a nutshell)



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

Statistical model with USU

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

Experimental info:
multivariate normal

Exact (non-linear) “model”
(e.g. ratios)

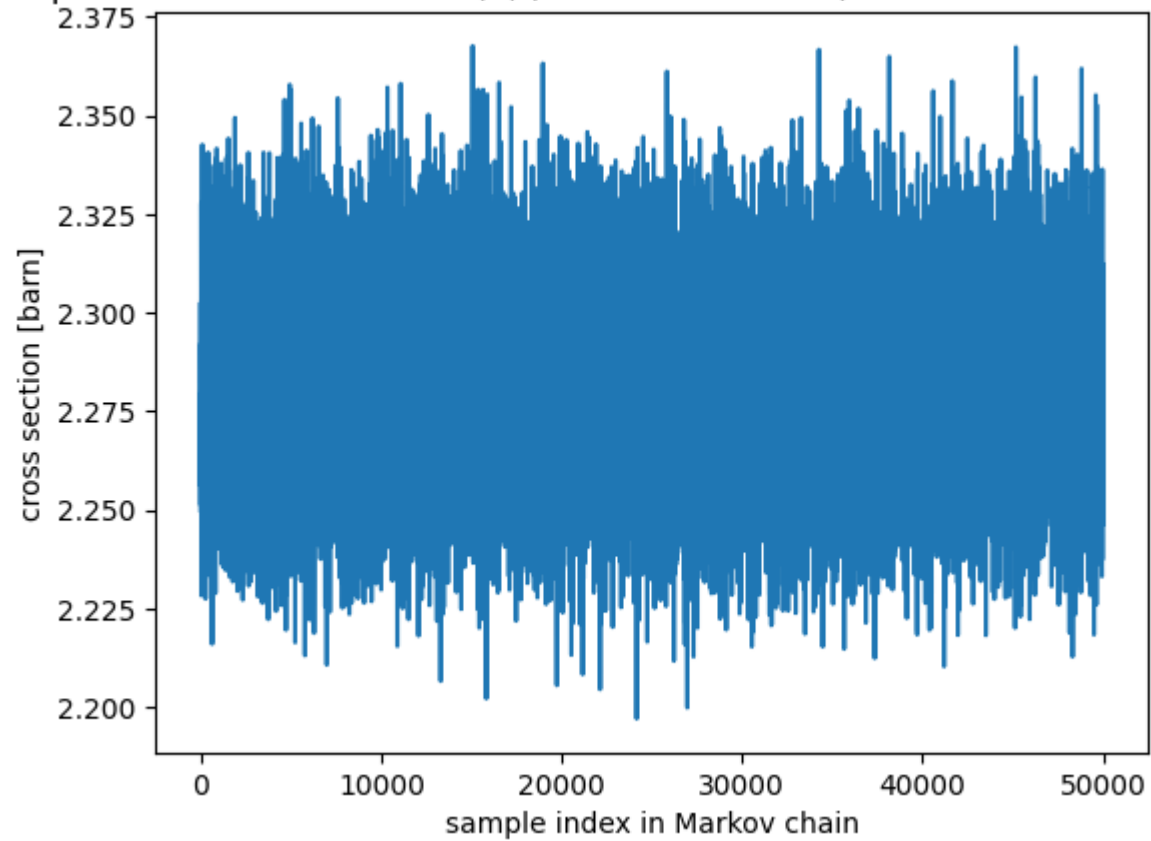
Prior:
multivariate normal

uniform prior

Samples from posterior by Hamilton Monte Carlo

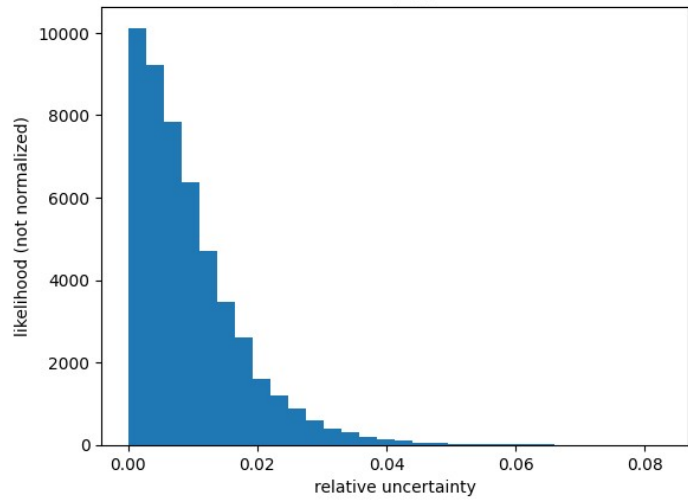
Convergence of Markov chain

traceplot for cross section PU9(n,f) abs at 10.0 MeV (effsize: 14586.53632370605)

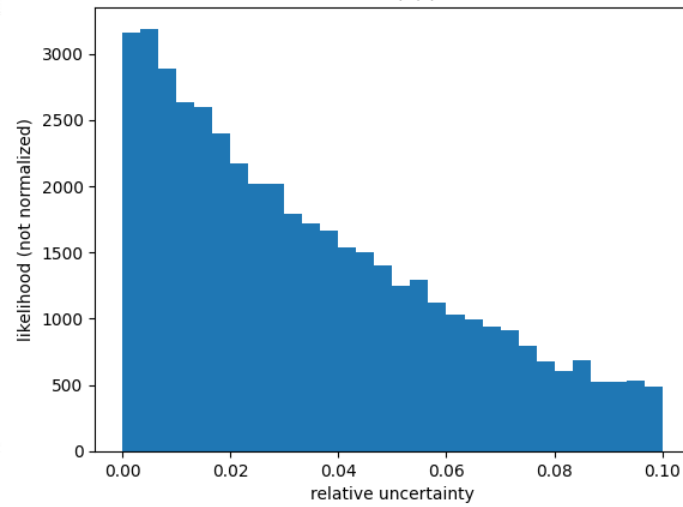


Is USU present?

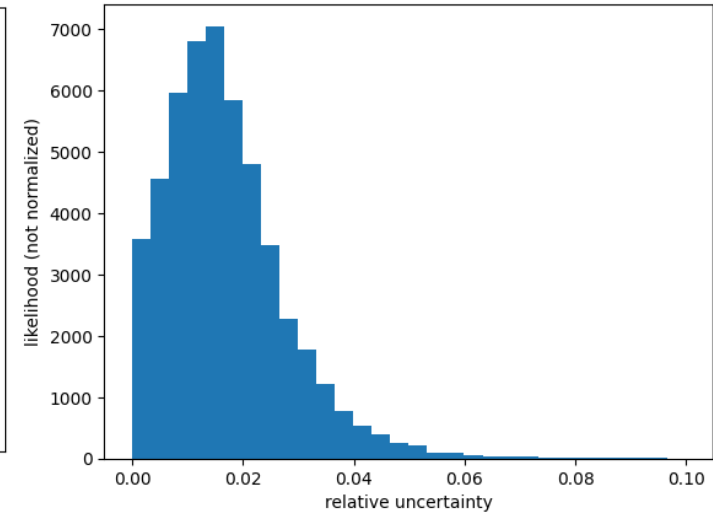
Posterior USU for U5(n,f) abs at 14.5 MeV



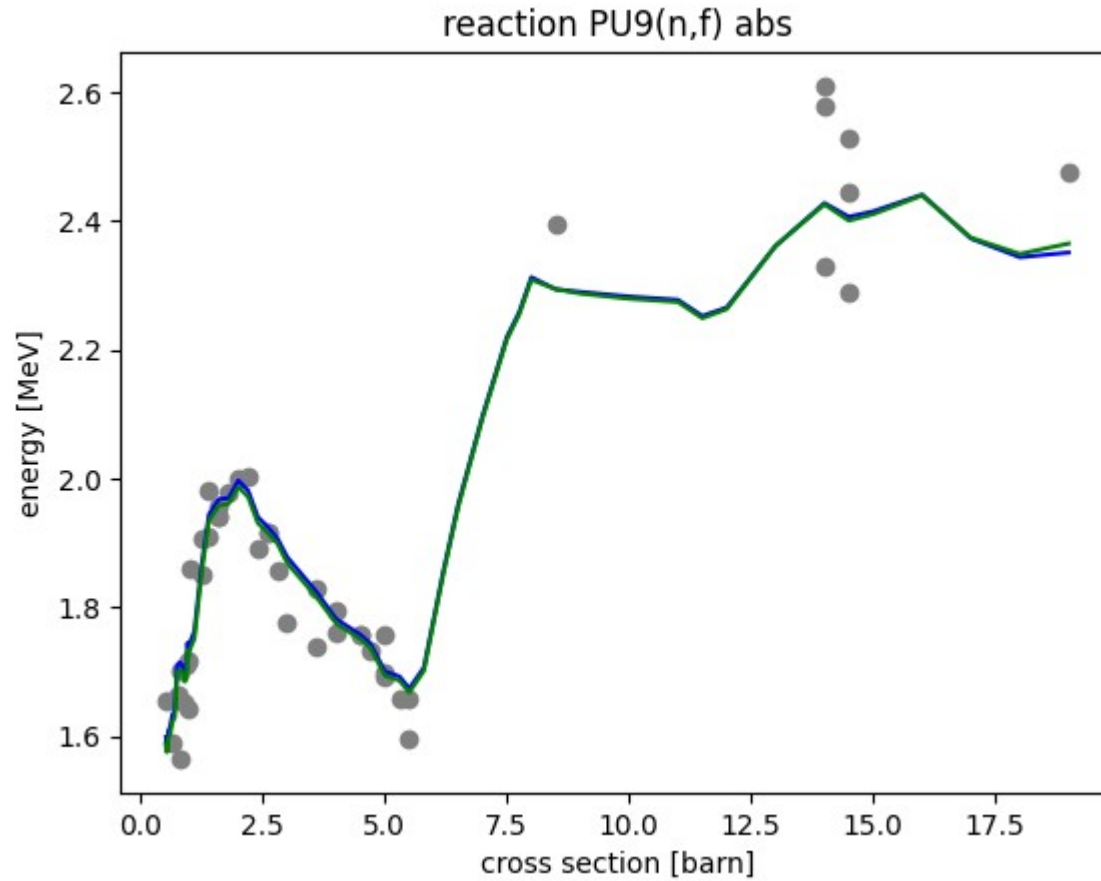
Posterior USU for PU9(n,f) abs at 14.5 MeV



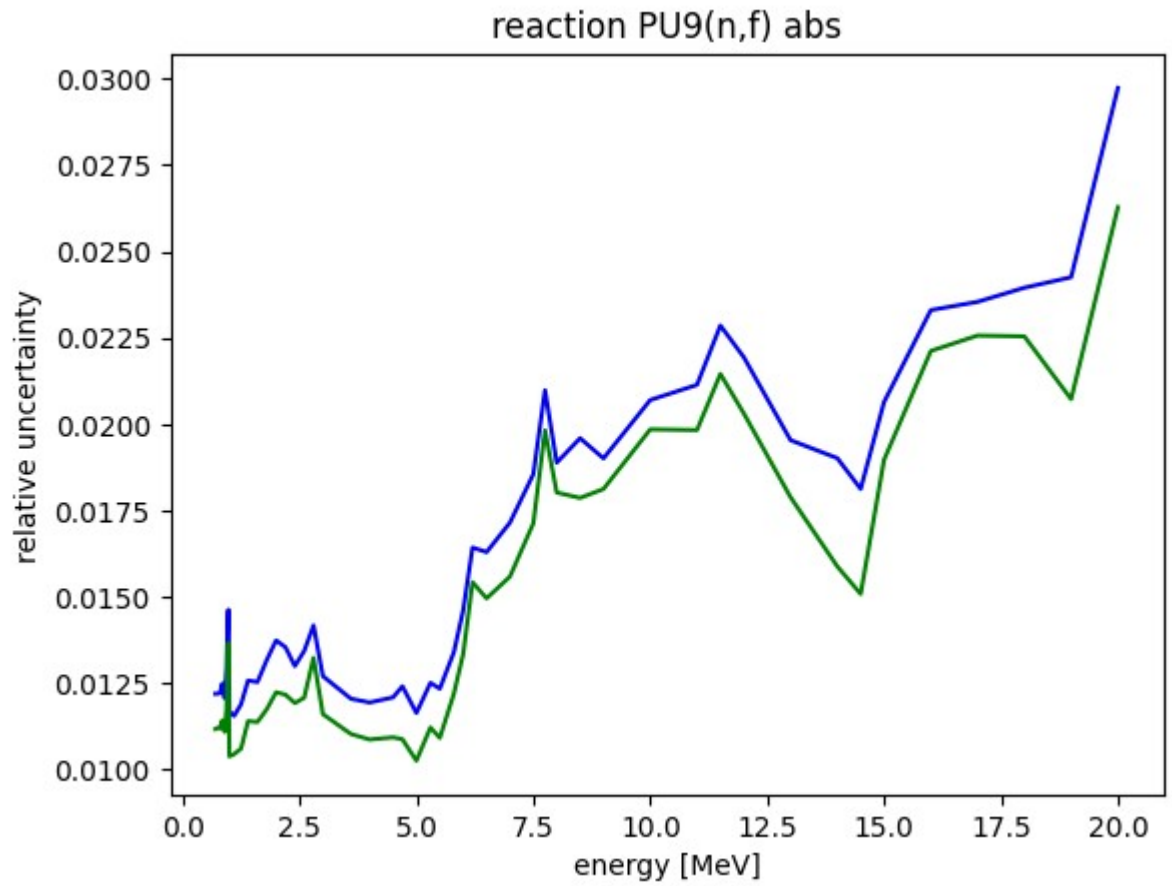
Posterior USU for PU9(n,f)/U5(n,f) abs at 14.5 MeV



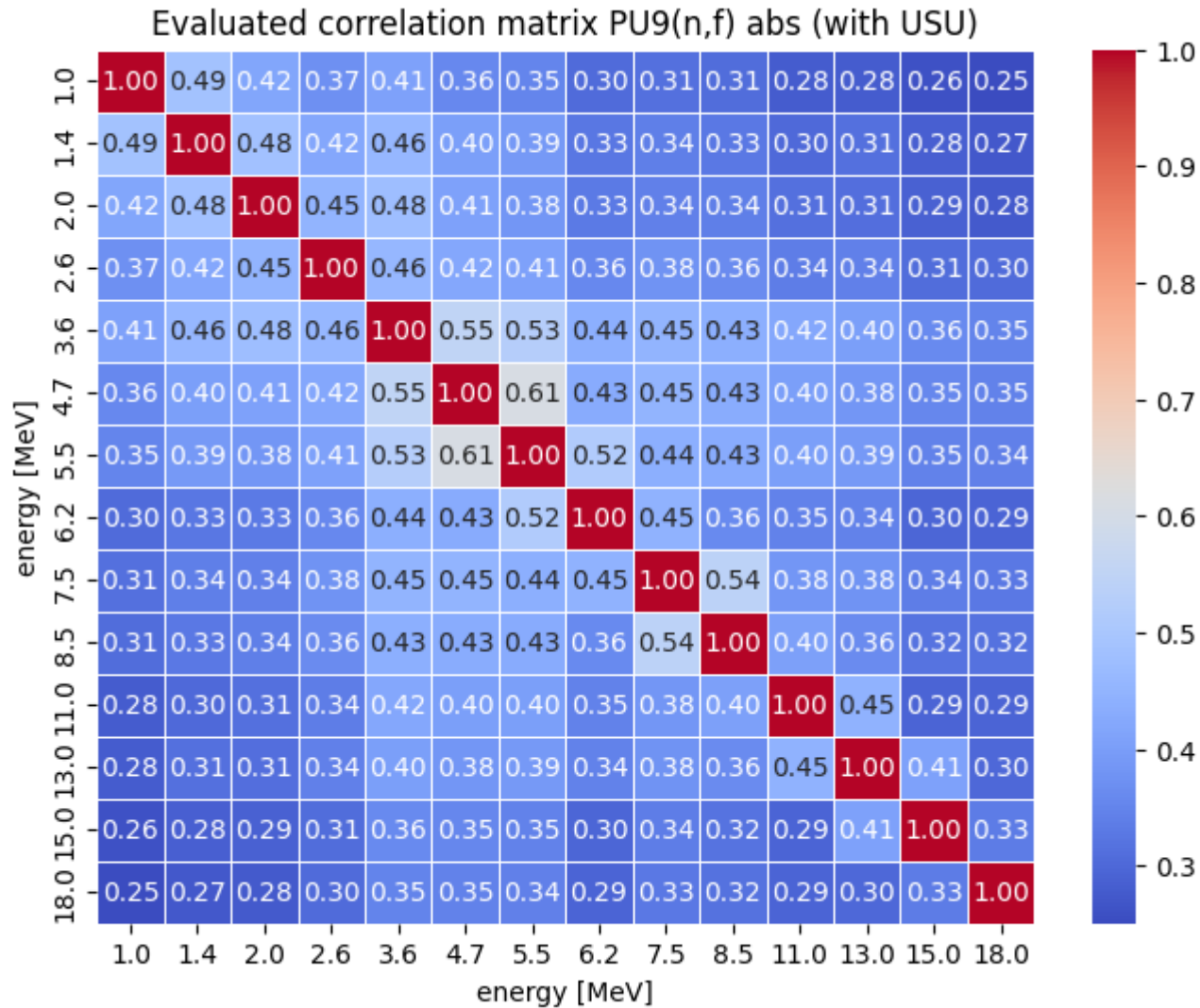
Impact of USU on cross section evaluation



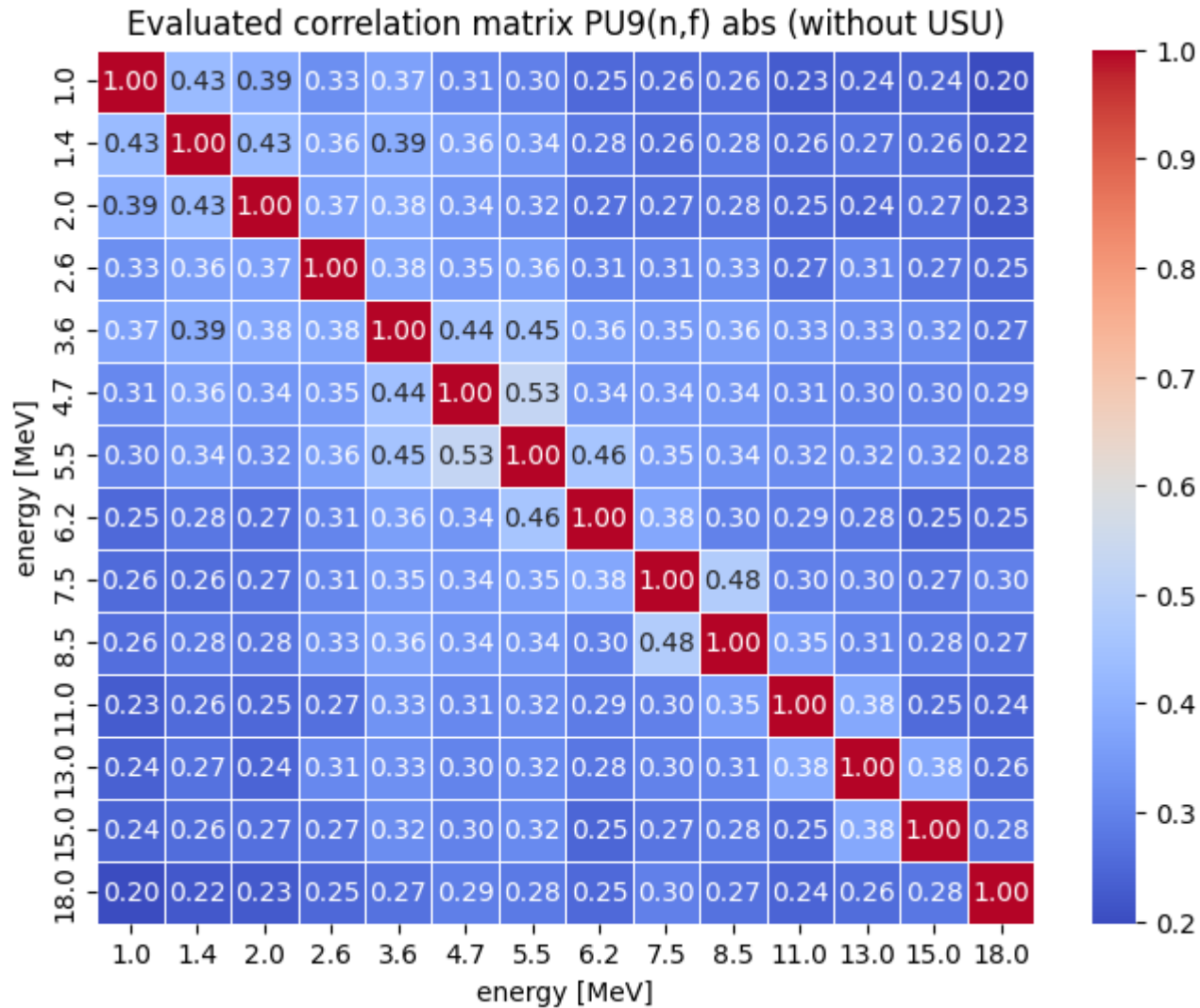
Impact of USU on evaluated cross section uncertainty



Correlation matrix



Correlation matrix



How to update the covariance matrix of existing evaluation?

Multivariate normal distribution (MVN)

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

center vector
(evaluated cross sections)

covariance matrix

Evaluation process gives us consistent μ and Σ

Multivariate normal distribution (MVN)

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

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:

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

“Distance” between two distributions

KL divergence = 0: distributions are identical

Specialized to case of two MVN distributions:

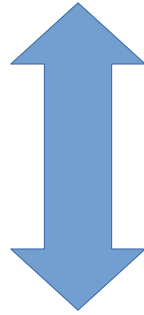
$$D_{\text{KL}}(\mathcal{N}_0 \parallel \mathcal{N}_1) = \frac{1}{2} \left\{ \text{tr}(\mathbf{\Sigma}_1^{-1} \mathbf{\Sigma}_0) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^{\text{T}} \mathbf{\Sigma}_1^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \ln \frac{|\mathbf{\Sigma}_1|}{|\mathbf{\Sigma}_0|}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



Richard Leibler

Nuclear data case

$$\mathcal{N}(\vec{\mu}_{eval}, \Sigma_{eval})$$

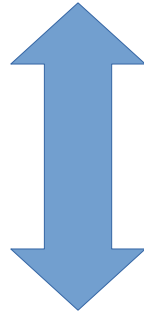


$$\mathcal{N}(\vec{\mu}_{lib}, \Sigma_{lib})$$

Adjust Σ_{lib} to make distributions as similar as possible measured by KL divergence

Nuclear data case

$$\mathcal{N}(\vec{\mu}_{eval}, \Sigma_{eval})$$



$$\mathcal{N}(\vec{\mu}_{lib}, \Sigma_{lib})$$

Adjust Σ_{lib} to make distributions as similar as possible measured by KL divergence

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

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