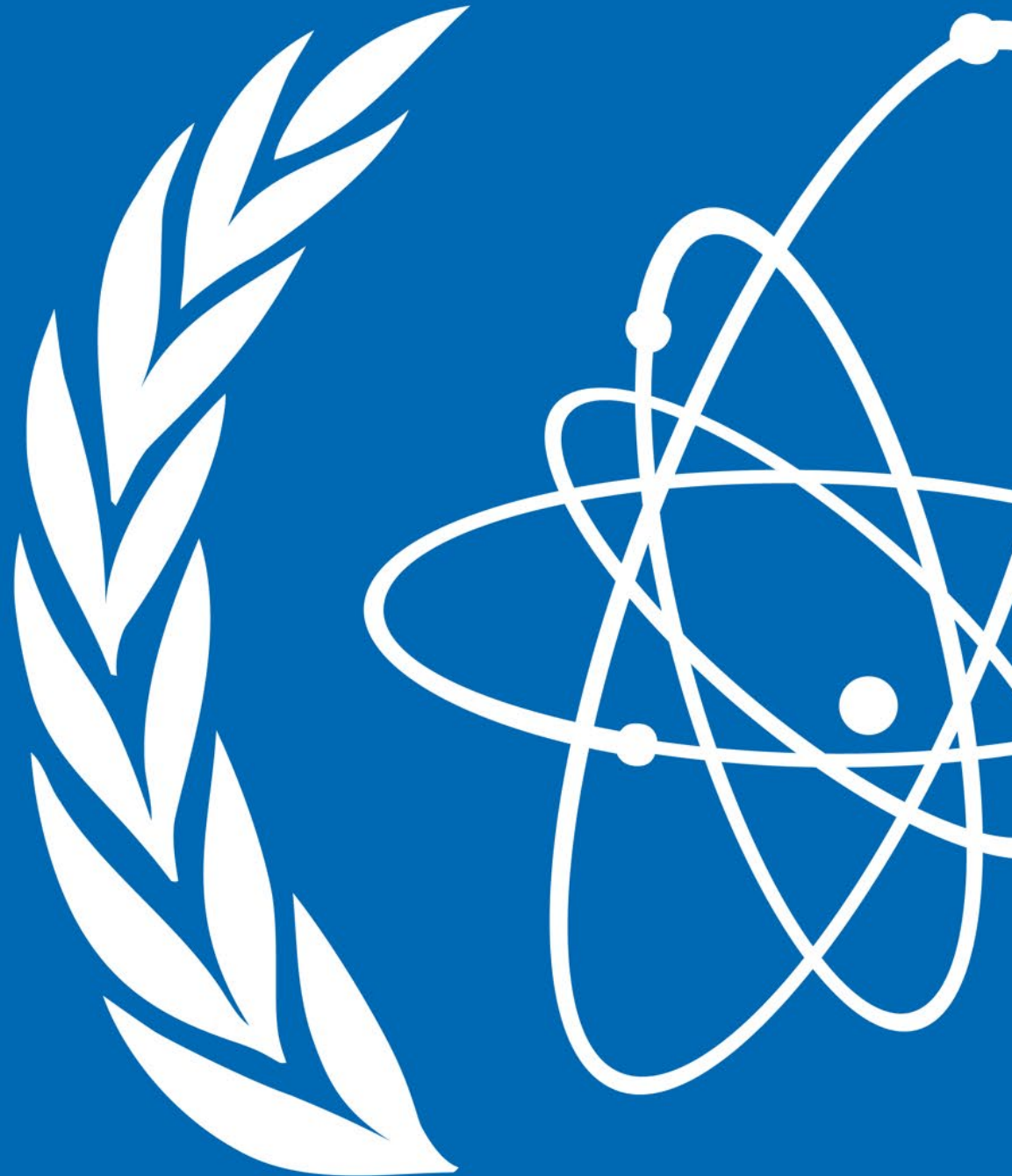


USU and Covariance

Georg Schnabel

NAPC-Nuclear Data Section, IAEA



More than 40 years of GMA

BNL-NCS-51363 VOL. I OF II
DOE/NDC 23
NEANDC(US)-209
INDC(USA)-85
UC-80
(General Reactor Technology - TIC-4500)

PROCEEDINGS OF THE CONFERENCE ON NUCLEAR DATA EVALUATION METHODS AND PROCEDURES

HELD AT
BROOKHAVEN NATIONAL LABORATORY
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*

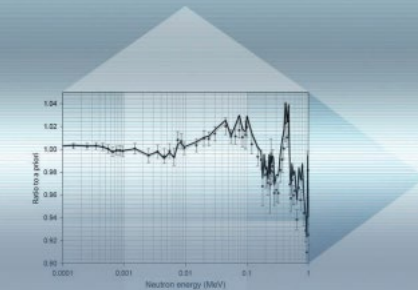
W. P. Poenitz

Applied Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439 USA.

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.

International Evaluation of Neutron Cross-Section Standards



IAEA
International Atomic Energy Agency



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Nuclear Data Sheets 148 (2018) 143–188

Nuclear Data
Sheets

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Evaluation of the Neutron Data Standards

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Generalized Least Squares equation

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

Experimental Covariance Matrix

Measurements

Sensitivity matrix

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

Underlying statistical model

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

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

How to estimate the “truth”?

$$\vec{d} \sim \mathcal{N} (f(\vec{\sigma}_{\text{true}}), \Sigma_{\text{exp}})$$

Maximize this...

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

... by adjusting this

Giving GMA a pie (GMA modernization)



IAEA-NDS / gmapy

Code Issues 1 Pull requests Actions Projects Wiki Security Insights

gmapy Public Edit Pins Watch 1 Fork 1 Star 6

dev Go to file Code

This branch is 379 commits ahead of master . Contribute

gschnabel remove examples/ folder from gma... e61c302 · 3 months ago

docs	first commit of documentatio...	2 years ago
gmapy	set experimental_use_pfor=Fa...	5 months ago
legacy-tests	rename gmapy to gmapy	2 years ago
tests	update test to use original Li...	5 months ago
.gitignore	add .gitignore file to repo	2 years ago
DOCUMENTATION.md	correct variable name in DOC...	2 years ago
LICENSE	add MIT license	2 years ago
README.md	correct install instruction	2 years ago
environment.yml	fix spelling error in package n...	last year
poetry.lock	update poetry.lock	5 months ago
pyproject.toml	bump version of pytest to 7.2...	5 months ago

About

gmapy: a Python package for nuclear data evaluation

- Readme
- MIT license
- Activity
- Custom properties
- 6 stars
- 1 watching
- 1 fork

Report repository

Releases

18 tags

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Becoming more uncertain

$$\vec{d} \sim \mathcal{N} (f(\vec{\sigma}_{\text{true}}), \Sigma_{\text{exp}})$$

Maximize this...

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

... and by adjusting this

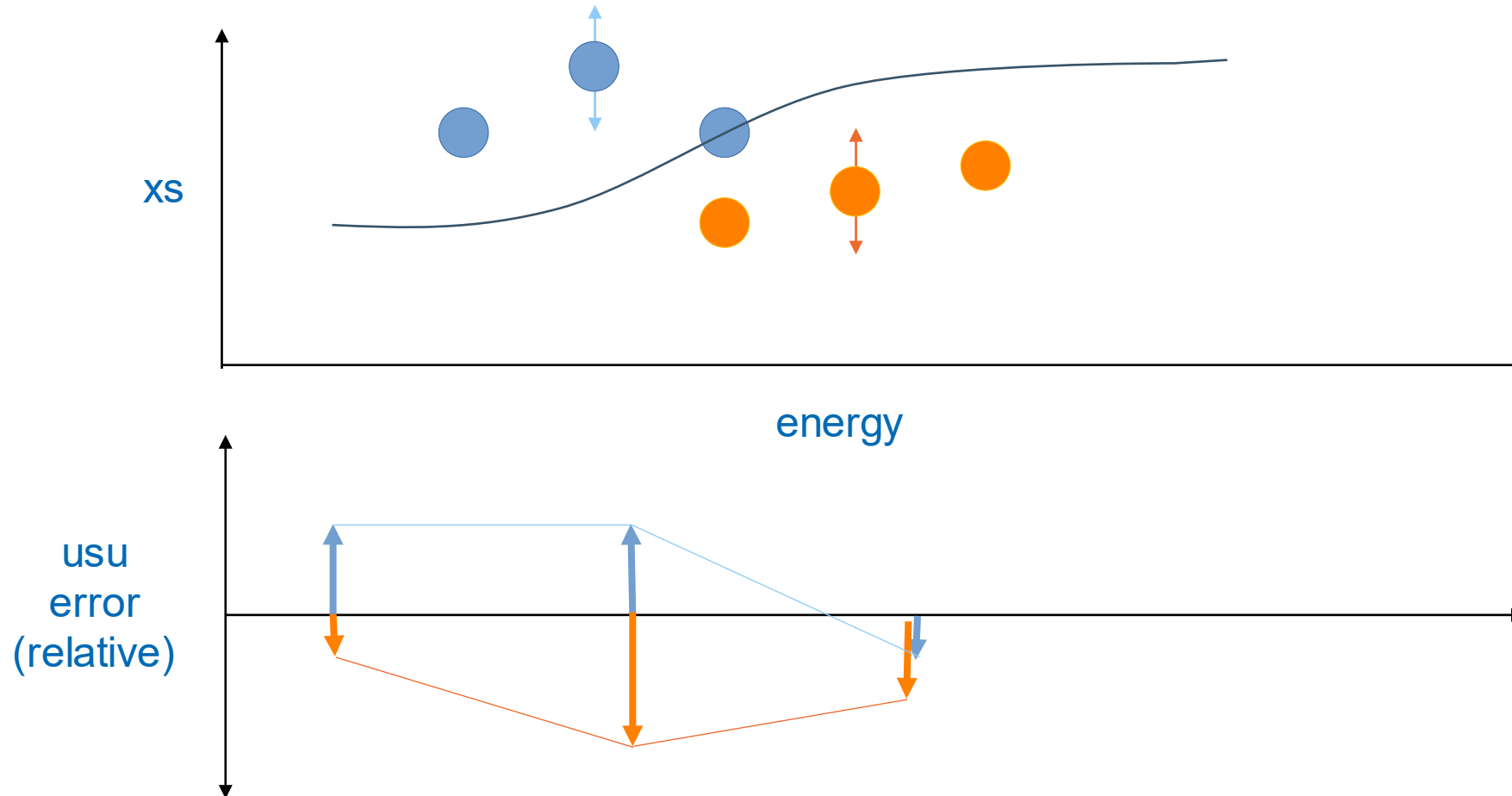
... by adjusting this ...

USU-augmented covariance matrix

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

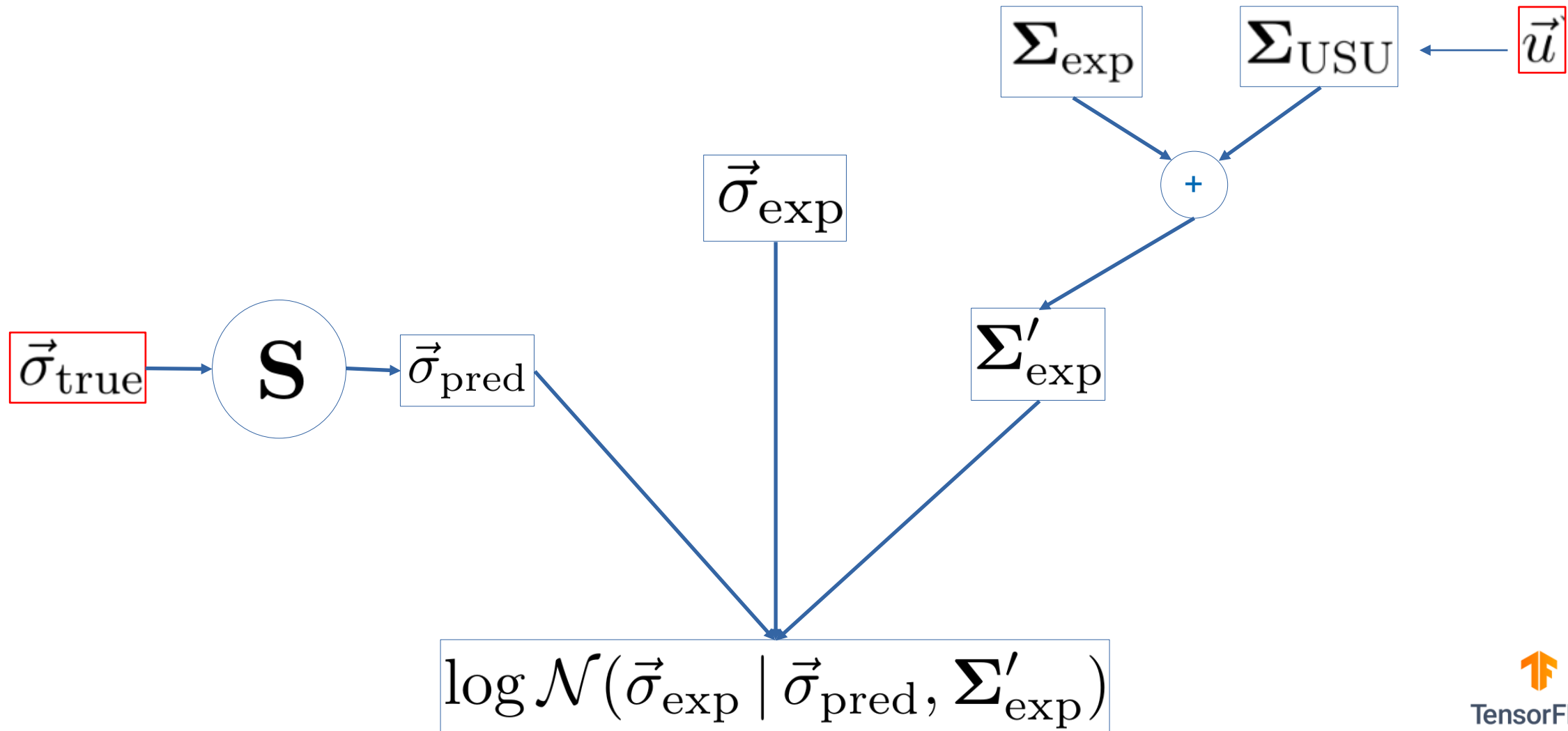
$$\Sigma_{\text{USU}}(\vec{u}) = \text{Diag}(u_1^2, u_2^2, \dots)$$

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



Beyond optimization

$$\rho(\vec{\sigma}_{\text{true}}, \Sigma'_{\text{exp}} \mid \vec{\sigma}_{\text{exp}}) \propto \rho(\vec{\sigma}_{\text{exp}} \mid \vec{\sigma}_{\text{true}}, \Sigma'_{\text{exp}}) \rho(\vec{\sigma}_{\text{true}}) \rho(\Sigma'_{\text{exp}})$$

Metropolis-Hastings to sample from posterior distribution

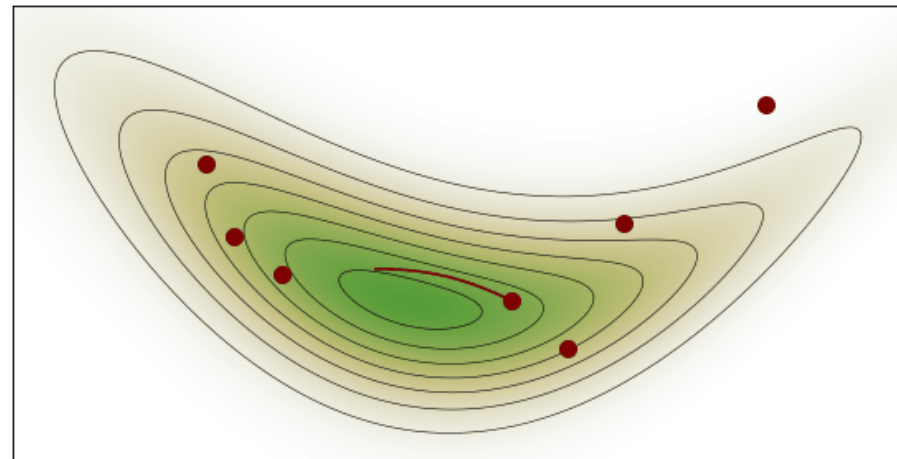
Hamiltonian Monte Carlo

- 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

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}$$

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

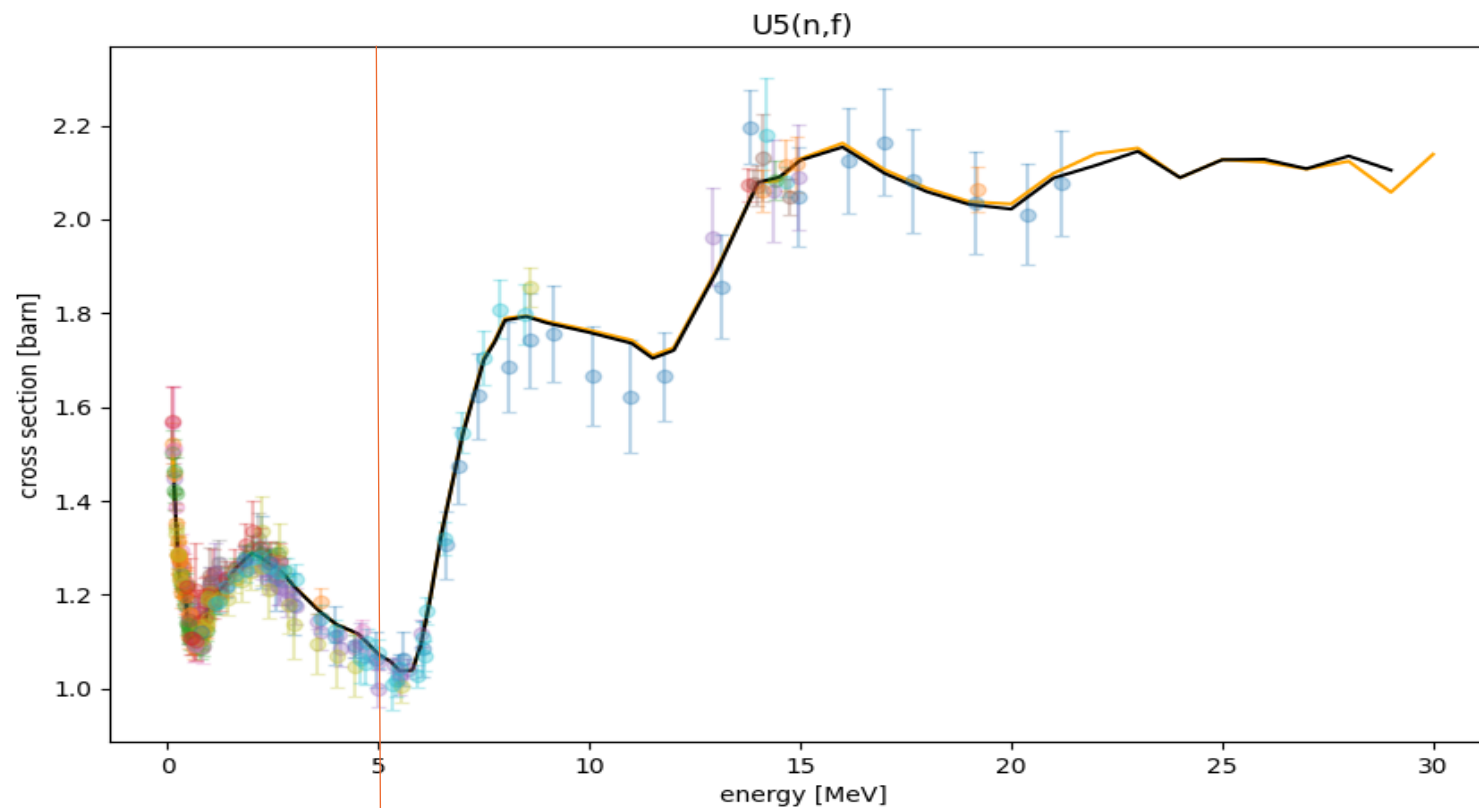
$$U(\mathbf{x}) = -\ln f(\mathbf{x})$$



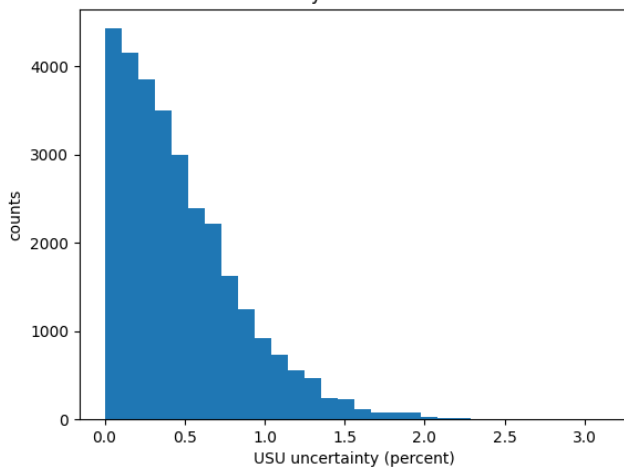
GMA database updates (from STD2017 until ENDF/B-VIII.1 submission)

- **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 $^{252}\text{Cf}(sf)$ neutron field (EPJ WoC 281)

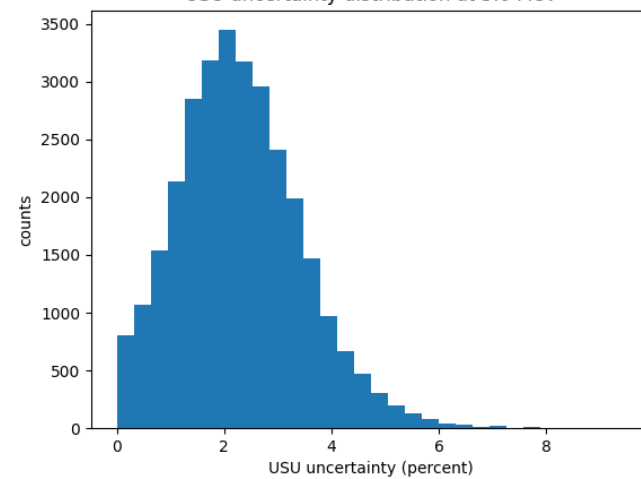
U5(n,f)



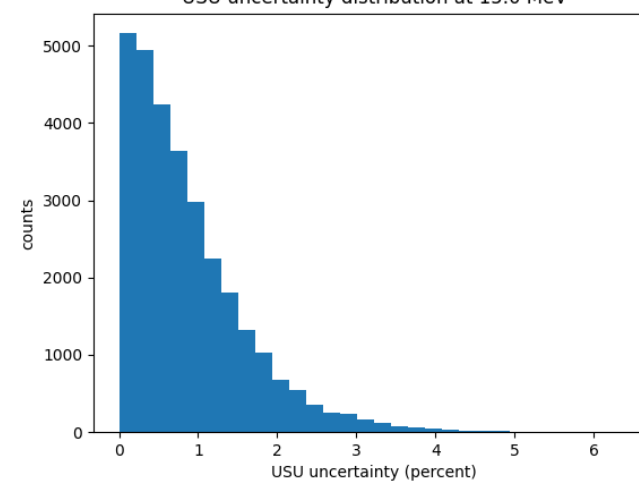
USU uncertainty distribution at 1.0 MeV



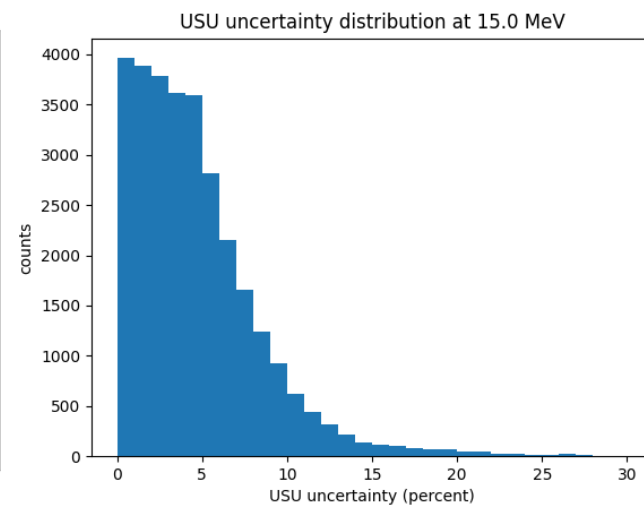
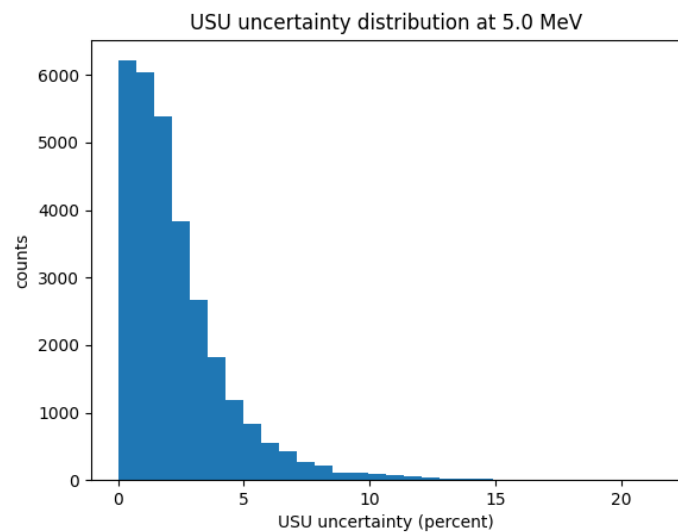
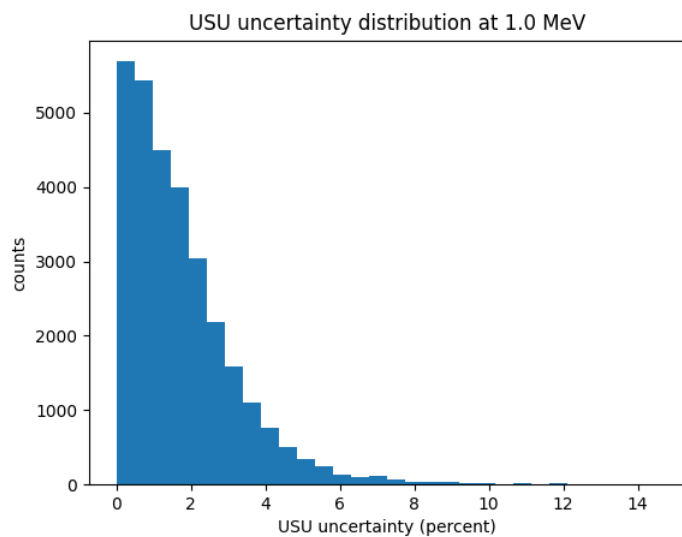
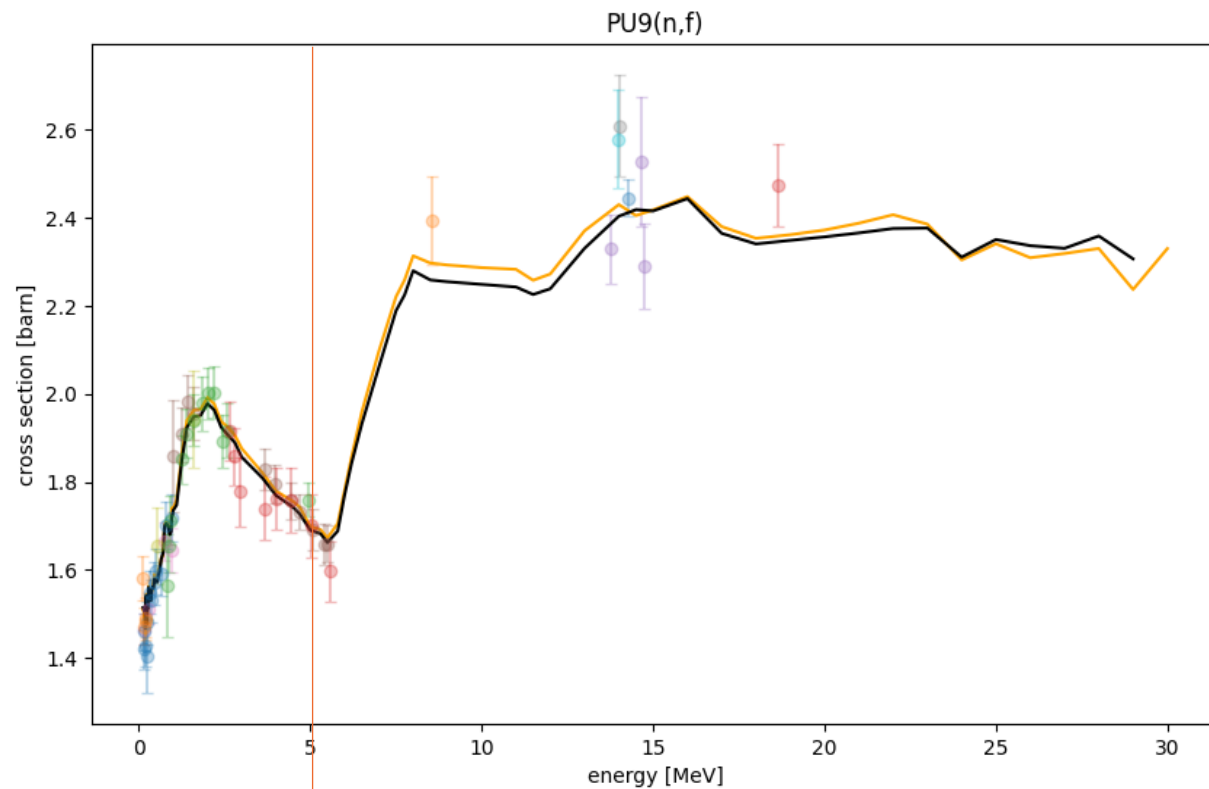
USU uncertainty distribution at 5.0 MeV



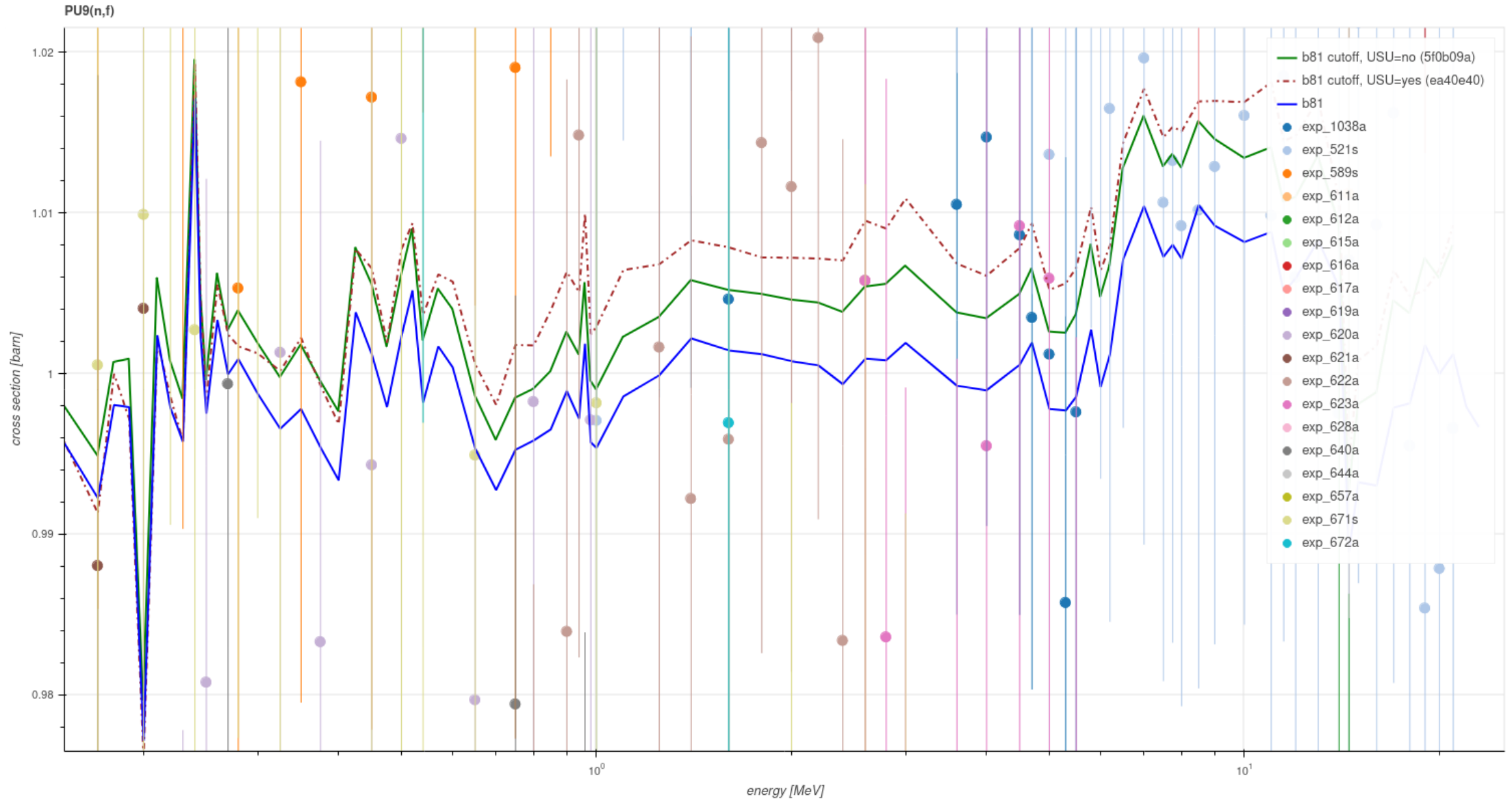
USU uncertainty distribution at 15.0 MeV



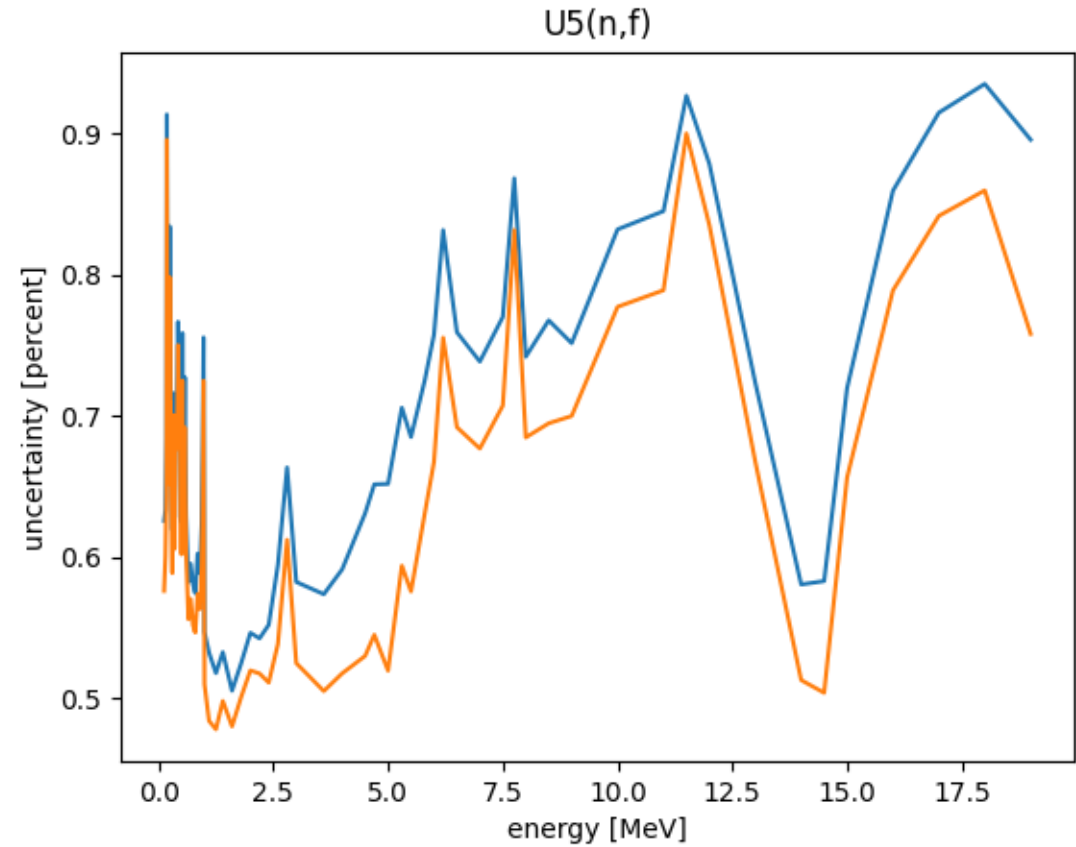
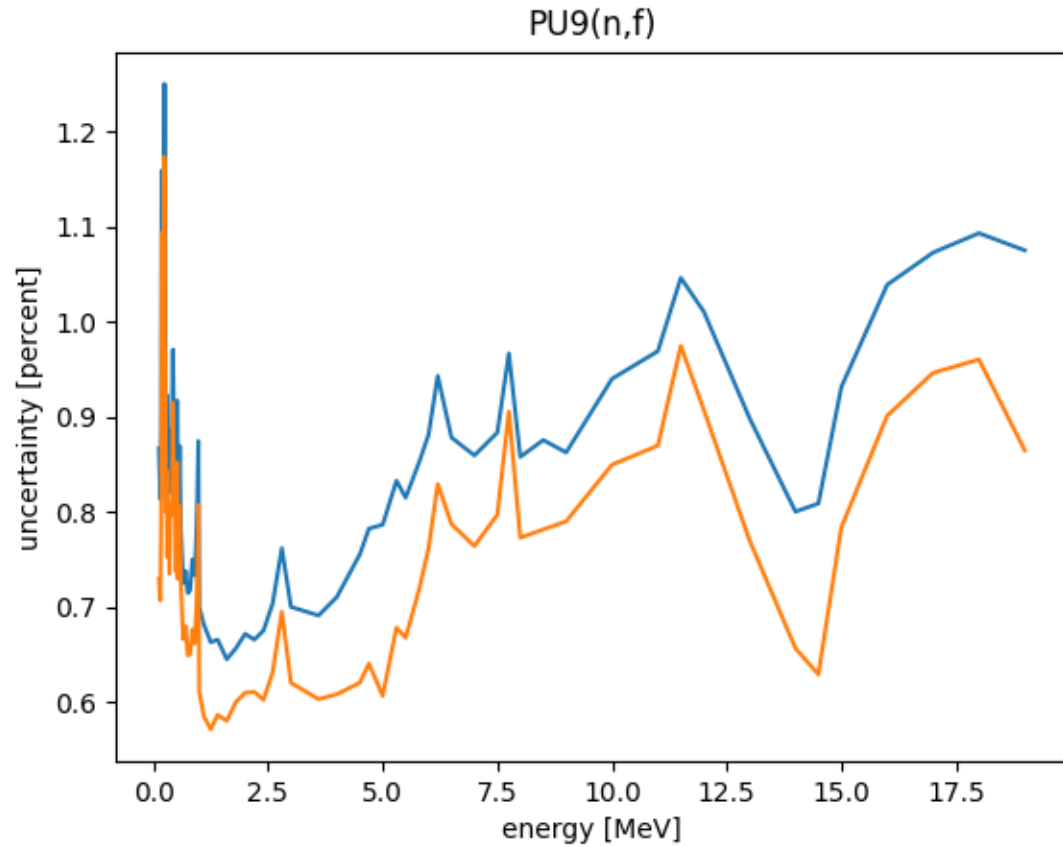
PU9(n,f)



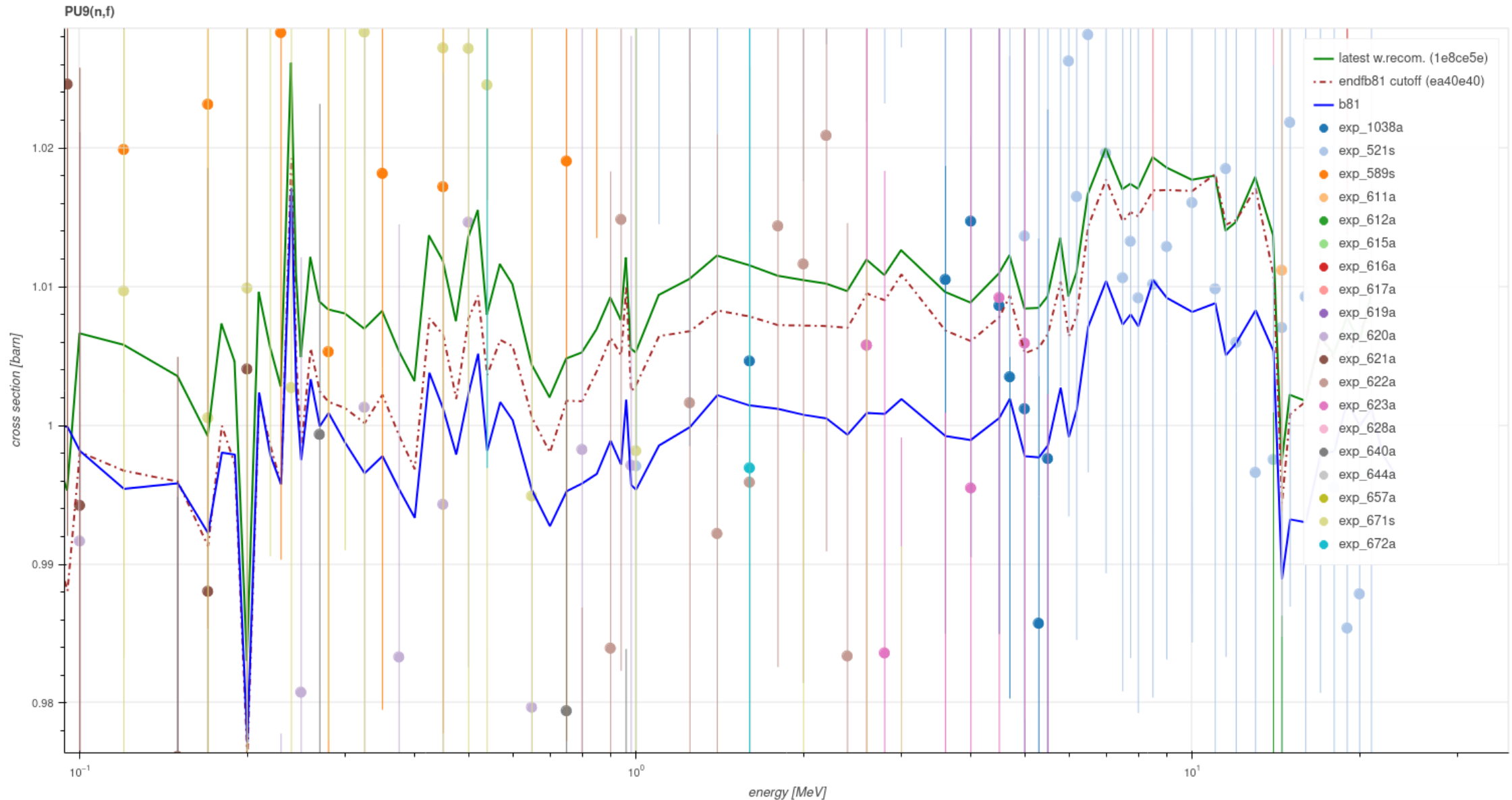
PU9(n,f) comparison



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...)

IAEA-NDS / **gmapy** Public

<> Code Issues 1 Pull requests Actions Projects Security Insights

master 10 Branches 18 Tags

gschnabel fix one unittest for MCMC ✓ 1afed81 · last year 1,281 Commits

File/Folder	Description	Last Commit
docs	first commit of documentation stub	2 years ago
examples	change interface of CompoundMap class	last year
gmapy	improve MH algo stuff: relativ errors, seeding and par...	last year
legacy-tests	rename gmapy to gmapy	2 years ago
tests	fix one unittest for MCMC	last year
.gitignore	add .gitignore file to repo	2 years ago

About

gmapy: a Python package for nuclear data evaluation

- Readme
- MIT license
- Activity
- Custom properties
- 6 stars
- 1 watching
- 1 fork
- Report repository

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

```
* 1de8a7c (eval_liso_rel_low_unc) switch Lisowski (1028) to shape
* 003a588 (eval_liso_abs_low_unc) strongly reduce uncertainty of lisowski (1028)
* 55c975c (eval_liso_abs) switch Lisowski (U5, 1028) to absolute
* 0f6dfb0 (eval_only_le_50_mev) only include prior & data smaller/equal 50 MeV
* bd98c9a (eval_only_le_39_mev) only include prior & data smaller/equal 39 MeV
  * 4199563 (eval_only_ge_20_mev) only use prior and experiments >= 20 MeV
//
* 6653c69 (eval_only_le_35_mev) only use prior and experiments <= 35 MeV
* afd2267 (eval_only_29_30_mev) only include points between (and including) 29 and 30 MeV
  * 8a600bd (eval_abs_nousu_drop1012) regard uncs constituing likelihood as absolute
//
* 5a3a340 (eval_rel_nousu_drop1012, eval_abs_liso_lowunc) remove USU treatment completely
* 04cc6d2 (eval_drop_1012) remove Scherbakov PU9/U5(n,f) data (1012)
//
* 4174ee3 (eval_no_tpc_below_20mev) remove NIFFTE TPC (6001) below 20 MeV
* cfc7e61 (eval_no_tpc_above_20mev) remove NIFFTE TPC data (6001) above 20 MeV
* 7eb0fac (eval_no_tpc_below_7mev) remove NIFFTE TPC (6001) below 7 MeV
* fc8634c (eval_no_tpc_above_7mev) remove NIFFTE TPC (6001) above 7 MeV
* 01a02a0 (eval_8007_removed) eval_8007_removed
//
* f42e55d (eval_1013_to_shape) make Scherbakov (1013) shape
//
* 1e8ce5e (eval_recommend) remove USU component from NIFFTE TPC PU9/U5 fission measurement (6001)
* c8a7746 remove Maslov's patch
  * b3876f1 (eval_decreased_tpc_weight) decrease NIFFTE TPC PU9/U5 weight
    * 4944a70 (eval_increased_tpc_weight) increase NIFFTE TPC PU9/U5 weight
  //
  * 89dc6bf (eval_drop_tpc) remove dataset 6001 - NIFFTE TPC Pu9(n,f)/U5(n,f)
  //
  * 0f2311f (eval_recommend_no_shape_usu) removed USU on shape data
  //
* 649a9e8 (tag: eval_recommend_baseline) implement recommendations
//
* ea40e40 (main) add STD2017 evaluation
* 9fa5b21 add evaluation scripts
* b443f80 add current database and explaining README.md
* ed1f2a8 add STD2017 data
* 96ab7e1 add gmapy submodule
```

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



IAEA

Thank you
