USU and Covariance

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NAPC-Nuclear Data Section, IAEA

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More than 40 years of GMA

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PROCEEDINGS OF THE CONFERENCE ON NUCLEAR DATA EVALUATION METHODS AND PROCEDURES

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UPTON, NEW YORK 11973
September 22-25, 1980

Conference Chairman:
R.J. Howerton
Lawrence Livermore National Laboratory

Proceedings Editors:
B.A. Magurno and S. Pearlstein
Brookhaven National Laboratory

March 1981

DATA INTERPRETATION, OBJECTIVE EVALUATION PROCEDURES AND MATHEMATICAL TECHNIQUES FOR THE EVALUATION OF ENERGY-DEPENDENT RATIO, SHAPE AND CROSS SECTION DATA*

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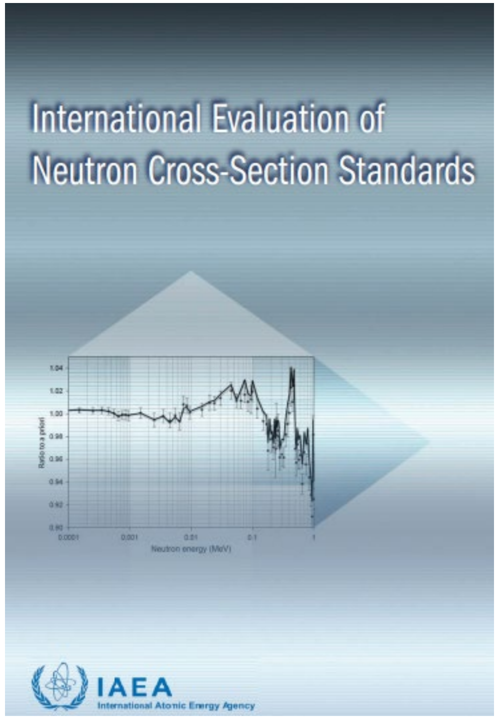
ABSTRACT

The evaluation of several energy-dependent cross sections which are of importance for practical applications is considered. The evaluation process is defined as the procedure which is used to derive the best knowledge of these cross sections based on the available direct experimental data information, and, using theoretical models, on the auxiliary data base. The experimental data base represents a multiple overdetermination of the unknown cross sections with various correlations between the measured values. Obtaining the least-squares estimator is considered as the standard mathematical procedure to derive a consistent set of evaluated cross section values. Various approximations made in order to avoid the monstrous system of normal equations are considered and the feasibility of the exact solution is demonstrated. The variance - covariance of the result, its reliability and the improvements obtained in iterative steps are discussed. Finally, the inclusion of auxiliary, supplementary information is considered.



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Evaluation of the Neutron Data Standards

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Generalized Least Squares equation

Experimental Covariance Matrix

Measurements

Evaluation

$$\vec{\sigma}_{\text{std}} - \vec{\sigma}_{\text{ref}} = \left(\mathbf{S}^T \mathbf{\Sigma}_{\text{exp}}^{-1} \mathbf{S}\right)^{-1} \mathbf{S}^T \mathbf{\Sigma}_{\text{exp}}^{-1} (\vec{d} - \vec{d}_{\text{ref}})$$

Sensitivity matrix

$$\vec{d}_{\text{ref}} = f(\vec{\sigma}_{\text{ref}})$$

Underlying statistical model

$$\vec{d} \sim \mathcal{N}\left(f(\vec{\sigma}_{\text{true}}), \mathbf{\Sigma}_{\text{exp}}\right)$$

$$\rho(\vec{d}\,|\,\vec{\sigma}_{\text{true}}) = \frac{1}{\sqrt{(2\pi)^N \det(\mathbf{\Sigma}_{\text{exp}})}} \exp\left(-\frac{1}{2}(\vec{d} - f(\vec{\sigma}_{\text{true}}))^T \mathbf{\Sigma}_{\text{exp}}^{-1} (\vec{d} - f(\vec{\sigma}_{\text{true}}))\right)$$

How to estimate the "truth"?

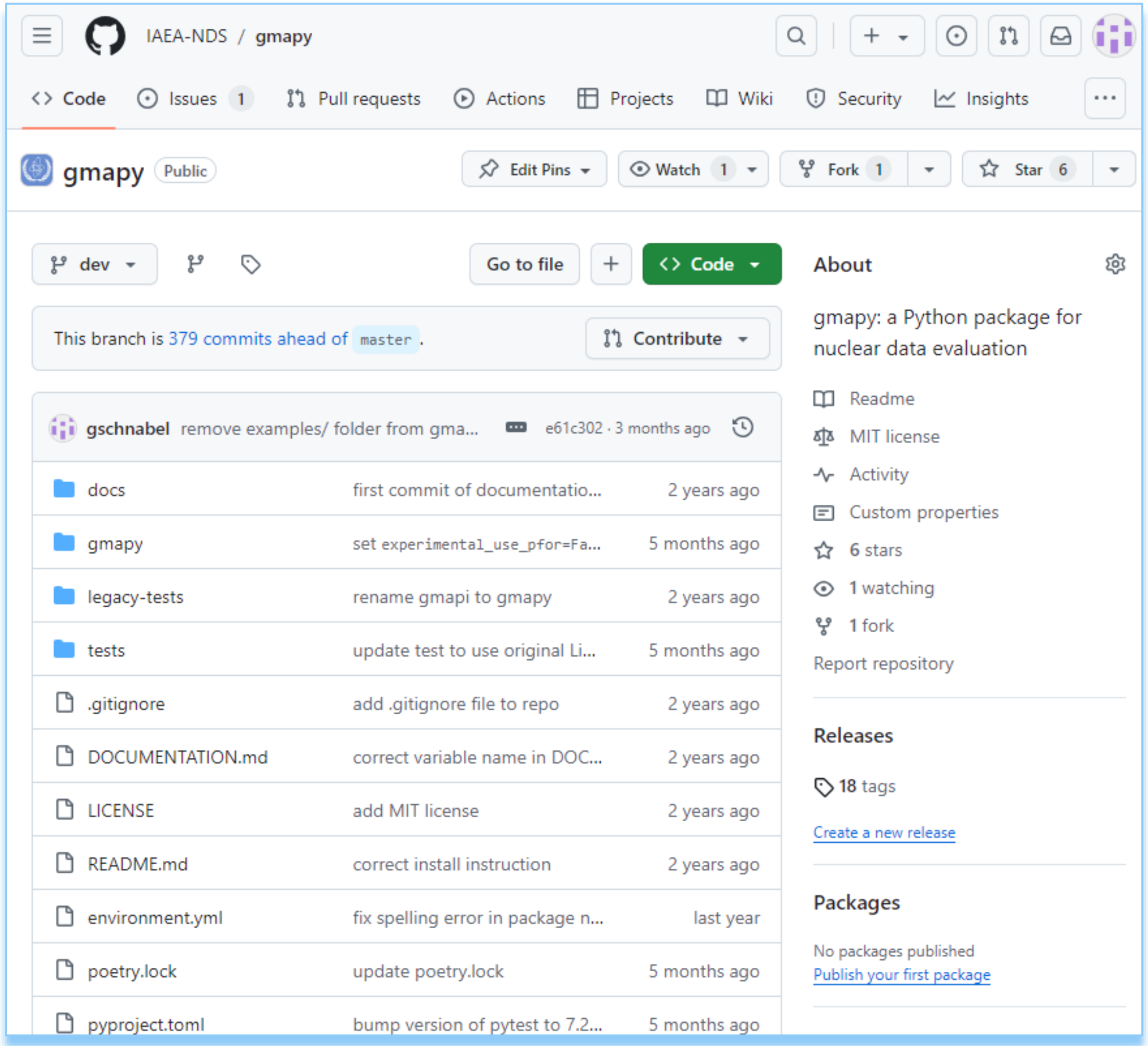
$$\vec{d} \sim \mathcal{N}\left(f(\vec{\sigma}_{\text{true}}), \boldsymbol{\Sigma}_{\text{exp}}\right)$$

Maximize this…

$$\rho(\vec{d}\,|\,\vec{\sigma}_{\text{true}}) = \frac{1}{\sqrt{(2\pi)^N \det(\boldsymbol{\Sigma}_{\text{exp}})}} \exp\left(-\frac{1}{2}(\vec{d} - f(\vec{\sigma}_{\text{true}}))^T \boldsymbol{\Sigma}_{\text{exp}}^{-1} (\vec{d} - f(\vec{\sigma}_{\text{true}}))\right)$$

… by adjusting this

Giving GMA a pie (GMA modernization)



Becoming more uncertain

$$\vec{d} \sim \mathcal{N}\left(f(\vec{\sigma}_{\text{true}}), \boldsymbol{\Sigma}_{\text{exp}}\right)$$

Maximize this…

… and by adjusting this

$$\rho(\vec{d}\,|\,\vec{\sigma}_{\text{true}}) = \frac{1}{\sqrt{(2\pi)^N \det(\boldsymbol{\Sigma}_{\text{exp}})}} \exp\left(-\frac{1}{2}(\vec{d} - f(\vec{\sigma}_{\text{true}}))^T \boldsymbol{\Sigma}_{\text{exp}}^{-1} (\vec{d} - f(\vec{\sigma}_{\text{true}}))\right)$$

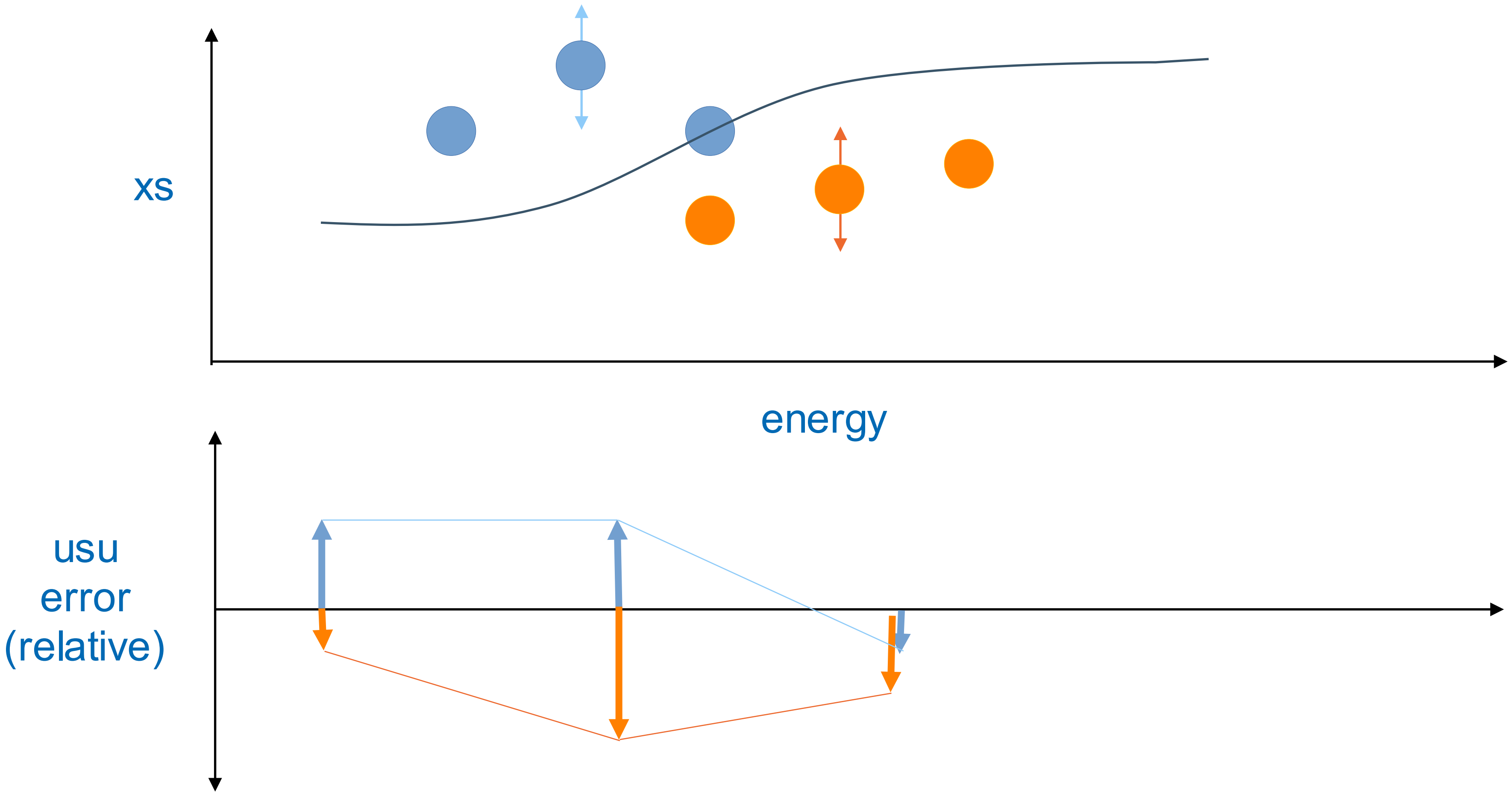
… by adjusting this …

USU-augmented covariance matrix

$$\mathbf{\Sigma}'_{\text{exp}}(\vec{u}) = \mathbf{\Sigma}_{\text{exp}} + \mathbf{\Sigma}_{\text{USU}}(\vec{u})$$

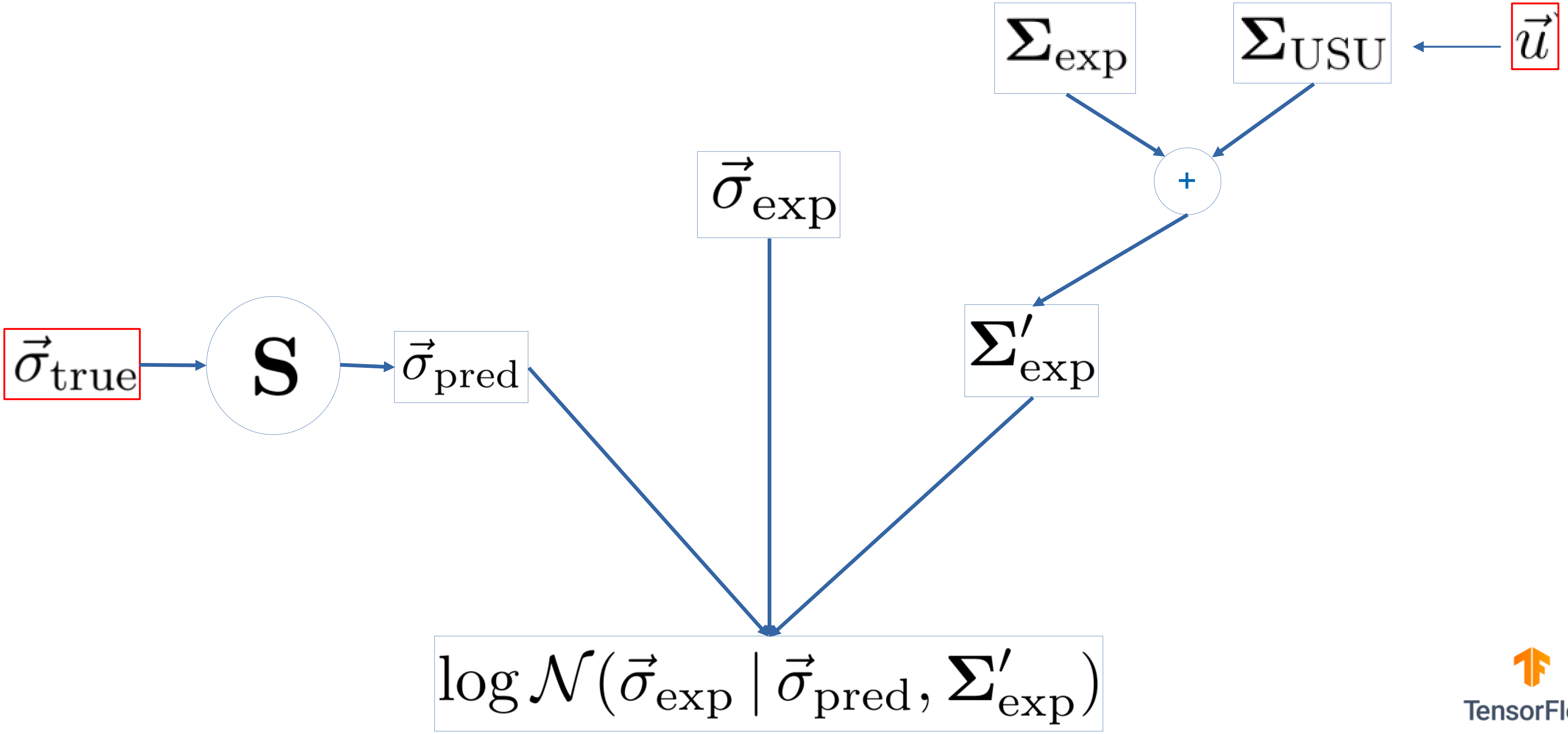
$$\mathbf{\Sigma}_{\text{USU}}(\vec{u}) = \text{Diag}(u_1^2, u_2^2, \cdots)$$

USU-augmented covariance matrix



Per energy USU uncertainty can be estimated by considering ensembles of USU errors associated with different datasets (implicitly done by Bayesian formulas)

Side note: TensorFlow and computational graph



TensorFlow

Beyond optimization

$$\rho(\vec{\sigma}_{\mathrm{true}}, \boldsymbol{\Sigma}'_{\mathrm{exp}} \,|\, \vec{\sigma}_{\mathrm{exp}}) \propto \rho(\vec{\sigma}_{\mathrm{exp}} \,|\, \vec{\sigma}_{\mathrm{true}}, \boldsymbol{\Sigma}'_{\mathrm{exp}})\, \rho(\vec{\sigma}_{\mathrm{true}})\rho(\boldsymbol{\Sigma}'_{\mathrm{exp}})$$

Metropolis-Hastings to sample from posterior distribution

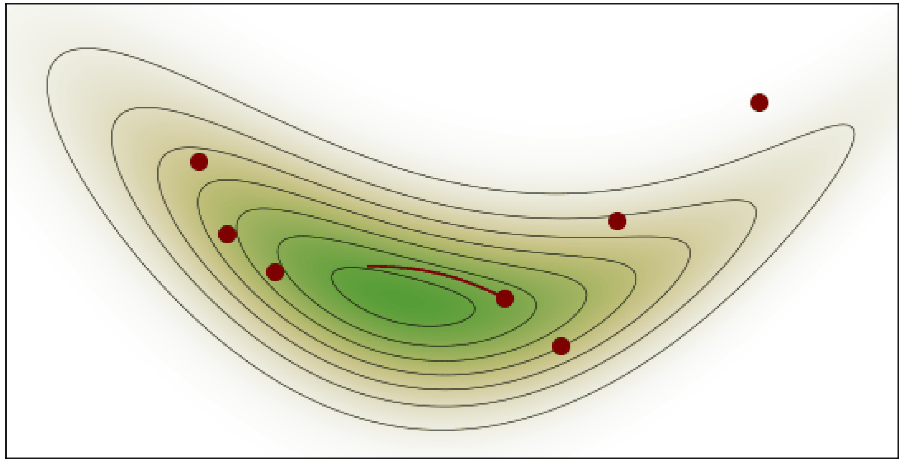
Hamiltonian Monte Carlo

- Specific instance of Metropolis-Hastings algorithm
- Augment "phase space" (cross section vectors) with momentum variables
- MH Proposal step: Simulate Hamiltonian dynamics with potential given by logarithmized posterior pdf

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial x_i}$$

$$H(\mathbf{x}, \mathbf{p}) = U(\mathbf{x}) + \frac{1}{2}\mathbf{p}^{\mathrm{T}} M^{-1} \mathbf{p}$$

$$U(\mathbf{x}) = -\ln f(\mathbf{x})$$

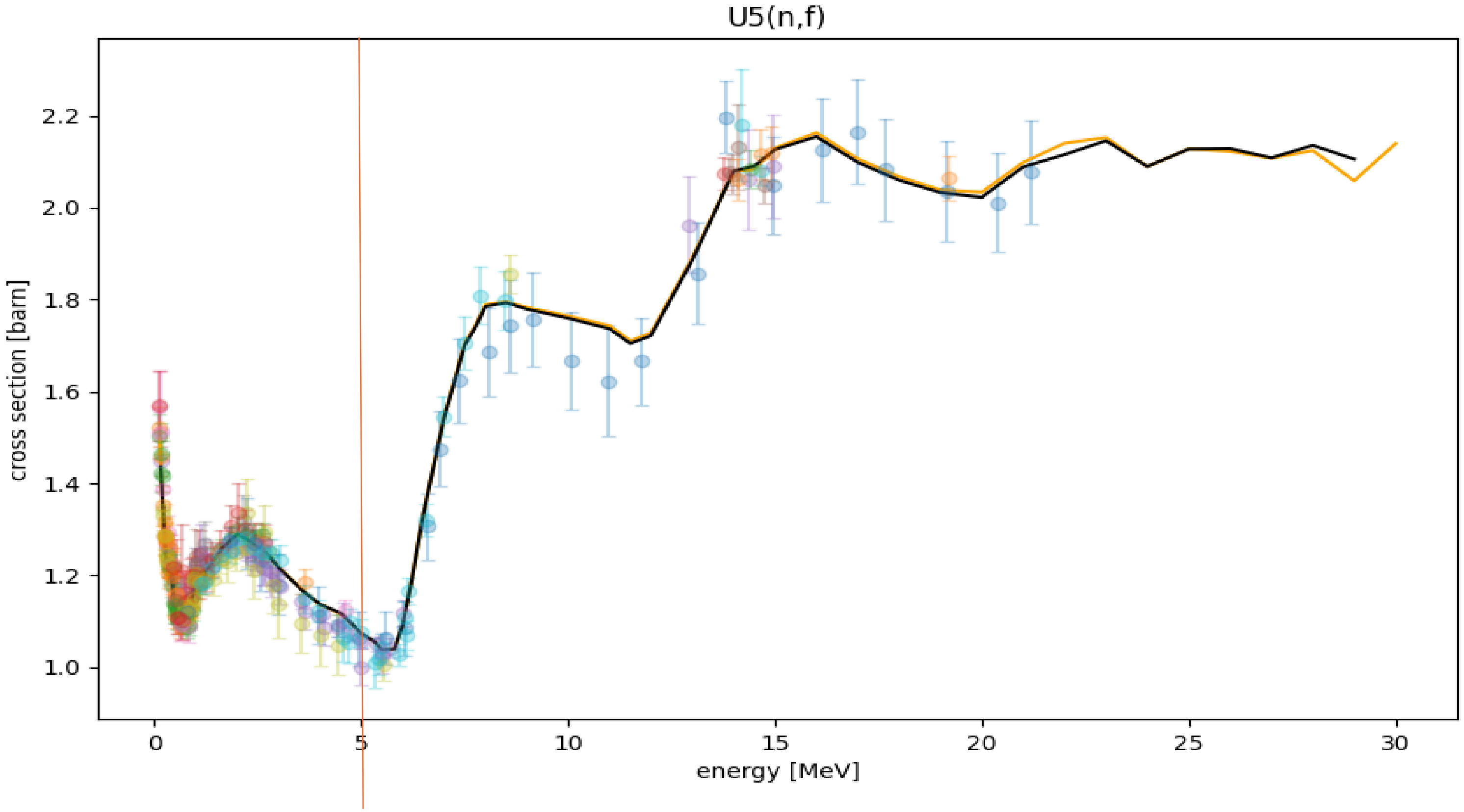


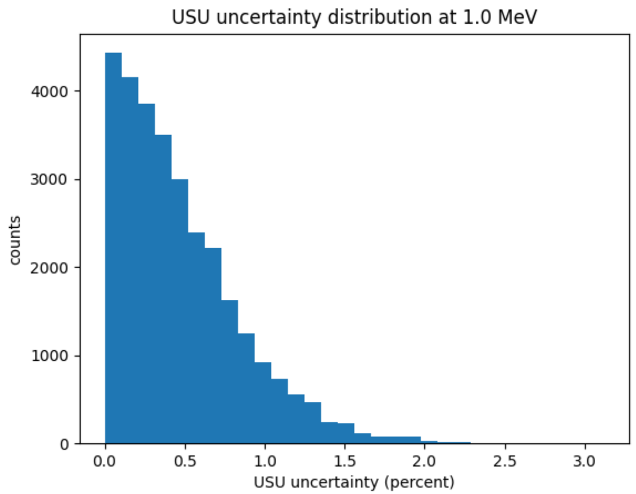
TensorFlow Probability

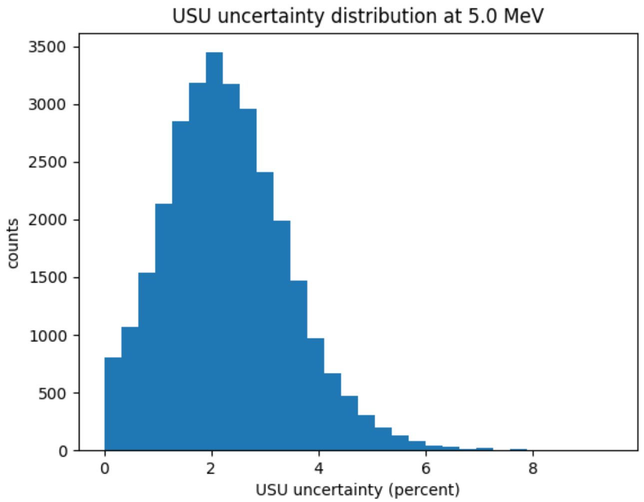
GMA database updates (from STD2017 until ENDF/B-VIII.1 submission)

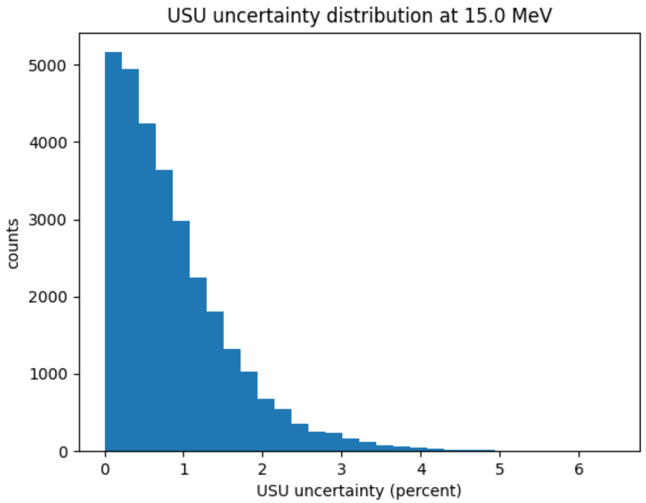
- **2020:** Neudecker et al: Revision of PU9(n,f) cross sections based on uncertainty templates (Nuclear Data Sheets 163)
- **2022**: Neudecker et al: Inclusion of relative U8(n,f) and PU9(n,f) TPC measurements from NIFFTE collaboration in GMA database (LA-UR-21-24093; TRN: US2216234)
- **2023**: Capote et al: Evaluation of experimental spectrum averaged cross sections (SACS) in ^{252}Cf(sf) neutron field (EPJ WoC 281)

U5(n,f)

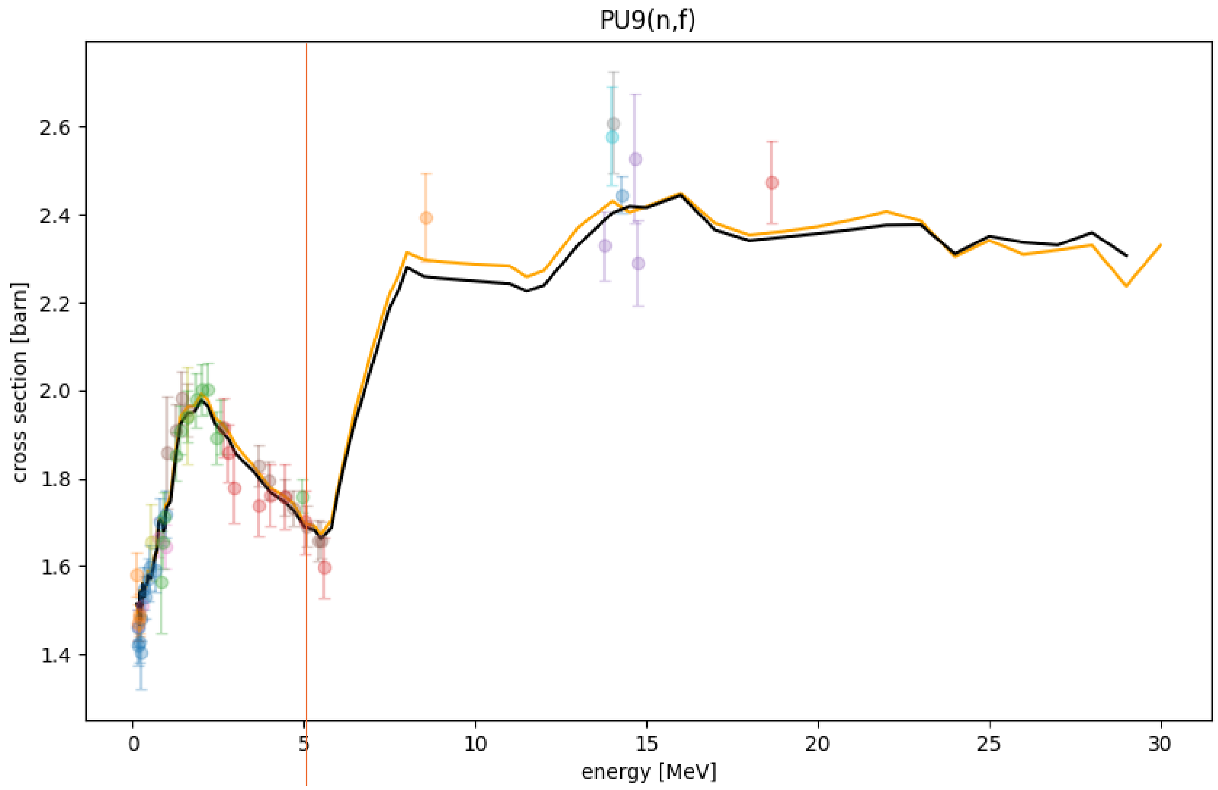

U5(n,f)
cross section [barn]
energy [MeV]
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0
5
10
15
20
25
30


USU uncertainty distribution at 1.0 MeV
counts
USU uncertainty (percent)
4000
3000
2000
1000
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0

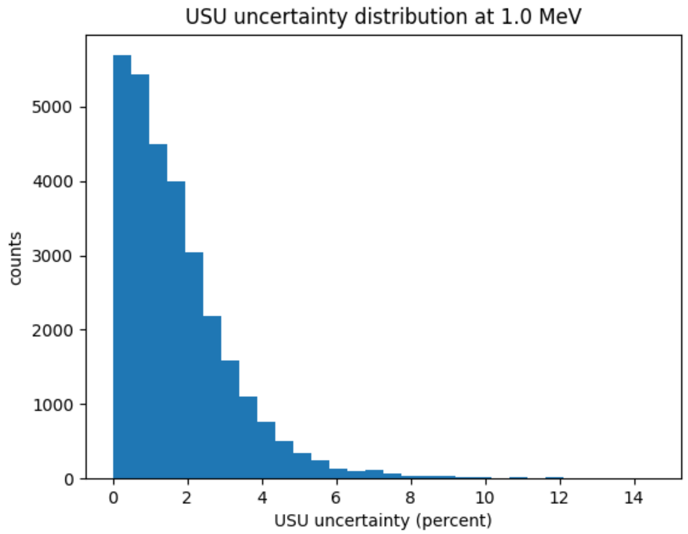

USU uncertainty distribution at 5.0 MeV
counts
USU uncertainty (percent)
3500
3000
2500
2000
1500
1000
500
0
0
2
4
6
8


USU uncertainty distribution at 15.0 MeV
counts
USU uncertainty (percent)
5000
4000
3000
2000
1000
0
0
1
2
3
4
5
6

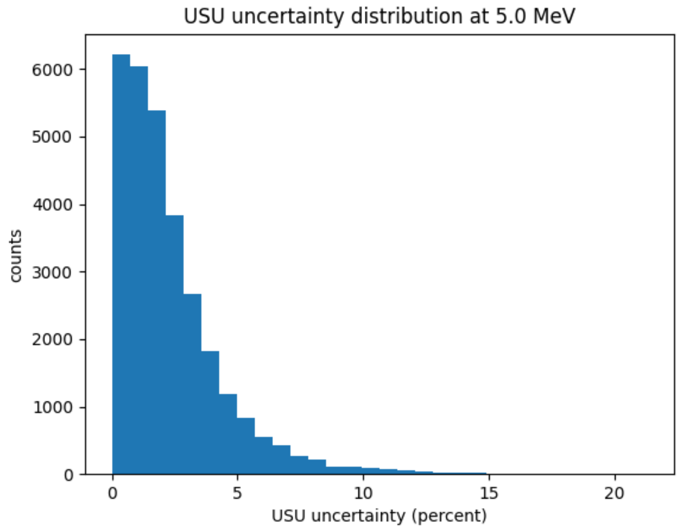
PU9(n,f)



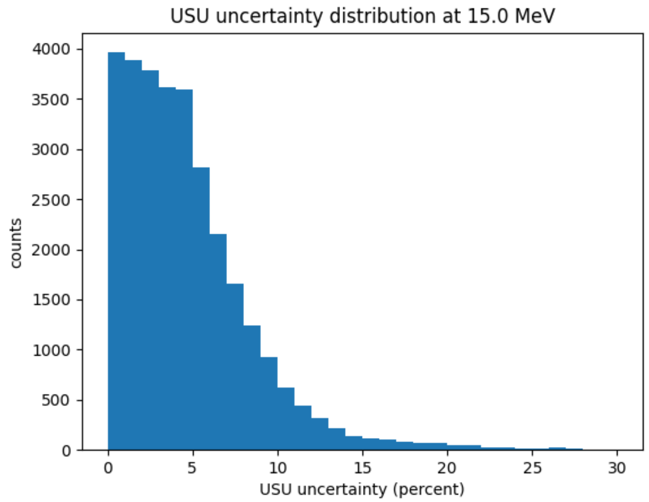
PU9(n,f)
cross section [barn]
energy [MeV]



USU uncertainty distribution at 1.0 MeV
counts
USU uncertainty (percent)

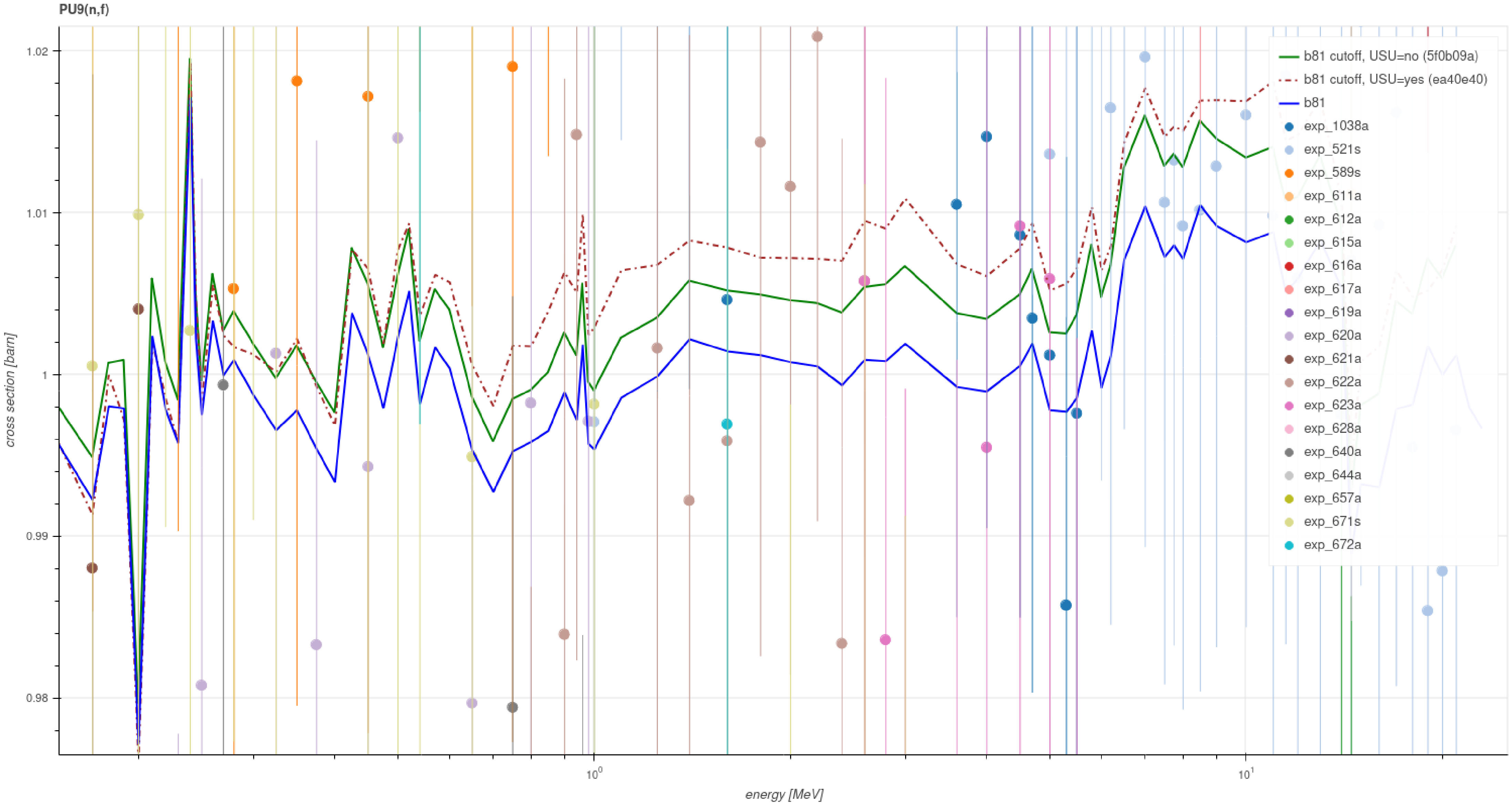


USU uncertainty distribution at 5.0 MeV
counts
USU uncertainty (percent)

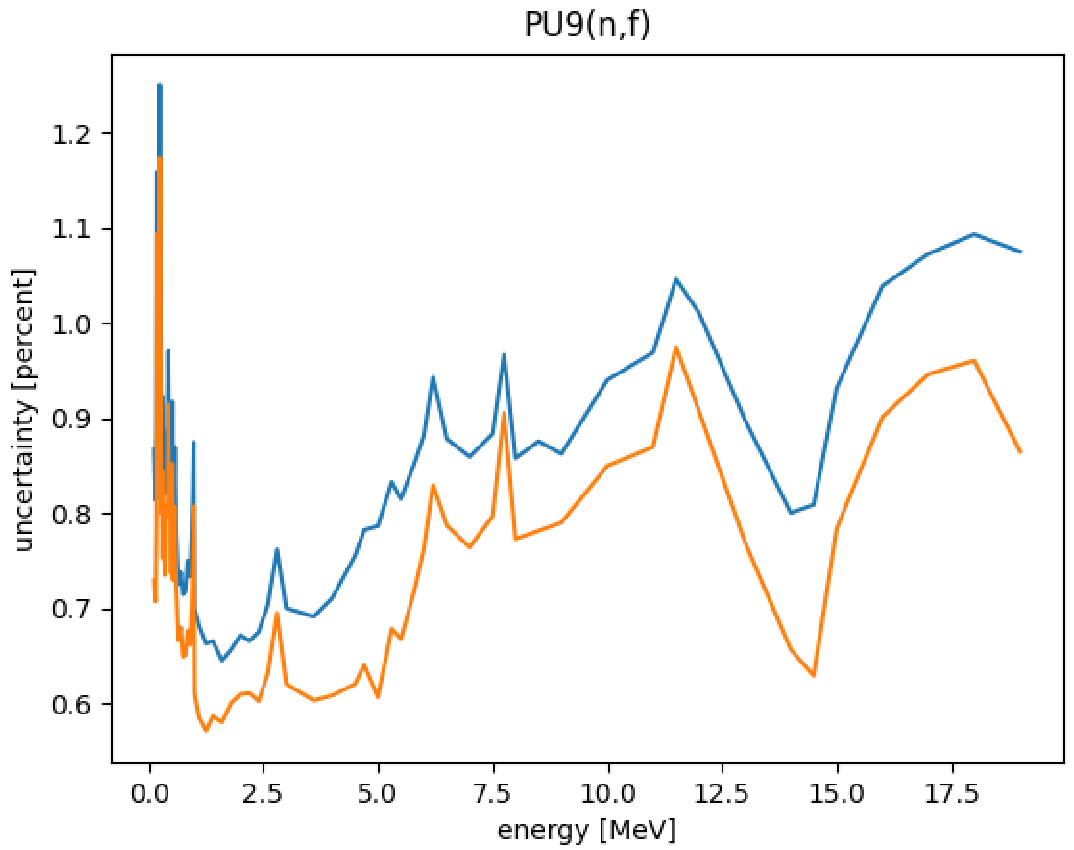


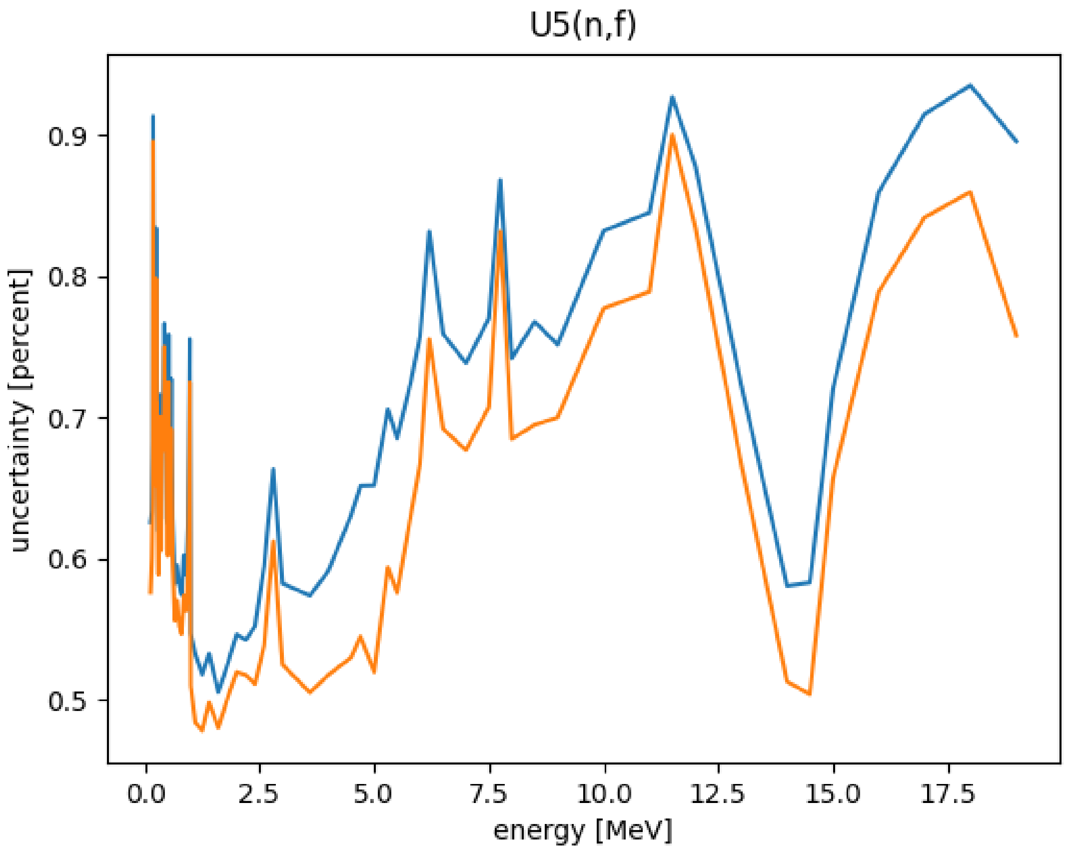
USU uncertainty distribution at 15.0 MeV
counts
USU uncertainty (percent)

PU9(n,f) comparison

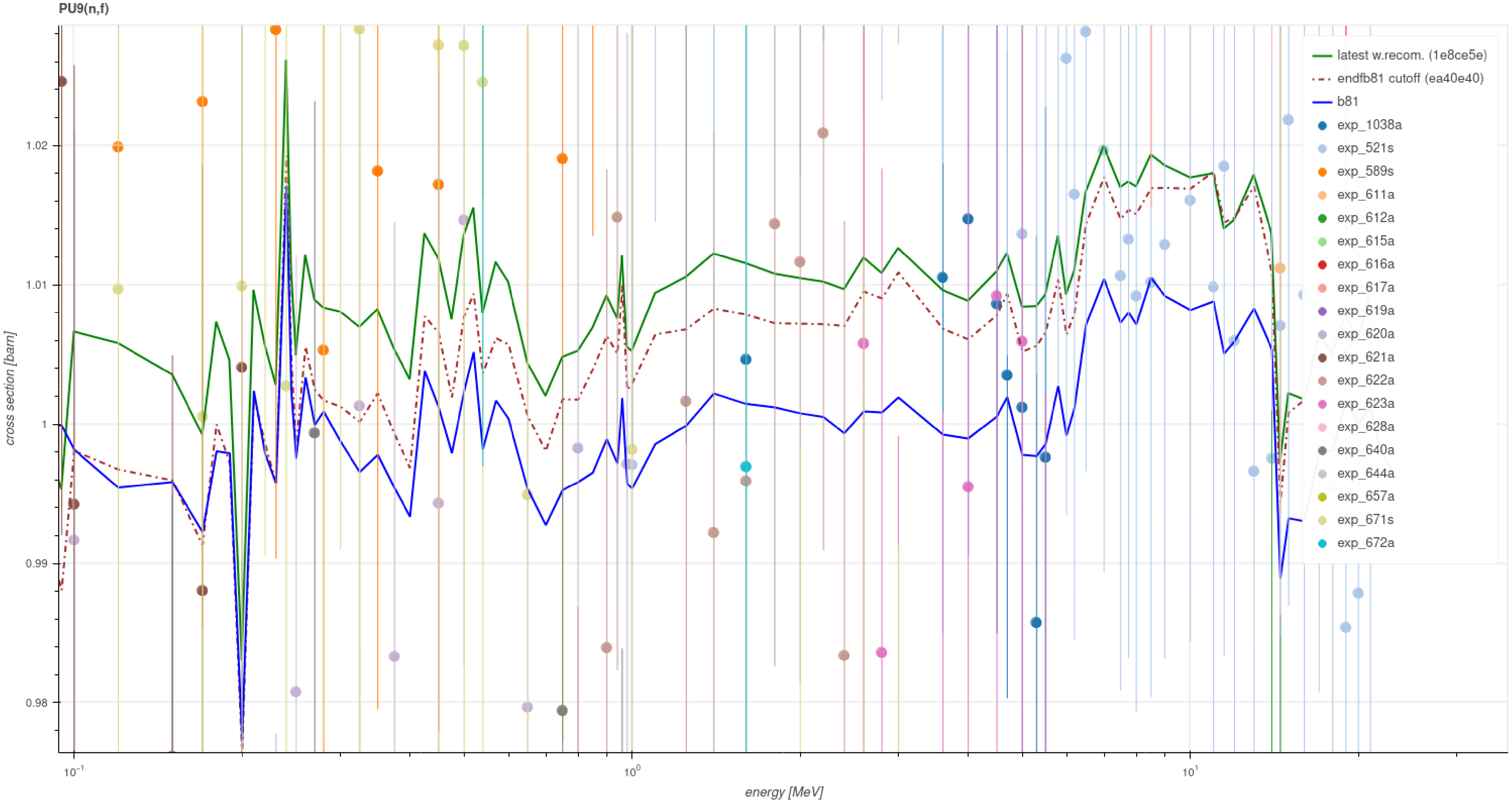


Evaluated uncertainties (USU vs no-USU)





PU9(n,f) comparison – latest prelim. STD eval



SACS comparison

latest w.recom (1e8ce5e) (git: 1e8ce5e)

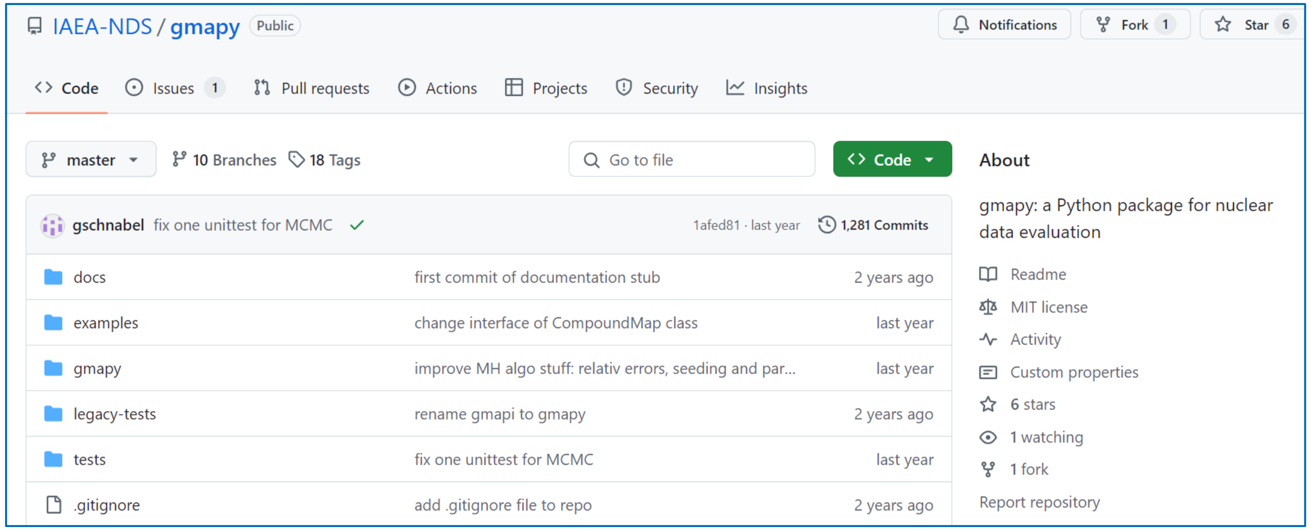
#	Reaction	Optim	MCMC
0	U5(n,f) SACS	1.2203	1.2248
1	PU9(n,f) SACS	1.8187	1.8257
2	U8(n,f) SACS	0.3224	0.3247
3	PU9(n,f) / U5(n,f) SACS RATIO	1.4903	1.4907
4	U8(n,f) / U5(n,f) SACS RATIO	0.2642	0.2651

b81 cutoff (ea40e40) (git: ea40e40)

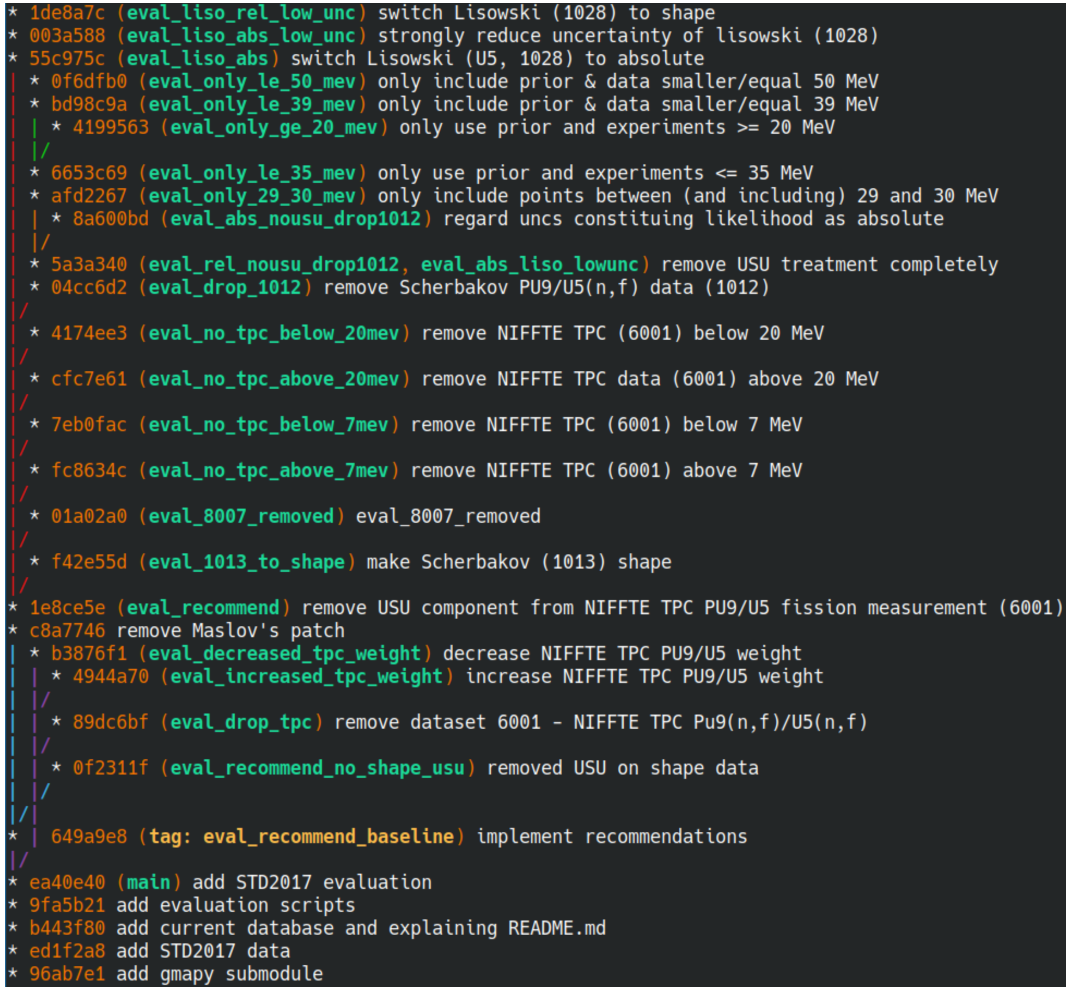
#	Reaction	Optim	MCMC
0	U5(n,f) SACS	1.2216	1.2256
1	PU9(n,f) SACS	1.8043	1.8126
2	U8(n,f) SACS	0.3218	0.3241
3	PU9(n,f) / U5(n,f) SACS RATIO	1.4770	1.4790
4	U8(n,f) / U5(n,f) SACS RATIO	0.2634	0.2644

Summary

- GMA modernized and validated (now **gmapy**)
- Supports rigorous optimization and MCMC at scale
- Inclusion of SACS ratios possible
- Energy-dependent USU treatment
- Everything open-source and reproducible (once there is sufficient documentation…)



https://github.com/iaea-nds/gmapy



https://github.com/iaea-nds/neutron-standards-evaluation

Thank you