



IAEA

60 Years

Atoms for Peace and Development


Activities in the IAEA Neutron Data Standards Project

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7th International Workshop on
Compound-Nuclear Reactions and Related Topics
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Neutron data standards (NDS) project

- No-model evaluations based purely on experimental data of well measurable cross sections
- Main purpose: Conversion of relative to absolute cross sections

[Nuclear Data](#)
 IAEA Nuclear Data Services Home Page
STANDARDS 2017
[HOME](#)
[Nuclear Data Sheets 148 \(2018\) 143-188](#)
[Neutron Standards Data in the ENDF-6 Formatted Files, presentation by V.G. Pronyaev, December 2019](#)
STANDARDS 2006
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Technical Report
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[Most recent calculations](#)
Documents
[Documents and Reports](#)

IAEA NEUTRON DATA STANDARDS (2017)

A.D. Carlson, et al., [Nuclear Data Sheets 148 \(2018\) 143-188](#)

#	Reaction	Energy Range	ENDF-6 formatted data	Free text format
1	H(n,n)	Standard range: 1 keV to 20 MeV	std17-001_H_001.endf	std17-001_H_001.txt
2	³ He(n,p)	Standard range: 0.0253 eV to 50 keV	std-002_He_003.endf	not available
3	⁶ Li(n,t)	1e-5 eV to 4 MeV (Standard range: Thermal - 1 MeV)	std17-003_Li_006.endf	std17-003_Li_006.txt
4	¹⁰ B(n,α);(n,α ₁ γ)	1e-5 eV to 1 MeV (Standard range: Thermal - 1 MeV)	std17-005_B_010.endf	std17-005_B_010.txt
5	^{nat} C(n,n)	up to 6.45 MeV (Standard range: 1keV - 1.8 MeV)	std17-006_C_000.endf	std17-006_C_000.txt
6	¹⁹⁷ Au(n,γ)	2.5 keV to 2.8 MeV (Standard range: Thermal, 200keV - 2.5MeV)	std17-079_Au_197.endf	std17-079_Au_197.txt
7	²³⁵ U(n,f)	150 eV to 200 MeV (Standard range: Thermal, 150keV - 200MeV)	std17-092_U_235.endf	std17-092_U_235.txt
8	²³⁸ U(n,f)	0.5 to 200 MeV (Standard range: 2 - 200MeV)	std17-092_U_238.endf	std17-092_U_238.txt
9	Thermal Neutron Constants: nubar, (n _{th} ,f), (n _{th} ,el), (n _{th} ,g) cross sections for fissile targets ²³³ U, ²³⁵ U, ²³⁹ Pu, ²⁴¹ Pu. Total nubar ²⁵² Cf(sf).	0.0253 eV (2200 m/s)		Standards2017_TNC.txt
10	¹⁹⁷ Au(n,γ)	MACS (30 keV)= 620(11) mb		
11	²³⁵ U(n,f)	Integral from 7.8 eV to 11 eV = 247.5(3.3) b*eV		



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Nuclear Data Sheets 148 (2018) 143–188

Nuclear Data
Sheets

www.elsevier.com/locate/nds

Evaluation of the Neutron Data Standards

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S.P. Simakov,¹² P. Schillebeeckx,⁷ D.L. Smith,¹³ X. Tao,¹⁴ A. Trkov,³ A. Wallner,^{15,16} and W. Wang¹⁴

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With the need for improving existing nuclear data evaluations, (*e.g.*, ENDF/B-VIII.0 and JEFF-3.3 releases) the first step was to evaluate the standards for use in such a library. This new standards evaluation made use of improved experimental data and some developments in the methodology of analysis and evaluation. In addition to the work on the traditional standards, this work produced the extension of some energy ranges and includes new reactions that are called reference cross sections. Since the effort extends beyond the traditional standards, it is called the neutron data standards evaluation. This international effort has produced new evaluations of the following cross section standards: the H(n,n), ⁶Li(n,t), ¹⁰B(n,α), ¹⁰B(n,α₁γ), ^{nat}C(n,n), Au(n,γ), ²³⁵U(n,f) and ²³⁸U(n,f). Also in the evaluation process the ²³⁸U(n,γ) and ²³⁹Pu(n,f) cross sections that are not standards were evaluated. Evaluations were also obtained for data that are not traditional standards: the Maxwellian spectrum averaged cross section for the Au(n,γ) cross section at 30 keV; reference cross sections for prompt γ-ray production in fast neutron-induced reactions; reference cross sections for very high energy fission cross sections; the ²⁵²Cf spontaneous fission neutron spectrum and the ²³⁵U prompt fission neutron spectrum induced by thermal incident neutrons; and the thermal neutron constants. The data and covariance matrices of the uncertainties were obtained directly from the evaluation procedure.

Technical preparatory work

- **2020:** Capote et al: Unrecognized sources of uncertainty in experimental nuclear data (Nuclear Data Sheets 163)
- **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 U5(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 $^{252}\text{Cf}(\text{sf})$ neutron field (EPJ WoC 281)
- **2024:** Duran et al: Investigating new integral references for fission cross sections in actinides above 1 MeV (EPJ WoC 294)
- **2020 – ongoing:** Schnabel: Modernization of GMA database, evaluation code and statistical algorithms

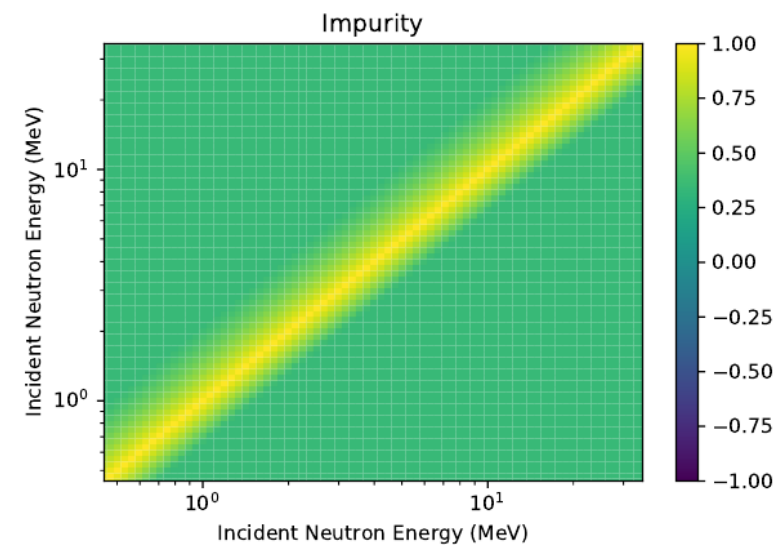
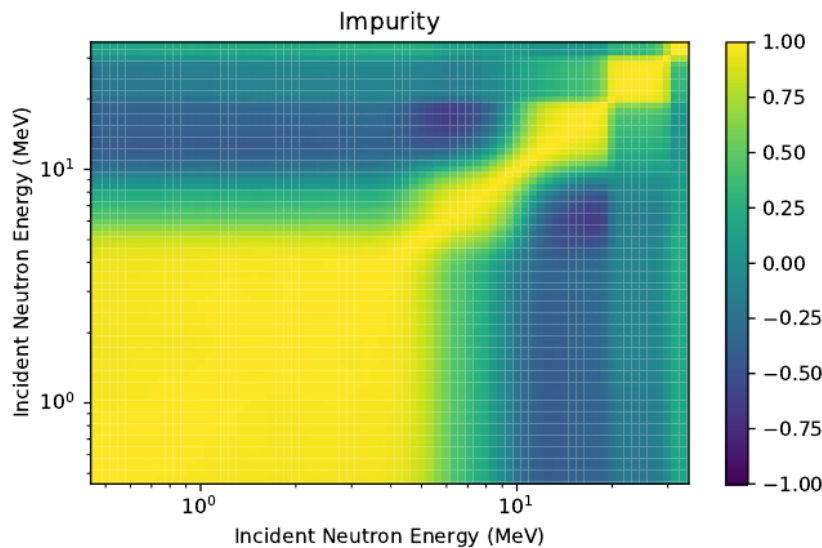
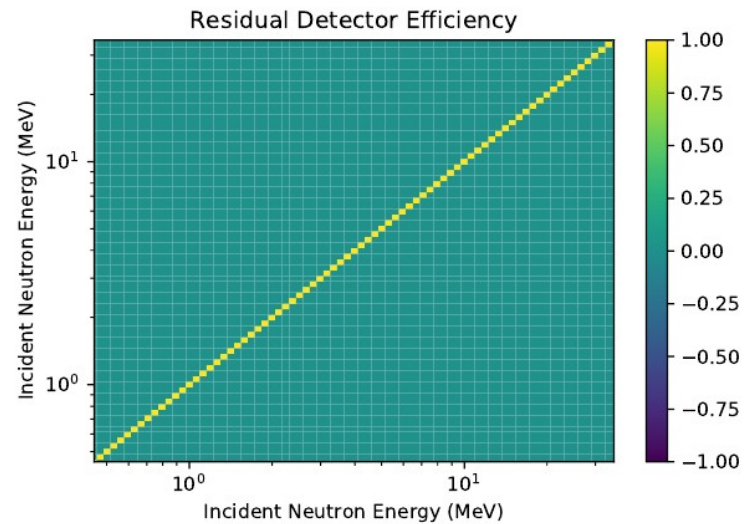
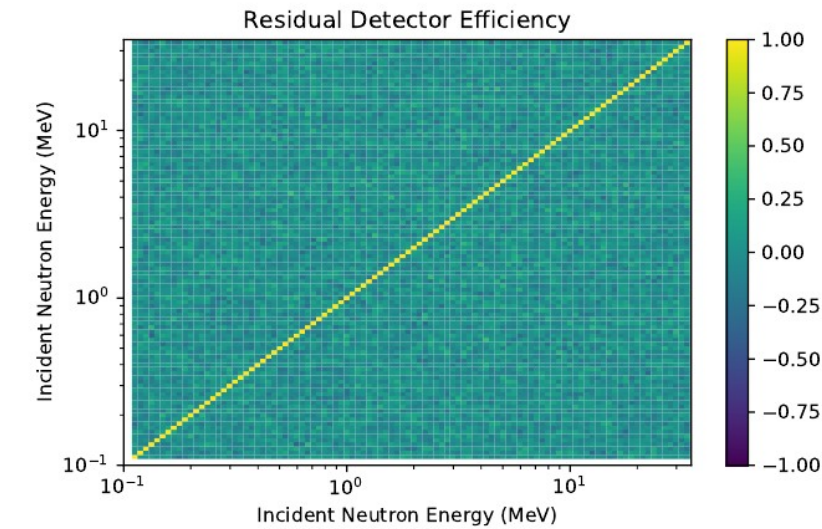
Experimental work

Recent experimental campaigns considered in the standards project have been summarized by A. Carlson et al in [1]:

Author	Institution	Energy	Quantity
Jiang et al	CSNS	6 MeV – 52 MeV	H(n,n)
Kornilov et al	OUAL	14.9 MeV	H(n,n) DA
Bai et al	CSNS	1 eV – 3 MeV	${}^6\text{Li}(n,t)$
Anastasiou et al	NIFFTE TPC	0.1 – 3 MeV	U5(n,f)/ ${}^6\text{Li}(n,t)$
Jiang et al	CSNS	1 eV – 2.5 MeV	${}^{10}\text{B}(n,a)$ / ${}^7,{}^6\text{Li}(n,t)$
Massey et al	LANSCE WNR	2 MeV – 20 MeV	${}^{10}\text{B}(n, p_x/t_x/a_x)$
Danon et al	RPI	150 keV – 400 keV	C(n,n)
Vanhoy	Univ. Kentucky		C(n,n)
Pirovano et al	n_TOF	20 MeV – 200 MeV	U5(n,f)
Manna et al	n_TOF	200 MeV – 500 MeV	U5(n,f)
Chen et al	CSNS	10 MeV – 60 MeV	U5(n,f), U8(n,f)
Wen et al	CSNS	1 MeV – 20 MeV	U8(n, f) / U5(n,f)
Casperson et al	NIFFTE/LANSCE	Up to 30 MeV	U8(n, f) / U5(n,f)
Snyder et al	NIFFTE/LANSCE	100 keV – 100 MeV	PU9(n,f) / U5(n,f)

5 [1] A. Carlson, R. Capote et al, “Database work for the new cross section standards evaluation,” EPJ Web of Conf. 284 (2023)

Experimental work



From D. Neudecker et al, Including $^{238}\text{U}(n,f)/^{235}\text{U}(n,f)$ and $^{239}\text{Pu}(n,f)/^{235}\text{U}(n,f)$ NIFFTE fission TPC Cross-Sections into the Neutron Data Standards Database, Tech. Report, LA-UR-21-24093 (2022)

Application of UQ templates

Applying a Template of Expected Uncertainties to Updating $^{239}\text{Pu}(n,f)$ Cross-section Covariances in the Neutron Data Standards Database

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Templates of uncertainties expected in specific measurement types were recently developed. One aim of these templates is to help evaluators in identifying (1) missing or suspiciously low uncertainties and (2) missing correlations between uncertainties of the same and different experiments, when estimating covariances for experimental data employed in their evaluations. These templates also provide realistic estimates of standard deviations and correlations for a particular uncertainty source and measurement type that can be used by evaluators in situations where they are not supplied by the experimenters. This information allows for a more comprehensive uncertainty analysis across all measurements considered in an evaluation and, thus, more realistic evaluated covariances. Here, we extend a template that is applicable to uncertainties expected in neutron-induced fission, (n,f), cross-section measurements. It is applied to improving covariances of $^{239}\text{Pu}(n,f)$ cross-section measurements in the database underlying the Neutron Data Standards evaluations. This particular

Nuclear Data Sheets 163 (2020), 228-248

Excerpt from (n,f) templates

TABLE I. Typical uncertainty sources encountered in (n,f) measurements that involve detecting fission fragments are listed, including proposed realistic ranges of uncertainties and shapes of correlations if missing for a specific measurement. The modifications from the preliminary version of the template in Ref. [9] are highlighted in red. The energy uncertainties δE are understood to encompass energy calibration and time resolution.

Unc. source	Typical range	Cor($\text{Exp}_i, \text{Exp}_i$)	Cor($\text{Exp}_i, \text{Exp}_j$) $i \neq j$
$\delta N_{(a)}$	$> 1\%$	Full	$\neq 0$ if same technique/sample
$\delta N_{(b\&c)}$	0-0.5% (Vapor-deposited target) 1% (Painted/electro-plated target)	Full Full	$\neq 0$ if same technique/sample $\neq 0$ if same technique/sample
δc	Eqs. (3) and (5)	Diagonal	0
$\delta\beta$ & δm ; δm	0.02–2%	Gaussian [20]	0.5–0.75
$\delta\beta$ & δm ; $\delta\beta$	0.2–1%	Gaussian	0.5–0.75
$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1-4%	Close to full	0.5–1
$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Gaussian	0.75–1.0
δb	0.2–>10%	Gaussian	Possible
δE	1%, 1–3 ns (TOF, for given TOF length)	From conversion	Technique-dependent
$\delta\phi$	0%, >1%	0.5–Full	Technique-dependent
$\delta\zeta$	See Table III	0.9–1	0.5–0.75
δd	>0.1%	Full	0

From D. Neudecker et al, Nuclear Data Sheets 163 (2020), 228-248

GMA Code

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.

I. INTRODUCTION

The subject of the present considerations and review is the evaluation of neutron cross sections which are of specific importance and thus have to be known with lesser uncertainties than others. This involves cross sections used in practical applications such as $^{235}\text{U}(n, f)$, $^{238}\text{U}(n, \gamma)$ as well as the standard cross

*This work performed under the auspices of the U.S. Department of Energy.

IAEA-NDS / GMAP-Fortran Public

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gschnabel added test to compare gfortran and if... 6659931 · 4 years ago

source	moved source to subdirect...	4 years ago
tests/test_001	added test to compare gfo...	4 years ago
README.md	updated README	4 years ago

README

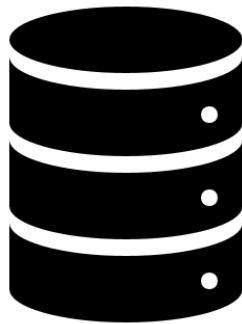
About GMAP

GMAP developed by Wolfgang P. Poenitz is a code to obtain evaluations of cross sections and their uncertainties based on the combined data from various experiments. The code employs the Bayesian version of the Generalized Least Squares method and is named after the mathematicians Gauss, Markov, and Aitken, who all contributed to the statistical theory around the linear least squares method. Input to GMAP are experimental data preprocessed by the [DATP](#) code, also developed by Poenitz.

<https://github.com/iaea-nds/gmap-fortran>

INDC(USA)-85 (March 1981)

Estimation problem



Estimate

Cross sections
on mesh

$\vec{\sigma}_{\text{mesh}}$

451 experimental datasets

7218 data points in total

+

Information on uncertainties
and correlations

33 reactions
963 variables

Assumptions in Neutron Data Standards project (so far)

Multivariate normal prior

$$\vec{\sigma}_{\text{true}} \sim \mathcal{N}(\vec{\sigma}_0, \mathbf{\Sigma}_0)$$

Multivariate normal likelihood

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

Linear model

$$\vec{f}(\vec{\sigma}_{\text{true}}) = \vec{f}(\vec{\sigma}_{\text{ref}}) + \mathbf{S}(\vec{\sigma}_{\text{true}} - \vec{\sigma}_{\text{ref}})$$

$$[\mathbf{S}]_{ij} = \frac{\partial f_i(\vec{\sigma}_{\text{ref}})}{\partial \sigma_{\text{ref},j}}$$

Generalized Least Squares equations

Multivariate normal posterior

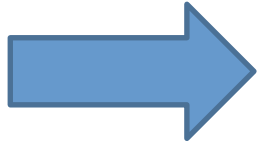
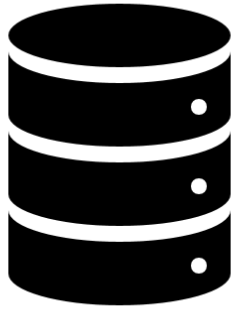
$$\vec{\sigma}_{\text{true}} \mid \vec{\sigma}_{\text{exp}}, \mathbf{\Sigma}_{\text{exp}} \sim \mathcal{N}(\vec{\sigma}_{\text{eval}}, \mathbf{\Sigma}_{\text{eval}})$$

with analytic equations for center vector and covariance matrix

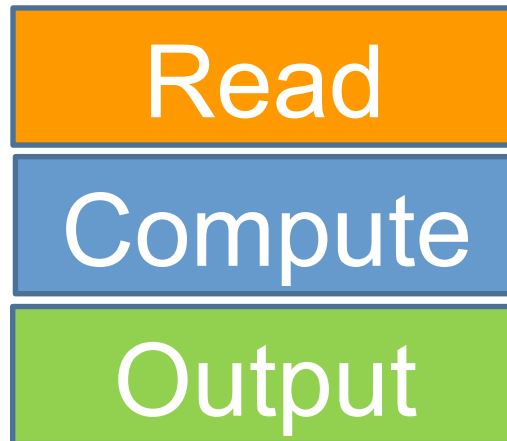
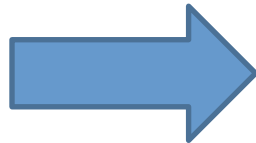
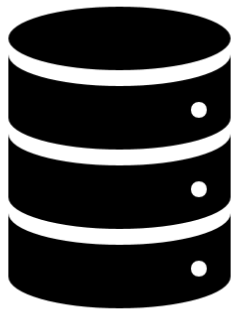
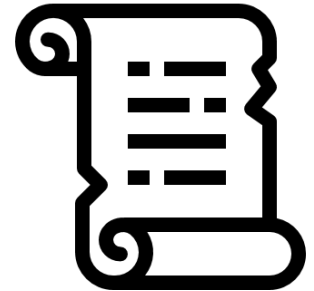
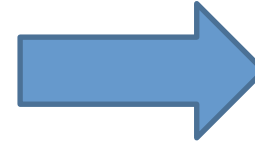
$$\mathbf{\Sigma}_{\text{eval}} = (\mathbf{S}^T \mathbf{\Sigma}_{\text{exp}}^{-1} \mathbf{S} + \mathbf{\Sigma}_0^{-1})^{-1}$$

$$\vec{\sigma}_{\text{eval}} = \vec{f}(\vec{\sigma}_{\text{ref}}) + \mathbf{\Sigma}_{\text{eval}} \left(\mathbf{S}^T \mathbf{\Sigma}_{\text{exp}}^{-1} (\vec{\sigma}_{\text{exp}} - \vec{f}(\vec{\sigma}_{\text{ref}})) + \mathbf{\Sigma}_0^{-1} (\vec{\sigma}_0 - \vec{\sigma}_{\text{ref}}) \right)$$

Code Modernization



GMAP (Fortran)



gmapy (Python)



Update with ratio of SACS data

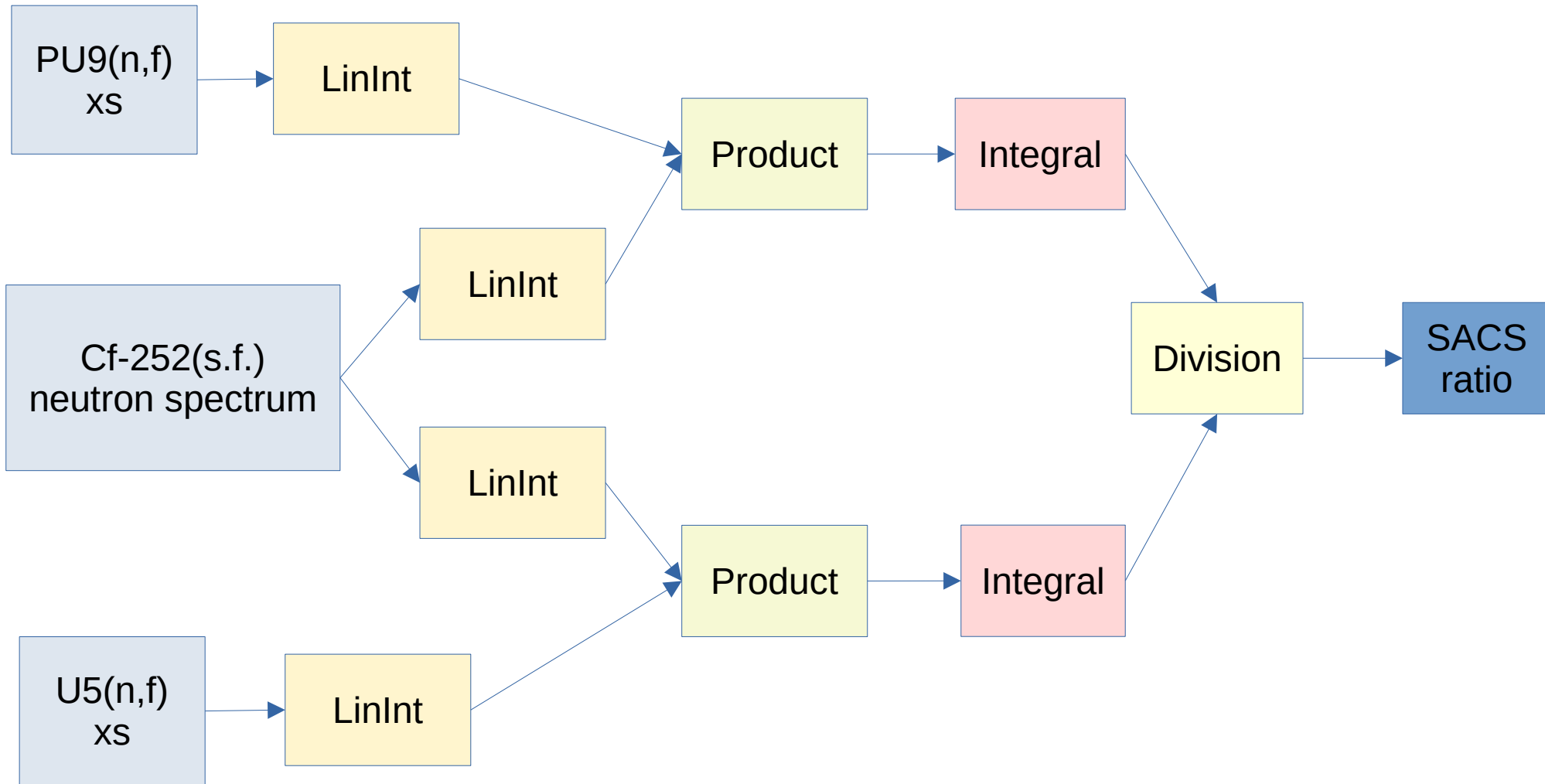
Table 5: Experimental $^{235}\text{U}(\text{n},\text{f})$, $^{238}\text{U}(\text{n},\text{f})$, and $^{239}\text{Pu}(\text{n},\text{f})$ SACS in $^{252}\text{Cf}(\text{sf})$ neutron spectrum: updated database.

Reaction index	Reaction	SACS [barn]	SACS uncert. [%]	Reaction label	Reference
1	$^{235}\text{U}(\text{n},\text{f})$	1216	1.62	U5F	Grundl 1983 [22, 23, 25]
2	$^{235}\text{U}(\text{n},\text{f})/^{238}\text{U}(\text{n},\text{f})$	3.73	1.20	U5F/U8F	Grundl-Gilliam 1983 [22, 24, 28], inverse = 0.2681
3	$^{235}\text{U}(\text{n},\text{f})/^{239}\text{Pu}(\text{n},\text{f})$	0.666	0.90	U5F/PU9F	Grundl-Gilliam 1983 [22, 24], inverse = 1.502
4	$^{239}\text{Pu}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	1.500	1.60	PU9F/U5F	Heaton 1976 [25]
5	$^{238}\text{U}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	0.2644	1.32	U8F/U5F	Heaton 1976 [25]
6	$^{238}\text{U}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	0.269	1.20	U8F/U5F	Schröder 1985 [16]
7	$^{239}\text{Pu}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	1.500	0.80	PU9F/U5F	Schröder 1985 [16]
8	$^{235}\text{U}(\text{n},\text{f})$	1234	1.45	U5F	Schröder 1985 [16]
9	$^{235}\text{U}(\text{n},\text{f})$	1215	1.79	U5F	Davis/Knoll 1978 [26]
10	$^{239}\text{Pu}(\text{n},\text{f})$	1790	2.26	PU9F	Davis/Knoll 1978 [26]
11	$^{238}\text{U}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	0.2741	1.66	U8F/U5F	Adamov 1977 [27]
12	$^{239}\text{Pu}(\text{n},\text{f})/^{235}\text{U}(\text{n},\text{f})$	1.475	1.50	PU9F/U5F	Adamov 1977 [27]

from R. Capote et al, EPJ-WoC 281, 00027 (2023)

Automatic Differentiation

(Example: ratio of SACS)



Some results based on database with SACS update

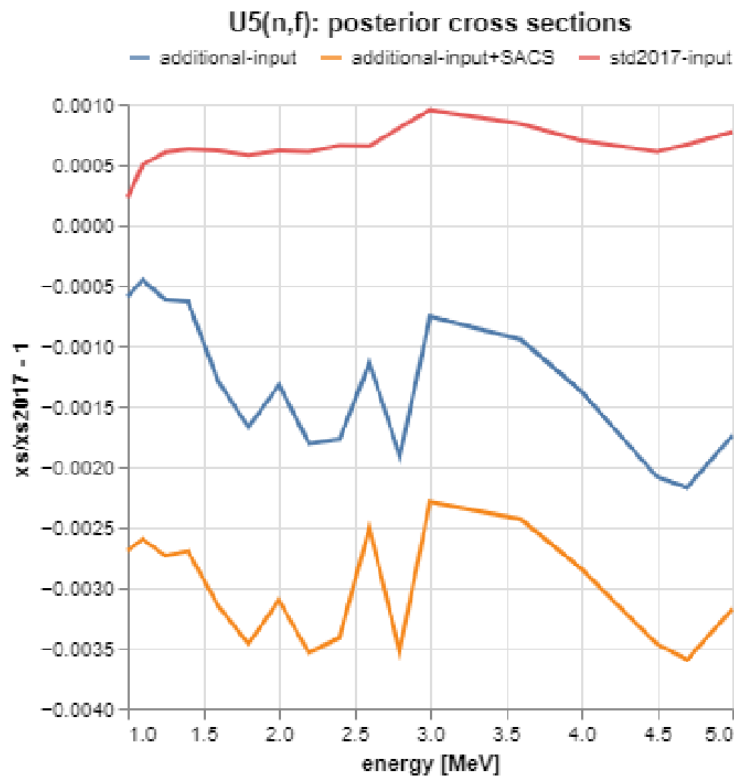


Figure 1: Evaluated $^{235}\text{U}(n,f)$ cross sections relative to the IAEA STD 2017 [3] from 1 MeV up to 5 MeV.

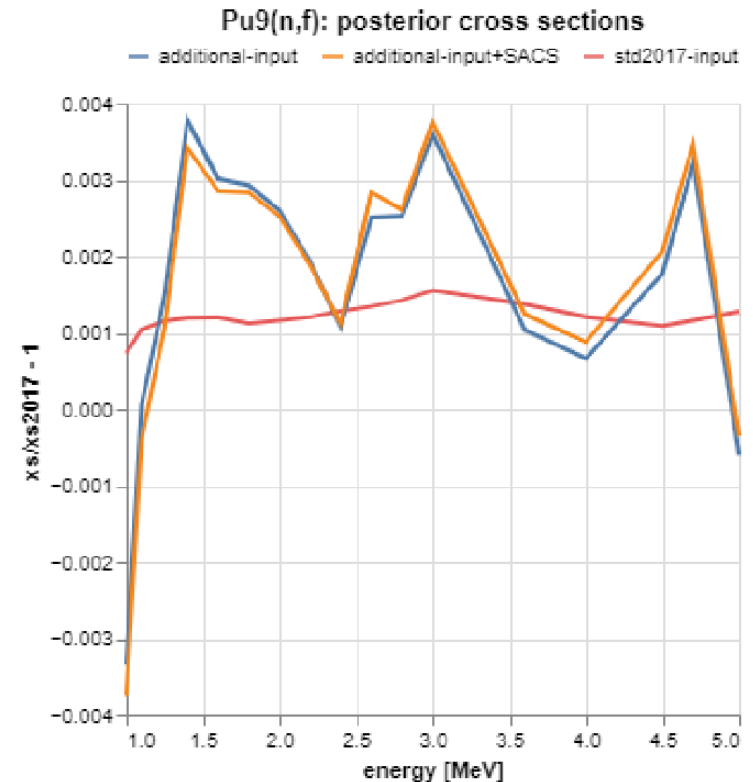




Figure 3: Evaluated $^{239}\text{Pu}(n,f)$ cross sections relative to the IAEA STD 2017[3] from 1 MeV up to 5 MeV.

Reaction	This work GMApy $\equiv C$ [barn]	This work, SACS exp. $\equiv E$ [barn]	C/E^1
$^{235}\text{U}(n,f)$	1.221 (0.3%)	1.221 (0.91%)	1.000 (0.96%)
$^{238}\text{U}(n,f)$	0.323 (0.4%)	0.327 (1.06%)	0.988 (1.13%)
$^{239}\text{Pu}(n,f)$	1.803 (0.4%)	1.826 (1.03%)	0.987 (1.10%)



¹ C/E uncertainties derived assuming C and E are independent quantities.


Treatment of “unknown unknowns”






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Unrecognized Sources of Uncertainties (USU) in Experimental Nuclear Data

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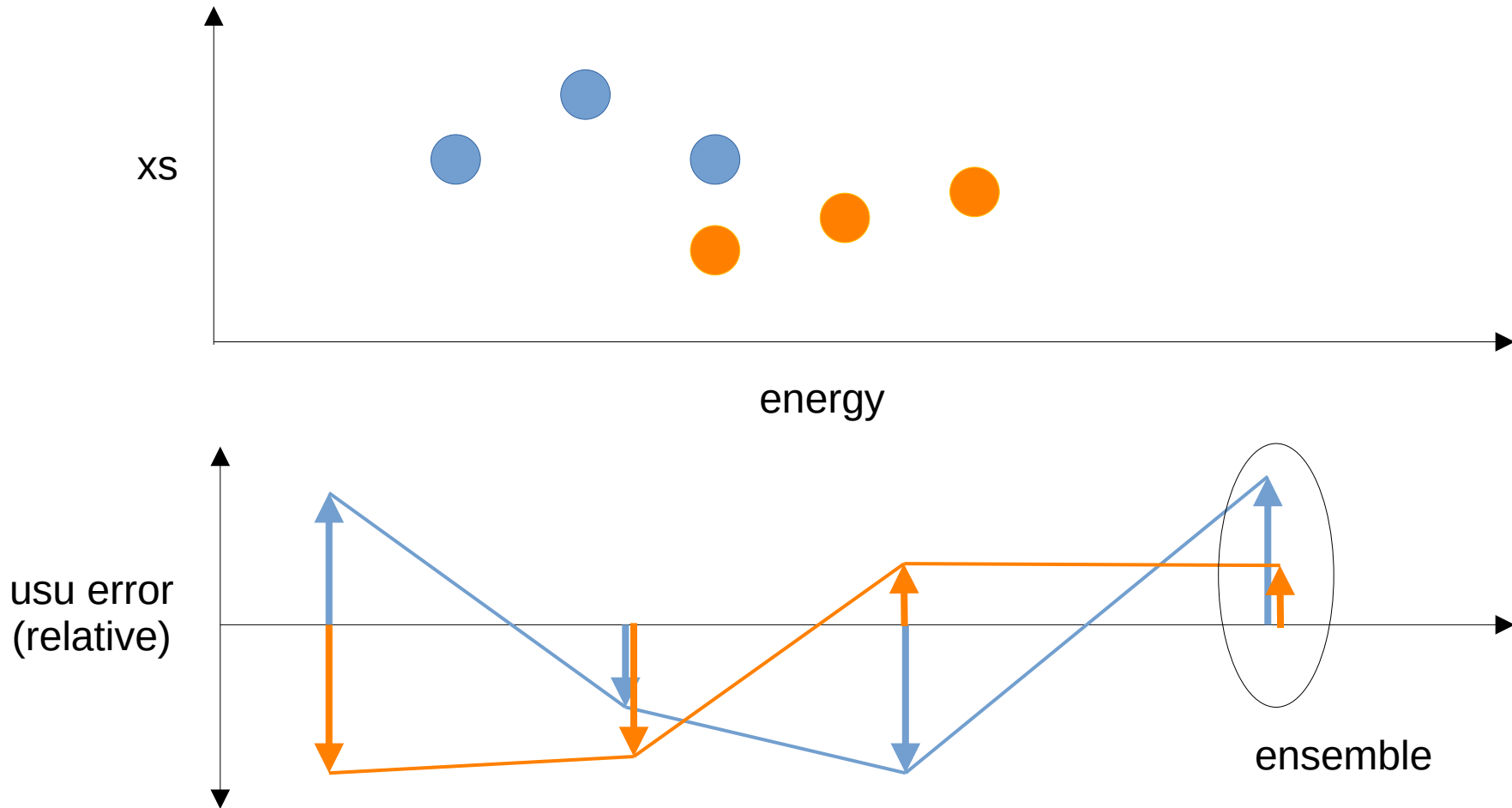
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<https://doi.org/10.1016/j.nds.2019.12.004> [Get rights and content](#) 

Abstract

Evaluated nuclear data uncertainties reported in the literature or archived in data libraries are often perceived as unrealistic, most often because they are thought to be too small. The impact of this issue in applied nuclear science has been discussed widely in recent years. Commonly suggested causes are: poor estimates of specific error components, neglect of uncertainty correlations, and overlooked known error sources. However, instances have been reported where very careful, objective assessments of all known error sources have been made with realistic error magnitudes and correlations provided, yet the resulting evaluated uncertainties still appear to be inconsistent with observed scatter of predicted mean values. These discrepancies might be attributed to significant unrecognized sources of uncertainty (*USU*) that limit the accuracy to which these physical quantities can be determined.

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 (implicitly done by Bayesian formulas)

Refined Bayesian modeling

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

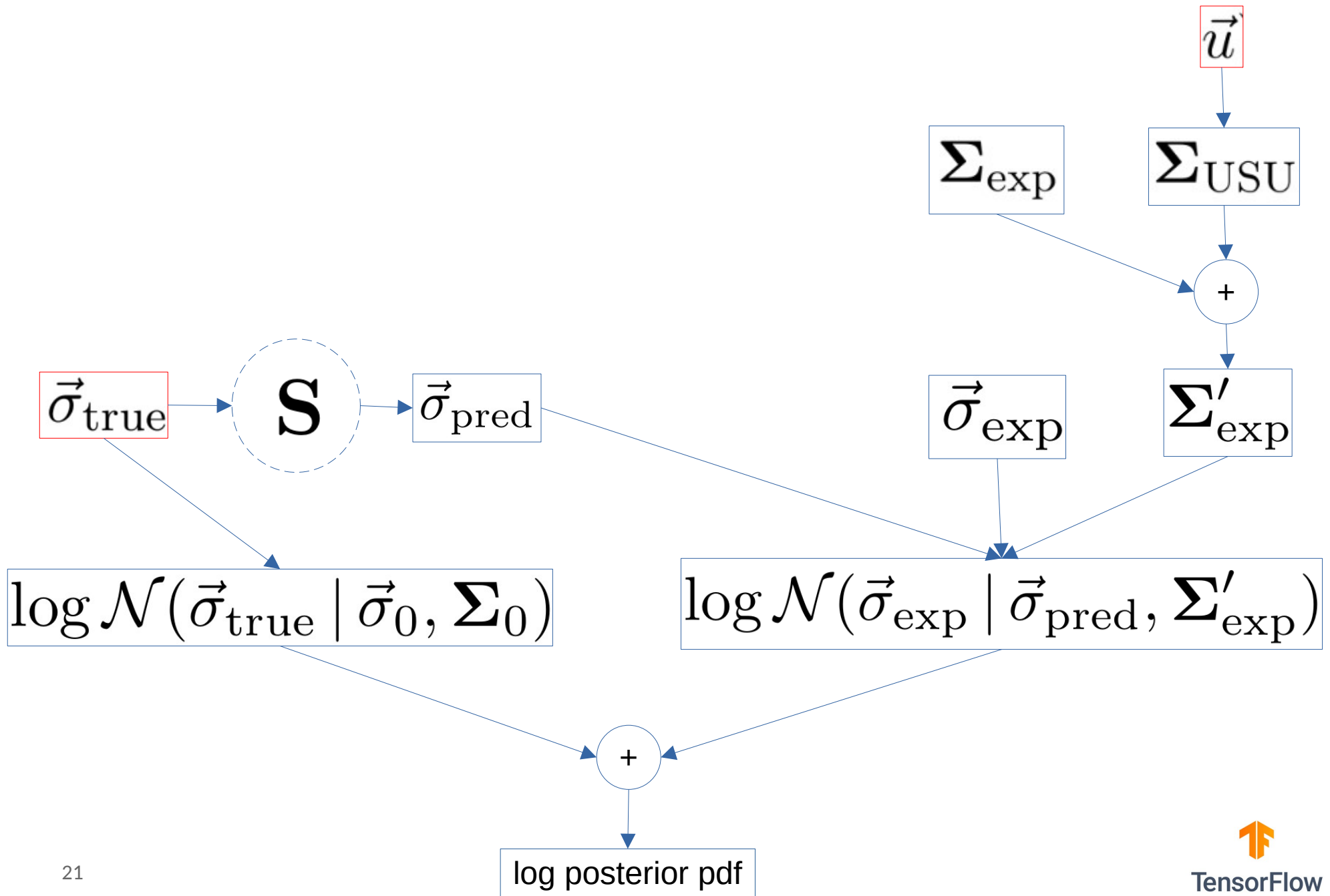
Remove the assumption that experimental covariance matrix is perfectly known

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

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

Improper uniform prior $[0, \text{inf}]$ on u_i

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

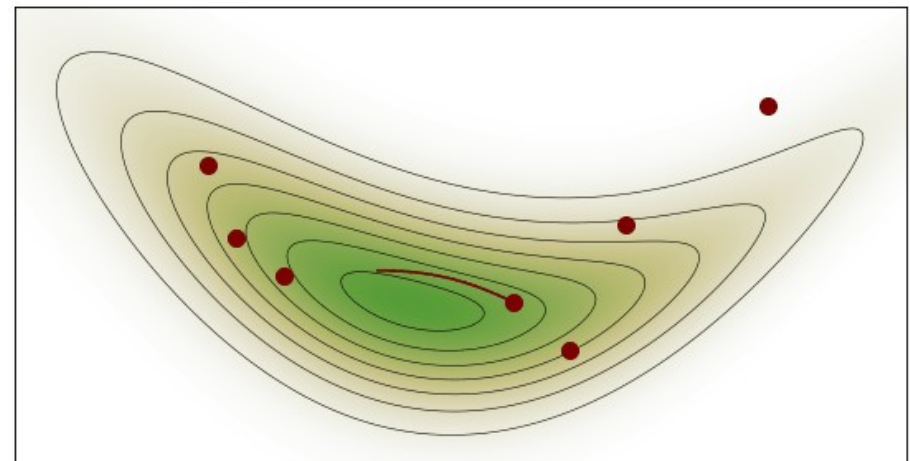
Hamiltonian Monte Carlo

- 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

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

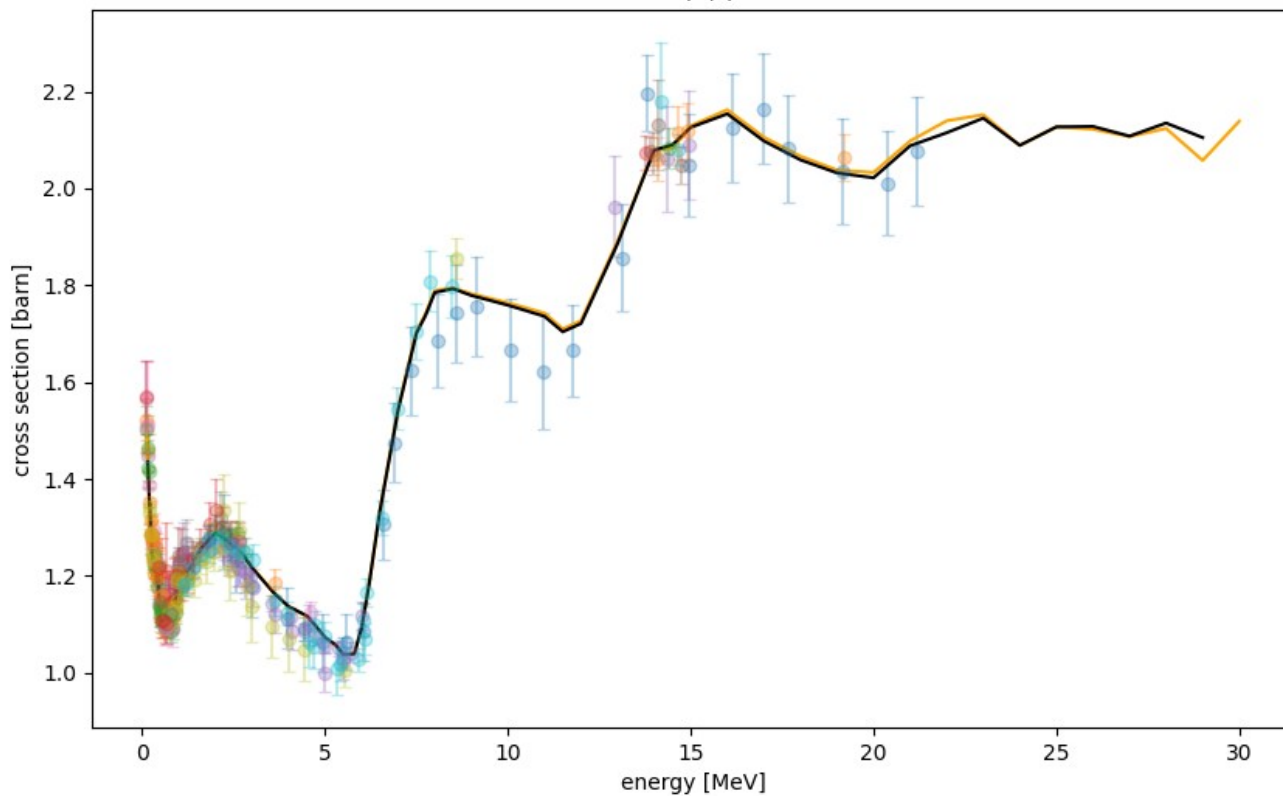
$$H(\mathbf{x}, \mathbf{p}) = U(\mathbf{x}) + \frac{1}{2} \mathbf{p}^T M^{-1} \mathbf{p}$$

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

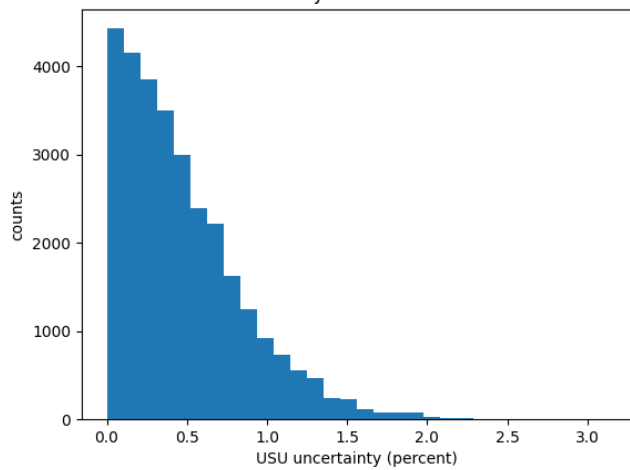


Example U5(n,f)

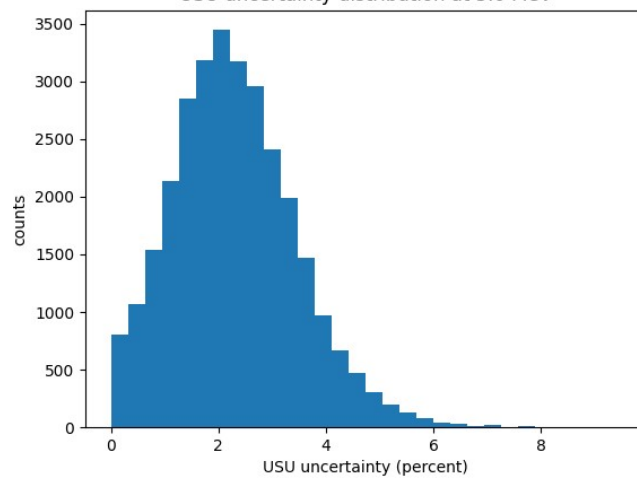
U5(n,f)



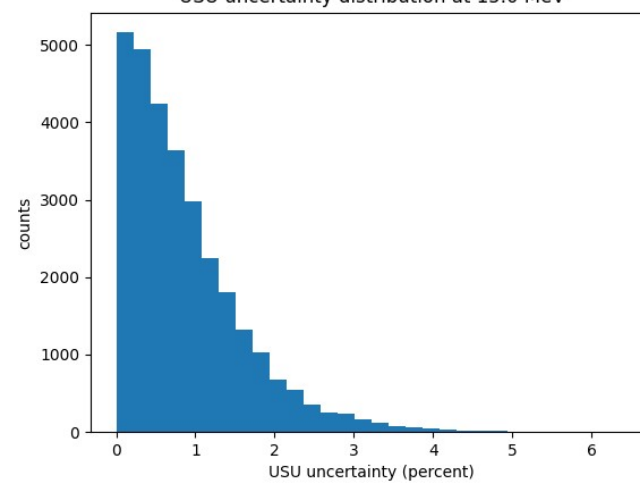
USU uncertainty distribution at 1.0 MeV



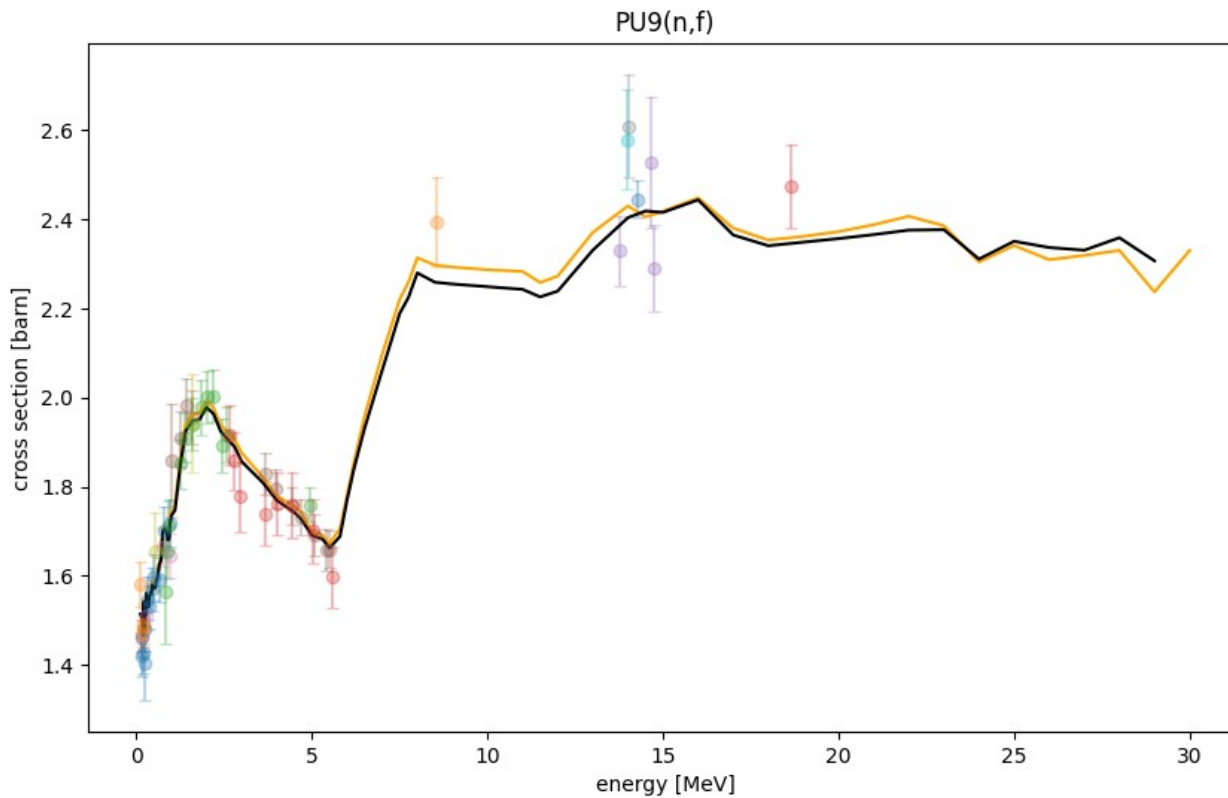
USU uncertainty distribution at 5.0 MeV



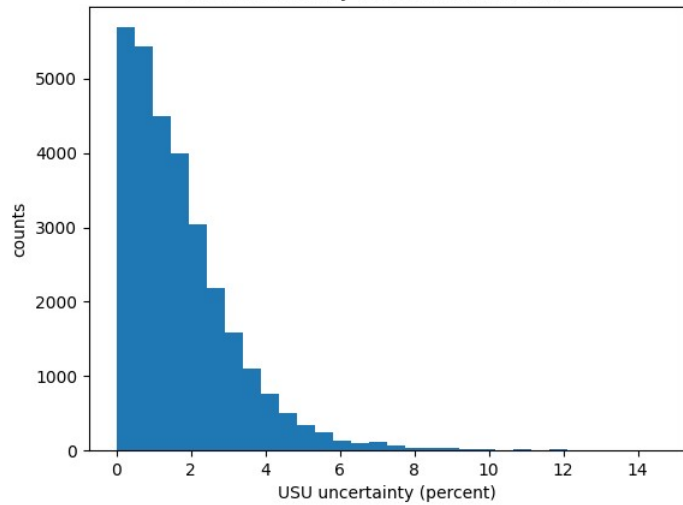
USU uncertainty distribution at 15.0 MeV



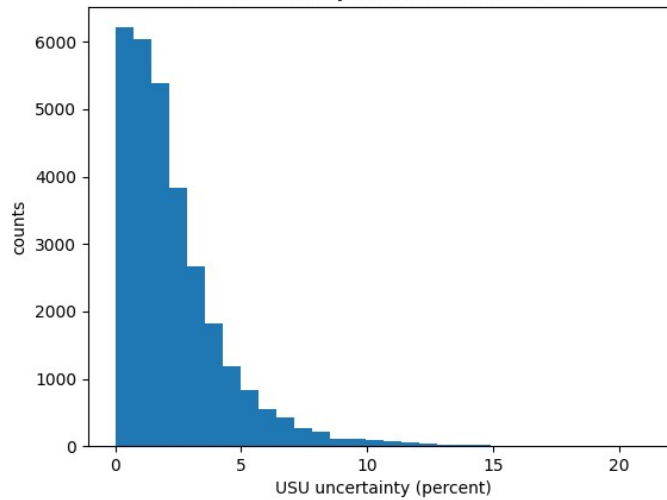
Example Pu9(n,f)



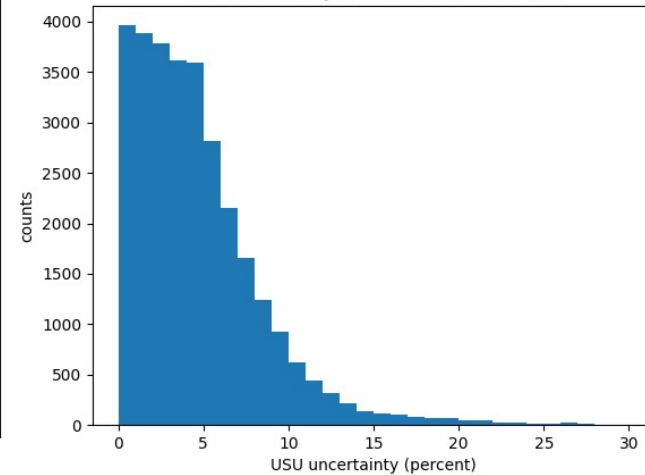
USU uncertainty distribution at 1.0 MeV



USU uncertainty distribution at 5.0 MeV



USU uncertainty distribution at 15.0 MeV



Conclusions

- New experimental data added but more work needs to be done
- Application of UQ templates
- Modernization of code (new observable types, MCMC methodology)
- Rigorous treatment of energy-dependent USU uncertainties