White paper for 5–10 Year Priorities on the Topic of Nuclear Data Covariances and Uncertainty Quantification for Users

March 11, 2024

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Chapter 1

Introduction

This white paper documents 5–10-year priorities on the topic of nuclear data covariances and uncertainty quantification (UQ) for users. Special emphasis was placed on identifying such needs that are cross-cutting across many users. These needs were identified at the virtual Nuclear Data Uncertainty Quantification Working Meeting (NDUQWM) from Oct. 11 to 13, 2022 by a group of thirty invited participants listed in Table I representing:

- Nuclear data producers: spanning from differential experiments, nuclear theory, evaluation, processing, validation, integral experiments,
- Nuclear data users: covering astrophysics, antineutrino physics, forensics, nuclear criticality safety, isotope production, neutron dosimetry, nuclear medicine, global security, reactor design, reactor operations and safety, safeguards, space applications, spent fuel inventory, stockpile stewardship, *etc.*

The Department of Energy (DOE) Office of Science asked that NDUQWM be convened because of the need for improved uncertainty quantification across many programs. In addition to the DOE Office of Science's advocacy for this meeting, ten other program managers were present for the first day to see the high-level needs presented by the participants in their advisory role.

The **goal** of this meeting was to draft this **white paper and prioritize nuclear data covariance and uncertainty quantification needs of users**. These needs are described herein in an actionable context (*i.e.*, a high-level plan is given to address them), and are feasible for the community to tackle the need (*i.e.*, high-level idea of funding is provided).

Chapter 2 provides a high-level summary of the priorities, while Chapter 5 describes them in more detail. Chapter 3 introduces nuclear data covariances and uncertainty quantification. Specific examples are provided in Chapter 4.

Table I: The advisory panel taking part, and presenting at the Nuclear Data Uncertainty Quantification Working Meeting is listed. The listed individuals were part of the discussion on and drafting this document.

Denise Neudecker (chair and editor)	Los Alamos National Laboratory
Robert C. Little (co-chair and co-editor)	Los Alamos National Laboratory
Lee Bernstein	Lawrence Berkeley National Laboratory
Rike Bostelmann	Oak Ridge National Laboratory
Dave Brown	Brookhaven National Laboratory
Robert Casperson	Lawrence Livermore National Laboratory
Stephen Croft	Lancaster University
Shaheen Dewji	Georgia Tech
Nathan Gibson (co-chair)	Los Alamos National Laboratory
Larry Greenwood	Pacific Northwest National Laboratory
Pat Griffin	Sandia National Laboratory
Lucas Kyriazidis	Nuclear Regulatory Commission
Amanda Lewis	Naval Nuclear Laboratory
Marco Pigni	Oak Ridge National Laboratory
Boris Pritychenko	Brookhaven National Laboratory
Brad Rearden	X-energy
Jo Ressler	Lawrence Livermore National Laboratory
Catherine Romano (co-chair)	The Aerospace Corporation; NDWG Chair
Tony Slaba	NASA Langley Research Center
Michael Smith	Oak Ridge National Laboratory
Vlad Sobes	The University of Tennessee, Knoxville
Alejandro Sonzogni	Brookhaven National Laboratory
Scott A. Vander Wiel	Los Alamos National Laboratory
Nicole Vassh	TRIUMF
Andrew Voyles	Lawrence Berkeley National Laboratory
Kyle Wendt	Lawrence Livermore National Laboratory

Chapter 2

High-level Summary of Priorities

Table I provides a high-level summary of those projects identified as high priority by the advisory panel. These projects are listed in order of their perceived importance for users. However, we advise that all of these projects should be tackled for maximal benefit to many users and the nuclear data community. In fact, the output of priority 1 (providing medium-fidelity covariances based on modeling for a wide number of isotopes and observables where covariances are currently missing) could be significantly enhanced by undertaking work addressing priority 3 (improving experimental uncertainties that serve as input for evaluations). Pairing that with priority 2 (quality assurances of covariances) would ensure that the covariances are properly tested and documented before their release to users, while priorities 4 and 5 provide the training and tools for users to utilize the resulting data most effectively.

Table I: High-priority projects are tabulated according to their priority. Their size, cost, duration and benefit to users are also briefly summarized.

Project	Chapter	Size	Cost	Duration	Benefit to Users
Medium-fidelity covariances	5.1.1 5.1.2 5.1.3	Large Medium Large	6 FTE/Y 3 FTE/Y 4 FTE/Y	4–5 Y 3 Y 5 Y	Nuclear data covariances are missing for many isotopes and reactions of interest to users in ENDF/B-VIII.0 or are of low fidelity. Part of the reason is that measured data are missing for many of these evaluations. These projects provide medium-fidelity covariances by modeling data across many isotopes and reactions and anchoring model parameters for those reactions where experiments exist. Confidence on application quantities will be increased by more complete and reliable input covariances.
Quality assurances of covariances	5.2.1	Small	0.25–0.5 FTE/Y	Sustained	Standardized testing of covariances before their release increases their quality for all users.
	5.2.2	Small	0.25 FTE/Y	1 Y	Consistent documentation of the reliability of covariances allows users to gauge the level of confidence they can have in their results.
Improved experimental UQ	5.3.1 5.3.2 5.3.3	Medium Small Medium	3 FTE/Y 0.25 FTE/Y 2 FTE/Y	3 Y Sustained 3 Y	Experimental uncertainties bound nuclear data covariances. These projects aim at improved experimental UQ that will result in more reliable evaluated covariances for users.
Covariance and UQ training for users	5.4	Small	0.5 FTE/Y	2 Y	A curriculum will be developed to educate users on covariances and UQ methods and tools.
	5.4	Small	0.5 FTE	Sustained	Various opportunities for users will be offered to learn about covariances, and UQ methods and tools.
Adjustment tools for general users	5.5	Medium	2 FTE/Y	3 Y	ENDF/B libraries are not formally adjusted, and, thus, can lead to large uncertainties in application-relevant quantities. This project provides tools to enable users to credibly reduce nuclear data uncertainties with experiments representing their application.

The projects were ranked according to the impact they would have on multiple users as well as their feasibility. The feasibility of the projects is addressed by providing detailed descriptions on how each could be executed in Chapter 5. The project's size is defined in Table II according to the time, funding level, and personnel needed to successfully finish the projects.

All high-priority projects share the common characteristic that they are expected to have a positive and cross-cutting impact across many application areas. Additional projects were identified that were of high importance for a more limited set of application areas. These needs were classified in a "medium tier" because of their more limited applicability to answer the critical needs of users. These needs are listed in Table III. They are listed in no particular order and are all considered to be of equal importance.

Some general recommendations that either apply to several projects or do not constitute a project are listed below:

- Students, Postdocs, early career scientists, and universities should be integrated into proposed projects in order to sustain a pipeline of young researchers for the field.
- If proposals by users are focused on assessing uncertainties on a quantity of interest due to nuclear data covariances, it is recommended that they include a nuclear data expert on the proposal to critically assess the interpretation of the results considering the current status of nuclear data at hand and inform users how to best leverage existing tools.
- To aid users in reporting and resolving issues, a contact list for various nuclear data issues on the NNDC or NDWG website would be helpful. A monitored forum on which to post issues and comments would be ideal.
- It is highly recommended that nuclear data evaluators document the quality of their nuclear data mean values and covariances when evaluating them. While covariance matrices should be used to capture the quality of the evaluated nuclear data, information should also be captured on the uncertainties and correlations in the underlying experimental data and/ or model parameter that were used to generate these final covariance matrices.
- Experimenters are highly encouraged, where applicable, to conduct a UQ study before executing a planned measurement. This study will highlight the potential impact of the new measurement on the evaluation or upon application quantities.

Table II: The size of the project (small, medium, large) is defined by years, funding level (in FTE per year), and personnel needed. It should be emphasized that the funding levels are preliminary estimates.

Size	Years	Funding Level (USD) & Personnel (per Year)
Small	1–2	< 1 FTE
Medium	2–4	1–3 FTE (including Postdocs/ students)
Large	> 4	Several staff/ Postdocs/ students

Table III: Medium-tier projects are tabulated. The order is arbitrary and each project is of equal, medium priority. Their size, cost, duration and benefit to users are also briefly summarized.

Project	Chapter	Size	Cost	Duration	Benefit to Users
Expanded sensitivity capabilities	5.6	4 small projects	0.75 FTE/Y	2 Y each	Having sensitivities for more quantities of interest enables users that have adjustment/ UQ tools to assess adjusted data/ bounds for these quantities.
Sampling from covariances	5.7	Medium	2 FTE	3 Y	This project provides users with open-source capabilities to sample from covariances, *e.g.*, for multi-physics purposes.
Thermal scattering law (TSL) covariances	5.8	Medium	2 FTE	3Y	This project would provide TSL covariances for users related to NCSP, nonproliferation, space reactors, Nuclear Regulatory Commission (NRC), and nuclear energy.
Fission yields covariances	5.9	Large	6 FTE/Y	5 Y	This project would provide fission yield covariances for the first time for users in the areas of anti-neutrinos, reactors, NRC, nonproliferation, safeguards, and astrophysics.
Decay constants & branching ratio covariances	5.10	Large	4 FTE/Y	5 Y	This project would provide decay constants & branching ratio covariances for users in the NRC, isotope production, nuclear medicine, nonproliferation, astrophysics, safeguards, and reactor physics.
Stopping power covariances	5.11	Medium	1 FTE	3 Y	This project would provide stopping power covariances for the first time for isotope production, space application, neutron dosimetry, nonproliferation, and detector technologies.
Delayed-neutron covariances	5.12	Small	1 FTE	2 Y	This project provides delayed neutron data covariances for safeguards, astrophysics, and nonproliferation users.
Re-evaluating cross-cutting integral data	5.13	Medium	2 FTE	2 Y	Expanding the suite of trusted integral data enables validation covering more application areas, and reduces via adjustment nuclear data uncertainties for these users.

Chapter 3

Introduction to Nuclear Data Covariances and Uncertainty Quantification

Nuclear data are the bridge between fundamental nuclear physics and nuclear application calculations. They tabulate physics reaction mechanisms of a nucleus for many isotopes or materials. For instance, the ^{56}Fe(n,p) cross section describes the likelihood that a neutron is absorbed by the ^{56}Fe nucleus, interacts with it, and emits a proton. Nuclear data across the chart of nuclides are collected in nuclear data libraries; for instance, ENDF/B-VIII.0 [1] is the current U.S. nuclear data library. These libraries are fed by a complex pipeline shown in Fig. 3.1. **Nuclear data are evaluated** by statistically combining information from differential experiments and nuclear theory. **Nuclear models** are fitted to existing differential data of the same or similar observables and auxiliary experimental data informing model parameters such as, *e.g.*, level densities. **Differential experimental data** measure nuclear data observables in a 1:1 correspondence, for instance the ^{56}Fe(n,p) cross section as a function of energy. They differ from **integral data** in that the latter integrate over several nuclear data observables but mirror applications on a small scale. **Integral data are used for validating nuclear data**, an essential step before libraries can be released to users. Validation calculations are undertaken with **particle-transport codes**, such as MCNP® Code Version 6.2[1], Mercury, *etc.* [2, 3]. Nuclear data are **processed** via codes such as AMPX or NJOY [4, 5] from their native format (ENDF-6, GNDS, *etc.* [6–8]) to be readable by transport codes. Processing is part of a larger verification effort to ensure that the format can be read and data pass basic tests, while validation counter-checks that nuclear data libraries perform as a whole reasonably well in predicting applications of specific subject areas.

After nuclear data are released as a library, some application users choose to **adjust** them with experimental data representing their application. Adjustment entails optimizing nuclear data and their uncertainties by means of a mathematical algorithm with experimental data. The resulting nuclear data library is then tied to the specific application represented by the experimental data and no longer a general purpose library (which is primarily based on differential data and theory rather than focused on one particular application).

Nuclear data covariances, Cov_{ij}, encode the uncertainties of nuclear data. They are formally defined as the second moment of a probability density $p(x_i, x_j)$ between data points x_i and x_j:

$$\mathrm{Cov}_{ij} = \int\int (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) p(x_i, x_j) \mathrm{d}x_i \mathrm{d}x_j, \tag{3.1}$$

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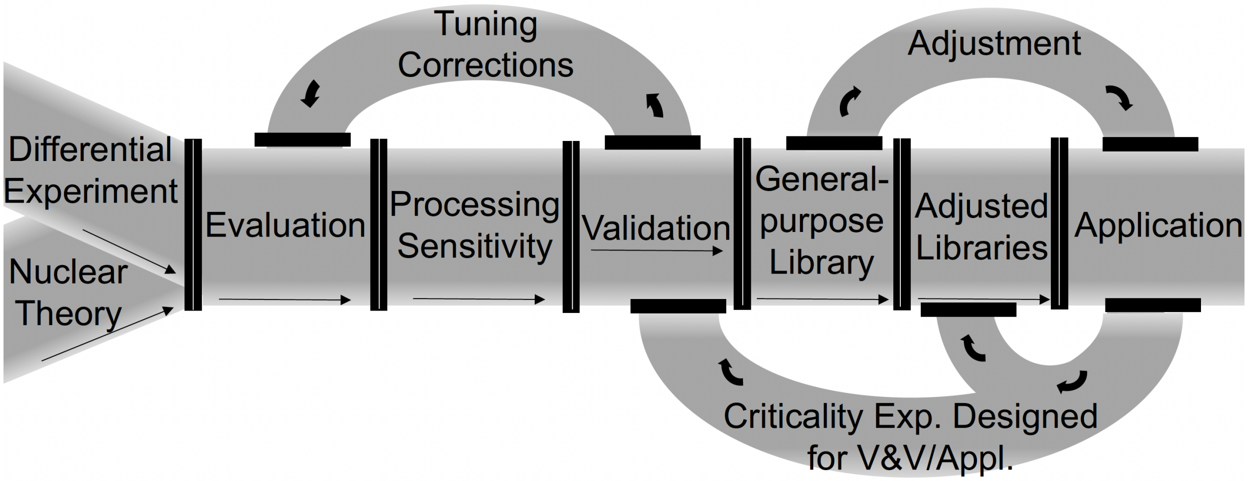


Figure 3.1: The various parts of the nuclear data pipeline are depicted. Differential experiments encompasses undertaking their experiments, documentation and their compilation into EXFOR. Validation encompasses transport codes.

with the mean value, $\langle x_i \rangle$, being the first moment:

$$\langle x_i \rangle = \int \int x_i p(x_i, x_j) \mathrm{d}x_i \mathrm{d}x_j. \tag{3.2}$$

A probability density function $p(x_i, x_j)$ gives the "complete probability information" for these two variables; sampling from it is akin to performing a measurement.

The diagonal of covariances stores the **variance**, var_i, of an individual nuclear data point:

$$\mathrm{var}_i = \int \int (x_i - \langle x_i \rangle)^2 p(x_i, x_j) \mathrm{d}x_i \mathrm{d}x_j. \tag{3.3}$$

Variances can be translated to **relative uncertainties**, δ_i, by:

$$\delta_i = \sqrt{\mathrm{var}_i} / \langle x_i \rangle. \tag{3.4}$$

The off-diagonal elements of a covariance matrix measure the linear dependence between x_1 and x_2, and can be translated to **correlation coefficients**, Cor_{ij}, by:

$$\mathrm{Cor}_{ij} = \mathrm{Cov}_{ij} / (\sqrt{\mathrm{var}_i \mathrm{var}_j}). \tag{3.5}$$

This correlation coefficient can assume values between 1 and -1. In simpler terms: The diagonal of the covariance matrix informs one how uncertain an individual data point is. The correlation coefficient encodes how x_i and x_j jointly vary together. If the correlation coefficient between x_i and x_j is, *e.g.*, 1, and one increases x_i, then x_j is expected to increase with it.

Uncertainties on nuclear data stem from uncertainties on differential experimental data and nuclear models (parameter uncertainties and model defects). They can be reduced by folding in knowledge from appropriate integral experimental data via adjustment algorithms.

Nuclear data covariances can be used together with nuclear data mean values for adjustment. Another use case is to employ them for uncertainty quantification where one estimates bounds on an application quantity of interest due to uncertain nuclear data, Δq. One uncertainty quantification approach is to apply the **"sandwich formula"**:

$$\Delta q = \sum_{ij} S_i^q \mathrm{Cov}_{ij} S_j^q, \tag{3.6}$$

where one folds nuclear data covariances with sensitivities, S_i^q, of an application quantity of interest, q, to nuclear data, x_i. Another approach is to build an approximate probability distribution function, $\hat{p}(x_1, x_2)$, using mean values and covariances and sampling from it. Then, these samples are used for calculating samples of the quantity of interest and then perform statistics analysis on it to obtain the needed bounds.

The sandwich formula depends on the availability of sensitivities (far from a given for some quantities of interest) and that the problem is linear, while the computational cost for the sampling approach can be prohibitive. Both UQ approaches can only provide reliable results if the mean values are reasonably accurate and covariances realistically reflect the uncertainties on mean values. If nuclear data covariances are unrealistically high or low, this can have significant impact on the reliability on application bounds. Examples of applying covariances are shown in Chapter 4.

Chapter 4

Examples Showcasing the Impact of Nuclear Data Covariances and Uncertainty Quantification on Use Cases

4.1 Impact of Experimental and Model Uncertainties on Effective Neutron Multiplication Factor

The example in Fig. 4.1 illustrates how over-simplified uncertainty quantification of differential experiment and model covariances can adversely impact nuclear data covariances and application quantities. To this end, simplified differential experiment covariances were estimated by extracting total uncertainties from the EXFOR [9–12] database for the ^{239}Pu prompt fission neutron spectrum (PFNS); a correlation coefficient of 0.5 was assumed between uncertainties of the same experiment, while 0 correlation was assumed between different data sets. If instead, detailed covariances are estimated following Ref. [13], the resulting evaluated mean values at incident-neutron energies of 0.5 MeV change by less than 10% until 10 MeV in the left-hand side of Fig. 4.1. While the impact on mean values is seemingly small, the corresponding impact on evaluated uncertainties is very large as shown in the bottom left-hand side panel of Fig. 4.1—those evaluated uncertainties would be underestimated by up to 70%! Even the relatively modest change in mean PFNS values leads to a change in the calculated criticality of Jezebel by 195 pcm (approximately 210 pcm is the difference between a controlled Jezebel assembly and one emitting lethal doses of radiation) [13] showing that the choices on **experimental covariances** can matter for applications. Improved uncertainty quantification of experimental data could be tackled by Priority 3 in Section 5.3.

Conversely, it matters if simplified versus detailed **model covariances** are used for evaluations as can be seen from the right-hand side of Fig. 4.1 [14]. In both cases the same model (the Los Alamos model) is used, but in the simplified version only uncertainties for 5 parameters are considered while they are considered for more than 20 in the case of the detailed model covariances [14]. Evaluated mean values change less distinctly as care was taken to get the same model mean values, but evaluated uncertainties are again up to 70% smaller if the simplified versus more detailed model covariances are used. This example highlights the importance of robust modeling for obtaining realistic evaluated uncertainties as proposed in Priority 1 of Section 5.1.

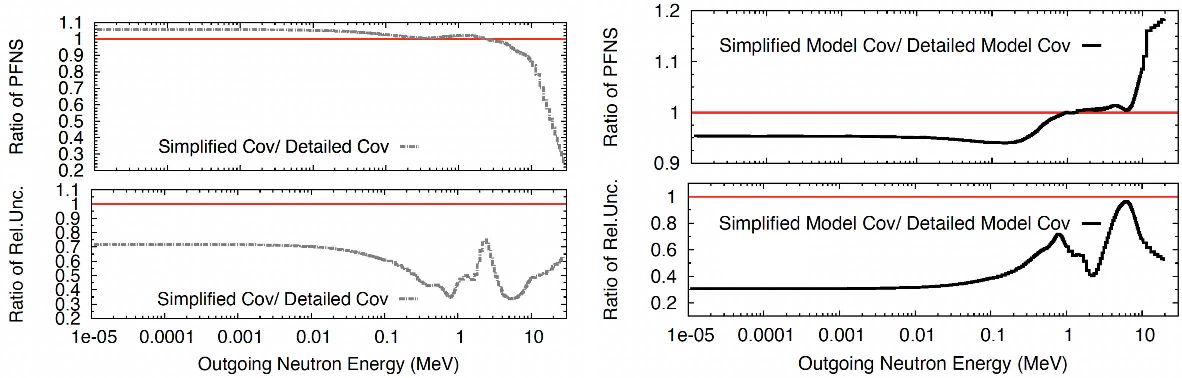


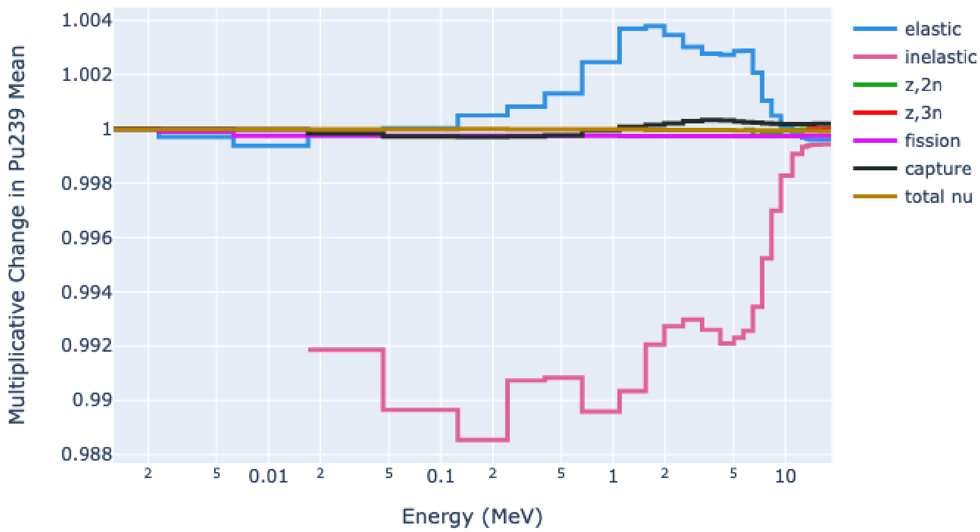
Figure 4.1: (Left) The change in evaluated ^{239}PFNS mean values (top) and uncertainties (bottom) at incident neutron energies of 0.5 MeV are shown if simplified versus detailed experimental covariances are used for the evaluation. (Right) The same as for the left-hand side except for using simplified versus detailed model parameter uncertainties.

4.2 Impact of Integral Experiments on Nuclear Data Covariances and Application Bounds

This example illustrates how adjustment of general purpose mean values and covariances can help reduce nuclear data uncertainties and tighten application bounds. The adjustment tool "EAT" developed by M. Grosskopf for the Experiments Underpinned by Computational Learning for Improvements in Nuclear Data (EUCLID) project [16] was used to adjust ENDF/B-VIII.0 nuclear data with respect to the experimental criticality values of the Jezebel and Flattop critical assemblies [18] via the generalized least squares algorithm [15, 16]. It can be seen from Fig. 4.2 that this adjustment with integral experimental data not only changes ENDF/B-VIII.0 ^{239}Pu mean values, but also significantly reduces ^{239}Pu nuclear data uncertainties by up to 40% compared to ENDF/B-VIII.0. If one uses unadjusted ENDF/B-VIII.0 covariances, the simulated criticality uncertainty of Dirty Jezebel is 908 pcm. If one forward-propagates these adjusted covariances via the sandwich formula in Eq. (3.6) to assess nuclear data uncertainties on simulated criticality values of the Dirty Jezebel assembly [18], this uncertainty is 272 pcm—70% lower! This latter example illustrates that users can effectively reduce nuclear data uncertainties on their quantity of interest by adjustment if appropriate experimental data are available to underwrite this uncertainty reduction. However, open-source adjustment tools and sensitivities beyond criticality are missing. These shortcomings could be addressed by Priority 5 (Section 5.5) or medium priority of Section 5.6.

4.3 Impact of Covariance Data in Nuclear Energy Applications

A recently concluded study assessed the impact of cross section covariance data on reactivity and power profile calculations of various non-light water reactors (non-LWRs) [17]. One part of the study quantified the uncertainties due to covariance data on the calculated metrics. Compared to traditional LWRs, significantly larger uncertainties were observed due to the use of different materials (*e.g.*, different moderator and fuel materials) and different neutron spectra (*e.g.*, fast neutron spectrum). Additionally, sensitivity analyses were performed to identify the key cross section uncertainties that are the top contributors to the observed output uncertainties. By identifying the top contributors, recommendations for additional measurements and evaluations for specific cross sections can be made. Furthermore, by performing analyses with different ENDF/B releases, the impact of updates in covariance data for important nuclide reactions can be observed.



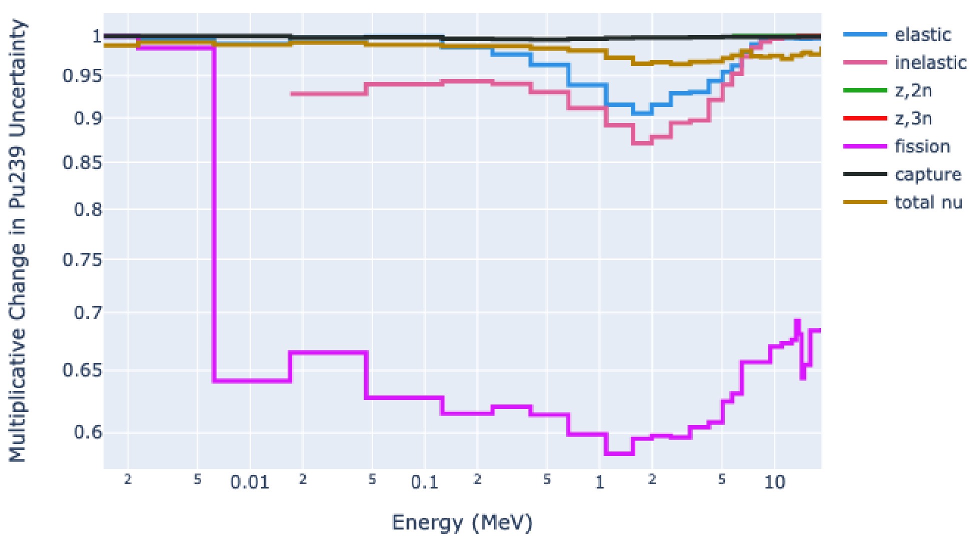


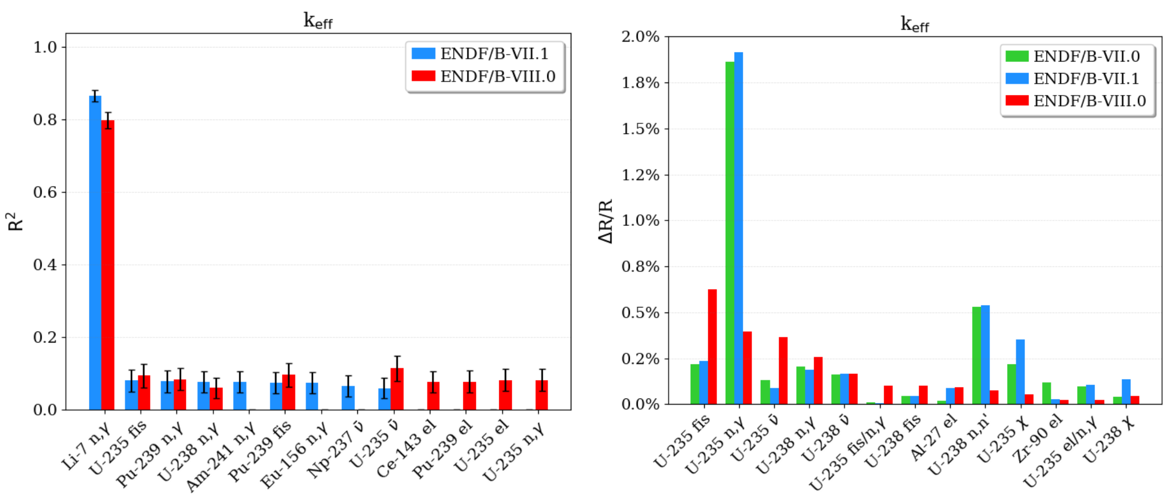
Figure 4.2: (Left) A modest % change of adjusted mean values as a ratio to ENDF/B-VIII.0 ^{239}Pu nuclear data is shown. (Right) The % reduction of adjusted uncertainties compared to ENDF/B-VIII.0 ^{239}Pu nuclear data uncertainties is significant. The adjustment was undertaken with the generalized least squares algorithm using the EAT tool [15, 16] using criticality values of Jezebel and Flattop assemblies.

Two examples are provided: the analysis of the effective neutron multiplication factor (or criticality) k_{eff} for a fluoride-salt cooled high temperature reactor (FHR) and a heat pipe reactor (HPR). The FHR is a graphite-moderated pebble-bed reactor operated with high assay low enriched uranium (HALEU) fuel and cooled by FLiBe salt. The HPR is an unmoderated fast spectrum reactor with HALEU metallic fuel cooled with potassium. Table I lists the k_{eff} uncertainties obtained in analyses using the latest three ENDF/B nuclear data library releases. It is noticeable that the uncertainties are a lot larger compared to commonly obtained uncertainty of approximately 0.5% in LWRs. It is also observed that the HPR uncertainty is cut in half with the ENDF/B-VIII.0 library compared to the previous releases.

Table I: k_{eff} uncertainty in FHR and HPR [17]

Library	FHR	HPR
ENDF/B-VII.0	-	2.01%
ENDF/B-VII.1	1.38%	2.08%
ENDF/B-VIII.0	1.43%	0.98%

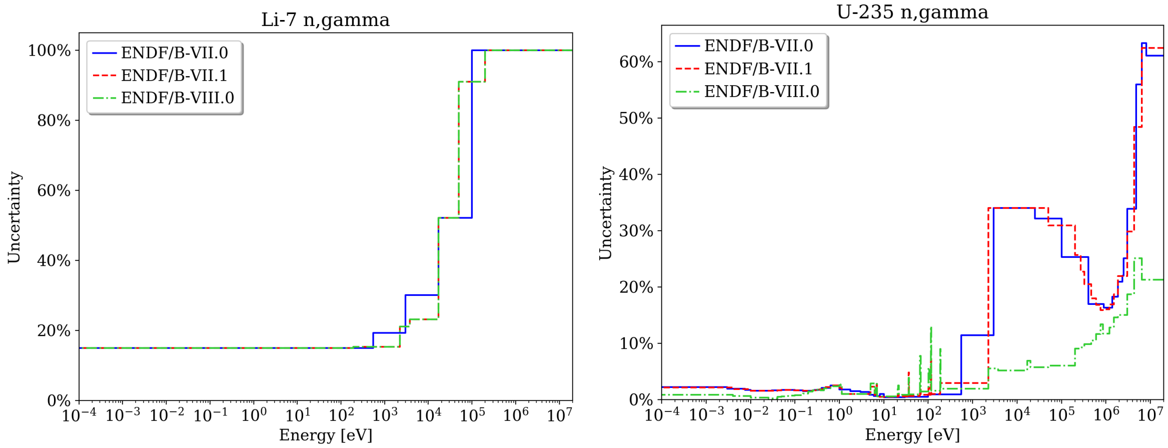
Sensitivity analyses revealed that the k_{eff} uncertainty in the FHR is dominated by the contribution of the uncertainty of radiative neutron capture (n,γ) in ^{7}Li (Figure 4.3). If the large uncertainty of this one reaction (see Figure 4.4) would be reduced, it is expected that the reactivity uncertainties for the FHR will be significantly reduced. Similarly, for the HPR the ^{235}U(n,γ) reaction was identified as top contributor when using ENDF/B-VII.0 and ENDF/B-VII.1 data. While this reaction has played a minor role in LWR uncertainty analysis, this reaction is the dominating contributor here because of the fast neutron flux in the HPR, *i.e.* large neutron flux in the energy range in which the ^{235}U (n,γ) uncertainty is especially large. This example further demonstrates the impact that a reduced uncertainty can have: This specific uncertainty was reduced in ENDF/B-VIII.0. This reaction is therefore no longer the dominating contributor to the k_{eff} uncertainty and consequentially the k_{eff} uncertainty is dramatically reduced.



(a) FHR (b) HPR

Figure 4.3: Top contributors to the k_{eff} uncertainty [17].

In conclusion, identifying specific uncertainties and spending effort in reducing these can dramatically improve the accuracy of predicted metrics in nuclear energy applications. This is especially valid for advanced reactors in which new materials and therefore different nuclear data are important. However, while such analyses can quantify uncertainties and identify key contributors, the uncertainty



(a) ^{7}Li (n,γ)

(b) ^{235}U (n,γ)

Figure 4.4: Cross section uncertainties.

propagation methods rely on the availability of complete and reliable nuclear data. For example, impacts of uncertainties for angular scattering distributions and thermal neutron scattering data could not be assessed due to the absence of these data in the ENDF/B libraries. All covariance data gaps need to be closed to allow accurate prediction of uncertainties. Such gaps could be, for instance closed with covariance data coming from Priority 1 in Sections 5.1 or 5.8.

4.4 Use of Nuclear Data Covariances Supporting Manufacturing

The focus of this example is an analysis of a proposed aliquot casting operation at the LANL plutonium manufacturing facility (PF-4) involving tantalum. The quantity of interest in this analysis was the simulated upper subcritical limit (USL) of the operation. The USL is defined as a limit on the calculated k_{eff} value established to ensure that conditions calculated to be subcritical will actually be subcritical. From an operational perspective, a higher USL might lead to increased criticality safety limits for fissile material mass that could support increased throughput for the analyzed operation.

The LANL sensitivity / uncertainty tool Whisper [68] was used to analyze the operation. Whisper ingests nuclear data sensitivities and calculated over experimental results from existing benchmarks as well as nuclear data sensitivities for the application of interest. Whisper also requires nuclear data covariances to perform statistical analyses. MCNP [2] is used to simulate the sensitivities.

The initial Whisper analysis for the tantalum aliquot casting operation resulted in a very low USL of approximately 0.94 (right-hand side of Fig. 4.5 with line "Whisper 1101"). This was largely because of very limited neutronically relevant benchmarks.The widely used quantity measuring similarity of application to benchmarks (c_k) had a maximum value of 0.64. Further exploration of using the Whisper capability to perform generalized least squares adjustment of nuclear data to existing benchmarks resulted in only modest improvement to the USL, suggesting the need to design a more relevant integral benchmark experiment.

An optimization technique was used to design such an experiment. The resulting design had a c_k of 0.9997 with 1.0 being maximally similar to the application of interest. The right-hand side of Fig. 4.5 shows how well the ^{181}Ta inelastic scattering sensitivity profile from that experiment matches the application. When incorporating that postulate experiment into the Whisper benchmark suite and re-analyzing the application, the USL was increased to 0.98 in the left-hand side of Fig. 4.5.

Covariance data are central throughout the entire Whisper analyses and design optimization process. It was known that the tantalum covariance data used were from the Low-Fidelity Covariance

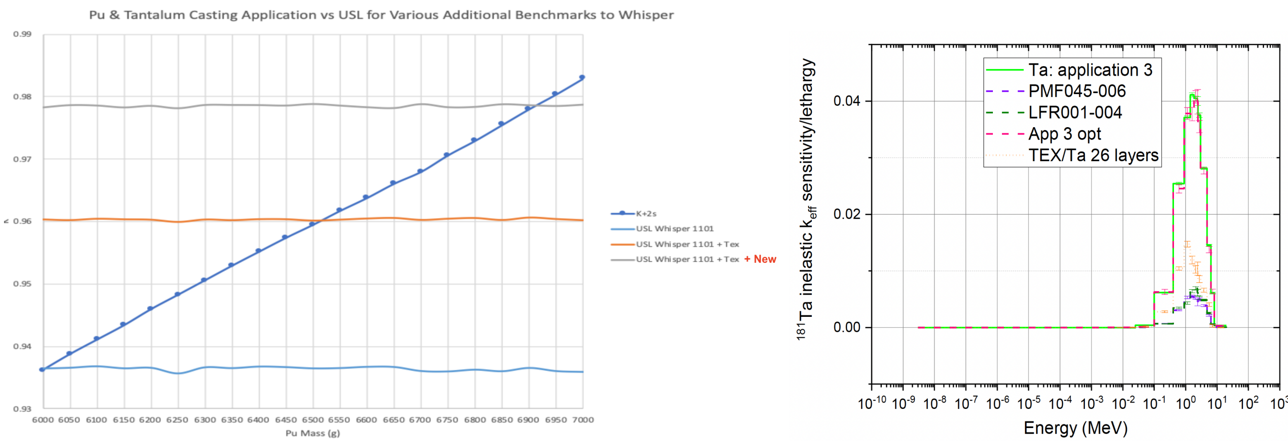


Figure 4.5: (Left)The original Upper Subcritical Limit using over 1100 benchmarks is less than 0.94. Adding the fastest TEX / Ta experiment increases the USL to 0.96. The addition of the optimized experiment increases the USL to almost 0.98. The possible Pu mass limit with this USL is about 1 kg greater than with the original benchmark suite, which could lead to improved throughput. (Right) Sensitivity profiles for ^{181}Ta inelastic scattering. The solid green line is the aliquot casting application. The dashed lines (PMF and LFR) are the highest c_k from 1000+ ICSBEP and IRPhEP configurations. Note how the sensitivity in these cases is extremely low compared to the application. The fastest TEX/Ta experiment is closer, but still lacking for the application. App 3 opt is from the optimized experiment design and shows a sensitivity extremely close to the application.

Project [19]. Before committing to the cost of performing a new integral benchmark experiment, there is a need for developing improved covariance data for tantalum to ensure maximum benefit for the application. Project 1 described in Section 5.1 could address such a need.

Chapter 5

Priority and Project Description

5.1 Priority 1: Medium-fidelity Covariances

5.1.1 Covariance Data for Neutron-induced Cross Sections, Neutron Multiplicities, and Prompt-fission Neutron Spectra

Description of Work Needed There is presently a severe lack of covariance data in our leading nuclear data libraries, such as ENDF/B-VIII.0 [1]. Of >500 neutron-induced reactions in ENDF/B-VIII.0, only about half of the reactions have any covariance data at all. Of those reactions that have some covariance data, many either have deeply approximate Low-Fidelity (Low-Fi) [19,30] covariances or have covariances of suspicious quality, often owing to the limited resources when that evaluation was performed. Reference [30] generated covariance information subsequently used to update two US nuclear data library releases [31] [1]. They were obtained by propagating estimated nuclear model parameter uncertainties to the reaction cross sections for an extensive set of materials. In that work the emphasis was on the completeness rather than on precision with minimal or limited reference to experimental data.

In an ideal world, one would re-evaluate all of the reactions with missing or suspicious data. However, this is an immense task given the sheer number of different reactions that need to be considered. Modernized approaches to medium fidelity surrogate covariances projects are needed to fill in the remaining gaps from thermal energies to 60 MeV and correct for some of the crude approximations used in the previous Low-Fi project. Additionally, extending these approaches to higher energies is essential to address the needs of many modern uncertainty quantification efforts, where reactions exceeding 50–60 MeV incident energies can be important. Building on using model parameter variation as a basis for medium fidelity covariances, modern statistical approaches can be used to implement these covariances in a statistically interpretable form as well as better account for uncertainties in experimental inputs to the evaluation. Exploring these statistical techniques should also entail recommendations on best practices which techniques and input yield more reliable covariances. Currently various approaches are taken (based on only experiment or model correlations, *etc.*) with various degrees of sophistication across the nuclear data libraries. Some simplified approaches can impact covariance quality and reliability. Because of the significant differences in how reactions are modeled in the resolved resonance and the fast incident neutron regime as well as for prompt fission observables, there are three parallel medium fidelity approaches needed to address these disparate regions and observables.

Why is it Important to Address the Issue for Users Neutron-induced reactions are crucial inputs across a vast spectrum of applications ranging from fundamental science to large scale societal applications. Low energy reactions are essential to modeling astrophysical processes in neutron-rich environments where the s-process and r-process can occur, and quantifying the uncertainties in these reactions is key to disentangling where in the cosmos the heavy elements are produced. Neutrons interacting with detector materials are a significant background signal in many large scale neutrino experiments such as the Deep Underground Neutrino Experiment (DUNE). Accurate modeling of secondary neutrons—resulting from a neutrino interaction—is critical for assessing detector response and sensitivity in DUNE and enabling a robust determination of the neutrino mass ordering and charge conjugation and parity violation [34]. Other application needs concern the assessment of uncertainties on integral quantities such as for the design and operational parameters of nuclear power reactor followed by data adjustment used to generate nuclear data libraries optimized to specific applications. Improved precision of evaluations and associated uncertainties are needed at the low energies (< 3 MeV) relevant for nuclear astrophysics studies and the high energies (> 20 MeV) utilized to produce some isotopes in the national interest.

How Could this Issue be Tackled?

Cross sections for thermal and above resonance energies There is no unique way to approach the generation of medium fidelity covariances. One possible approach in the thermal-energy and fast incident neutron regime is to start from similar parameter variations used in previous efforts such as Low-Fi but using non-uniform prior distributions for the model parameters. Samples of model outputs from these priors can be used to train a response model which in turn can be used to forward propagate through an experimental likelihood function when experimental data are accessible. In these cases, any unknown widths in the parameter prior can be tuned and used for insight into expected widths of priors for nearby nuclei. Because cross sections are smooth in the thermal and fast incident neutron regime, techniques like Gaussian process regression can be used to build a parameterized response model which can be exactly forward propagated through the likelihood, but the correct treatment of correlated reaction channels will require deeper investigation.

Prompt fission neutron observables for thermal and above resonance energies Prompt fission neutron observables such as the PFNS or the average prompt fission neutron multiplicity are currently being modeled by fission event generators such as FREYA and CGMF [46, 47]. While the modeled average prompt fission neutron multiplicity in the fast range is of evaluation quality [48], the predicted PFNS is far from experimental data [49] and the Los Alamos model is frequently being used for evaluations [52]. In any case, all these models would need to be emulated if correlated covariances across many isotopes and observables need to be provided given their otherwise prohibitive computational cost. This emulation effort would need to include a fit to “anchor” experimental data of well-measured isotopes for a medium-fidelity assessment of model parameters. For the best possible assessment of model parameters, project 3 (Improving experimental uncertainty quantification capabilities in Section 5.3) could yield improved input. In addition to supporting the required broad parameter search, machine learning techniques could also be used to estimate model defects.

Resolved Resonance Range There are two sequential factors that strongly contribute to the generation of consistent covariance information. The first relies on the ability and fidelity of the theoretical model to reproduce measured quantities. R-matrix theory is an effective theoretical model to describe the resolved resonances. However, the lack of a theoretical model consistently extending the resolved resonance formalism to include measured data in the energy region where there are overlapping resonances, results in a very difficult task to first estimate and then evaluate nuclear data uncertainties and corresponding model correlations. The extension of the R-matrix theoretical model to describe the fluctuations in partial statistical regime, will allow by definition the inclusion of covariance information on any theoretical observable. This represents the second factor and it is devoted to the completeness of the covariance information—which is particularly important for adjustment methodologies.

Level of Funding Needed There are three medium scale projects that need to be funded, each requiring a Postdoc and significant time from several staff, around 1 FTE of a senior/ mid-career staff and 1 Postdoc / early career per project. Significant computation resources will be required as well.

5.1.2 Covariance Data for Angular- and Energy-distribution of Secondary Particles

Description of Work Needed An effort is required to estimate and populate the covariance information for the evaluated data of the angular- and energy-distributions of secondary particles. The ENDF-6 format [6] for this data type is defined and would currently store these data in Files 34, and 35 corresponding to the mean values stored in Files 4 (angular distributions), 5 (energy distributions) and 6 (energy-angle distributions). While Files 4, 5 and 6 are populated in ENDF/B-VIII.0, very little covariance data are currently available for them, and no covariance format for what would be "MF 36" currently exists. A notable example where data are found is File 34 for ^{56}Fe, representing the uncertainty on the evaluated moments of the Legendre expansion of the angular distribution for elastic scattering. While the format is defined in ENDF, due to the lack of use of these Files, the capabilities of nuclear data processing codes to correctly read, interpret and use these (rare) files should simultaneously be investigated and improved as necessary.

Why is it Important to Address the Issue for Users The angular- and energy-distribution of secondary particles have important impact on multiple applications, especially, for the design of small, advanced reactors where neutron leakage plays a large role. Angular distributions determine whether neutrons going out to the reflector will be reflected back into the core or will forward-scatter and leak out, impacting the criticality of the core. Energy-distributions affect moderation. Both of these effects also impact critical experiments, a strong foundation of the nuclear criticality safety program. In safeguards applications, angular- and energy-distributions affect the ability to accurately model and predict active interrogation measurement techniques. Predictive modeling of targetry for isotope production is also impacted by reliable modeling of angular- and energy-distributions of secondary particles. Finally, as the use of accelerator-driven neutron sources (e.g., deuteron breakup, Li(p,n), DT, DD) becomes more relevant for fusion science and aerospace shielding applications, characterization and evaluation of data generated in these facilities rely upon energy- and angular-distributions of all secondary particles [65]. No covariance information in Files 34, and 35 computationally results in zero propagated uncertainty for user applications. This is both misleading and not conservative. Therefore, for all of the applications mentioned above, it is very important to populate the ENDF library with some initial covariance values. That entails to develop a format for and populate File 36.

How Could this Issue be Tackled? A low- to medium-fidelity approach to covariance data is suggested to initially populate Files 34, 35 and/or 36 for the heavily-used isotopes (10–30 isotopes). That requires developing the format for File 36. Even a Low-Fidelity, bounding-(large uncertainty) approach initially will be sufficient in order to distinguish between zero propagated uncertainty for applications due to no covariance information and some (conservative) amount of propagated uncertainty for the applications. With feedback from the users, it will later become apparent for what applications and for which isotopes there will be a need to have these uncertainties reduced using higher-fidelity approaches.

Once some values are established for the uncertainties, MCNP6 [2] has the capability to calculate the sensitivities of k_{eff} with respect to the moments of the Legendre expansion of the angular distributions. Basic scripting allows this to be combined with the covariance matrix for linear-propagation of uncertainty. Alternatively, a Total Monte Carlo approach [20] can be used to propagate the uncertainty in the forward direction. For the inference problem, the Low-Fidelity work can be done by hand/expert-judgement. The medium-fidelity approach will require some custom code development.

Level of Funding Needed Initial effort level is suggested at 3 FTEs for 3 years including students and Postdocs. The code development (not expert judgment) part of this project is well suited for a PhD graduate student or Postdoc.

5.1.3 Covariance Data for Charged-particle-induced Reactions

Description of Work Needed In the US ENDF/B-VIII.0 nuclear data library, the status of charged-particle induced sub-libraries consists of some sparse evaluations but with a complete lack of covariance information. Most users in need of these data instead rely on a number of application-specific libraries (such as the IAEA medical libraries, the European Activation File, *etc.*). These are often very limited in evaluated reactions and are based on application needs. TENDL can be used for completeness (rather than correctness). Therefore, a comprehensive generation of these kinds of nuclear data libraries up to 250 MeV is needed—including covarianes. As detailed in a recent scoping study focusing particularly on α-particle induced reactions [60], there are recommended areas of improvements including a list of priority nuclei particularly relevant for (α, n) reactions. Nuclear data for incident particles of a minimum of protons, alphas, deuterons, ^{3}He, ^{7}Li, ^{6}Li, ^{12}C, and ^{16}O are needed.

Why is it Important to Address the Issue for Users Several types of application areas motivate the development of special nuclear data libraries such as for charged-particle induced reactions. For instance, in passive neutron calculations for verification of certain nuclear materials, an accurate description of the neutrons emitted in (α, n) reactions is essential. Another subject area interested in such libraries is isotope production. Complementary to this, nuclear forensics, treaty verification, nuclear material measurements for safeguards, reactor-based materials production detection, and nuclear test monitoring rely extensively on output responses from modeling codes using nuclear data libraries. Applications mentioned above focus on incident α-particle energies between about 1 and 8 MeV. However, there are important branches of studies in the low α-particle energy range up to 2 MeV such as the investigation of α-cluster structure in N$\neq$Z nuclei, as well as analyses and experiments devoted to improve the knowledge of nucleosynthesis and reaction rates in nuclear astrophysics and cosmochemistry. Additionally, ion beam analysis—which typically focuses on the broader energy incident α-particle spectrum—requires accurate knowledge of nuclear reaction cross sections of light elements. Lastly, the isotope production community likewise requires this same information, for a broad range of light ions on nearly all stable targets.

How Could this Issue be Tackled? To satisfy application needs, at least, for α-particle induced reactions, the aim is to generate a complete ENDF sub-library. Because of the limited number of incident alpha evaluations currently in ENDF, the focus in generating evaluated data will be on the completeness rather than the precision of the evaluation. To be clear, this project requires providing also mean values for some reactions for the very first time that must be accompanied by covariances. Moreover, the performance of the evaluated charged-particle ENDF library should be validated with integral quantities such neutron yield and emerging neutron spectra. To guarantee completeness in compiling the nuclear data libraries, the evaluation work devoted to it will be of medium-fidelity level to generate the mean values and of low-fidelity level to generate the related covariance information. The strategy to generate α-particle reaction cross sections, which can be extended to other needed incident charged particles, will consider existing libraries such as JENDL-AN [61] and their consistent update according to available recently measured experimental data together with nuclear reaction codes (*e.g.*, SAMMY [62] for R-matrix analyses and TALYS [63] for Hauser-Feshbach evaluations, where the latter might require some additional improvement to better predict the desired reactions). Particular focus will be devoted to the priority list compiled in Romano et al. [60] to satisfy application needs for commonly used U and Pu matrix compound fuel materials such as UO2, UF6, PuF4, and PuO2 for which the dominant neutron producing (α,nx) reactions are from oxygen and fluorine isotopes.

This work will include compilation of measured data but also improved completeness in types of data included in the evaluated nuclear data file such as angular distribution, and gamma and neutron energy spectra. Available nuclear reaction codes will be used to generate from the low-energy up to the 250-MeV energy range covariance information by propagating estimates on the nuclear model parameters. Verification of the evaluated nuclear data library and validation testing (using integral quantities such neutron yields or emerging neutron spectra) will be the final steps prior to the release of the library. The validation testing will require the update and development of neutron source codes such as SOURCES4C [64]. Updating SOURCES4C was listed as a priority in the (α, n) scoping study [60] but will be a larger task because the code uses hardwired nuclear cross section data of unknown origin; the need is to get this code to use ENDF, and also bring the numerical methods up to date and give it an easy-to-use user interface.

Level of Funding Needed This work is expected to be a large size project running over 5 years with a mix of senior and early or intermediate career staff for continued education of the workforce.

5.1.4 Roadmap for Nuclear Data Covariances

A complete and accurate nuclear data library with mean values and covariance matrices is desired by the applications community. When provided, nuclear data covariances can be propagated to assess confidence in application metrics. For some applications, notably those involving safety, conservative estimates are made when uncertainties are unknown or untrusted; accurate assessments of the uncertainty can improve design margins with significant cost (and often time) savings. Nuclear data covariances are also used in applied sensitivity studies to identify nuclear needs, providing direct feedback to the nuclear science community for high-impact improvements to the nuclear data. The importance of nuclear data covariances in creating higher-fidelity, predictive capabilities for applications cannot be overstated.

Nuclear data are shared across a broad range of applications, requiring extensive coverage over multiple physics regimes. Requesting or requiring mathematically and physically robust covariances is not immediately feasible. We outline a proposed "roadmap" below with four major objectives, ordered by priority, toward achieving important nuclear data covariances used by applications.

Objective 1: Complete Covariances for Incident-neutron Reaction Cross Sections

Neutron reactions are important to numerous applications, including the current and future nuclear power industry, medical community, astrophysics, and nuclear security applications.

Task 1-1: Complete Incident Energy Covariances Significant gaps in covariances exist, even for common isotopes. In 2008, a Low-Fidelity or "Low-Fi" effort was undertaken to fill gaps [19]. This effort should be revisited and augmented with new knowledge and methods from parameter studies and machine learning efforts, as well as new experimental data collected since the initial study. This update will improve confidence in these estimates and will provide needed values while full evaluations are completed.

Task 1-2: Establish Recommended Methods for Cross-reaction Covariances Correlated uncertainties frequently occur between nuclear reactions of a given isotope, often due to the total cross section having smaller uncertainty than the sum of individual reactions. A recommended procedure, beyond the computationally expensive Total Monte Carlo sampling, for defining these correlations must be developed.

Task 1-3: Establish Cross-isotope Covariances Changes to reactions in one isotope may affect reactions in a neighboring isotope. For example, first-chance fission data in an actinide isotope should also be reflected in the second-chance fission data of the heavier neighboring isotope.

Task 1-4: Establish thermal neutron covariances, through Thermal Scatter Law (TSL) data New measurements have expanded and improved TSL data, which are important for accurately describing very low energy neutron interactions. However, for all TSL data, covariances are lacking.

Objective 2: Complete covariances for neutron-induced reaction products

Neutron reaction products are also important to many applications, where the types (*e.g.* particles, photon), numbers (*e.g.* multiplicities), energies, and emission angles affect assessment metrics.

Task 2-1: Complete covariances for fission product yields For actinides undergoing fission, correlations between independent yields and cumulative yields with incident neutron energy, and between fission products, are needed. This effort is currently underway through a multi-institutional effort supported by NA-22 and led by LANL.

Task 2-2: Establish covariance data for multiplicities For reactions emitting more than a single particle or photon, the correlation between the number of outgoing particles/photons produced with the ingoing neutron energy is needed.

Task 2-3: Establish covariance data for energies (spectra) for outgoing particles The energetic emissions of a nuclear reaction can affect observations or subsequent reactions. Two-dimensional correlations between incident neutron energies and outgoing particle spectra are needed. This covariance should also address the emission multiplicities. Examples of recent evaluations are given in Refs. [48, 49].

Task 2-4: Establish covariance data for angle-dependent quantities The angular dependence of particle/photon emission can affect absorption/leakage from a system or detection rates for an application. Correlations to incident neutron energies, outgoing particle/photon energies, and multiplicities should be considered. This effort may need additional data for completeness; sampling techniques for sensitivity studies should also be considered.

Task 2-5: Establish branching ratio covariances For reactions and decays with two or more possible pathways, the relative probabilities (or branching) are important for application observables and/or final products. Covariance data between these observables are important, but significant questions remain for the evaluation of mean values. Establishing complete covariances for branching ratios is not recommended until data improvements, *e.g.*, consistent values in ENDF and ENSDF databases, are achieved first.

Objective 3: Provide covariances for charged particle reaction data

Incident reactions with charged particles, notably light ions with $Z <= 6$, are also important to reactions such as medical isotope production and astrophysics. Charged-particle data do not have the same broad use or scrutiny as neutron data. The nuclear data community is discussing databases and evaluation efforts for charged-particle data in a similar manner as has been done for neutron data.

While covariance data for charged-particle data are important, significant focus on complete covariance data is recommended to be a future endeavor. Methods and processes developed for neutron-induced reactions will establish a framework that can be followed,

Objective 4: Provide covariances for photon reaction data

Like charged-particle data, photon-induced reaction data lacks the compilation and database structures employed for neutron reactions. Complete covariance data is recommended for a future effort, following the framework for neutron data.

We are recommending, at first, a focus on neutron-induced data (reactions and products), as these data impact the most applications. Charged particle and photon data are also important and are included here for awareness but establishing full covariance data is recommended for a future date, following methods and techniques established by neutron reaction data. Our recommendation is for the broader, collaborative, nuclear data community focus in the near term on neutron data while considering aspects of charged particle and photon data in later years. Covariances for these latter types may be established through smaller-scope efforts driven by specific application needs.

5.2 Quality Assurance for Covariances

5.2.1 Proper Standard Validation of Covariances

Description of Work Needed Nuclear data covariances need to be stringently tested before their release to users to guarantee that (a) they satisfy mathematically required properties for a covariance matrix, and (b) are of a reasonable magnitude given the evaluation input. If covariances do not satisfy mathematical constraints, some application codes sampling from them will not be able to use them and users then have to apply ad-hoc fixes. Under- or over-estimated uncertainties or unphysical shapes of correlations are more difficult to identify, but can have far-reaching consequences. Unrealistic estimates of evaluated uncertainties can lead to poorly estimated bounds on application simulation, while unphysical correlations can lead to improper adjusted mean values [15, 39].

In short, users require stringently tested covariances for their UQ applications. CSEWG strives to carefully data, including covariances, before the release of an ENDF/B library. The current CSEWG workflow is:

- An evaluator commits to the appropriate ENDF project on the NNDC GitLab instance (`git.nndc.bnl.gov`),
- The ADVANCE CI/CD system performs automated physics and formatting checks including several covariance quality checks,
- Build reports are presented to evaluation reviewers who review the evaluation,
- The ENDF library manager, upon successful completion of the evaluation review, merges the evaluations into the Phase II testing branch,
- The Phase II testing is managed by the CSEWG Covariance and Validation Committees, Phase II testing included testing with the AMPX system [4] and the SCALE/ TSUNAMI [84, 85] package as well as testing with CovVal [51], testing using data from DICE, processing of covariances via FUDGE or NJOY [5], *etc.*

Description of Work Needed In order to guarantee that evaluated covariances are valid, the following tests should be included in either ADVANCE or similar systems:

- Testing whether all covariances can be fully processed. This will require enhancements and corrections of processing codes such as FUDGE and NJOY.

- Testing of correlations for mathematical constraints (diagonal is 1, off-diagonal values are between -1 and 1, positive semi-definiteness, and symmetry) and nuclear data imposed constraints (constraints on covariances resulting from sum-rules on mean values as well as obeying physically imposed limits),

- Testing of the magnitude of the evaluated uncertainties with respect to the bounds established based on experimental information [50, 51] and flagging those data that appear to violate these bounds,

- Expand the plots of 1D quantities such as cross sections and average prompt, delayed, or total neutron multiplicities to include accompanying uncertainty plots. These plots should include data expected lower/upper bounds on uncertainty values (see Ref. [51]) in addition to data extracted from EXFOR [9–12].

- An expansive covariance report including inventory of covariances per isotope and a listing of missing covariances per isotopes as well as per reaction within a file of an isotope. This inventory should be linked to plots of the correlation matrices and quantity cross correlations of quantities.

- Any evaluation documentation and metadata describing the covariances. This can include information about whether a given evaluation's covariance data were generated from one of the "Low fidelity" covariance projects such as "Low-Fi" [19], COMMARA or by Total Monte Carlo approaches based on parametric variation of nuclear model data used in evaluations such as TENDL. Structured documentation such as described in the GNDS-2.0 [8] specifications can simplify the programming task for newer evaluations, but providing that in ENDF-6 [6] is also important as that format is still widely used.

- Quickly assessing benchmark performance via the "sandwich formula" (first-order linear error propagation described in Eq. (3.6)) such as performed with the DICE system [66]. To this end, DICE is using an archive of SDF (sensitivity data files), generated with TSUNAMI, to rapidly calculate benchmark uncertainties due to those of nuclear data using the sandwich formula. This would require reading in various sensitivity libraries [66, 67],

- Processing with the code AMPX. The completion of efforts making AMPX open source should be of high priority to enable straightforward integration with codes such as ADVANCE.

Based on this, feedback for the evaluators of covariances will be generated. If the covariances are unrealistic or improperly formulated, it is always more advisable that the evaluator fixes them, rather than the user having to apply less informed ad-hoc fixes.

Why is it Important to Address the Issue for Users Fast, automated testing allows for rapid development of the ENDF/B library while ensuring a quality product. Every user of nuclear data covariances will benefit from adequately estimated and fully verified covariances. On the one hand, users do not have to spend valuable time to correct for violations of math properties. On the other hand, application simulation bounds are more realistic, if the input covariances are reasonable in size to begin with.

Level of Funding Needed Development of ADVANCE and the evaluation reviews are all performed with a combination of DOE-NP/SC base funding and funding from the NCSP. The changes listed above are planned to take place over the next few years. Development can be dramatically accelerated with dedicated funding. Inclusion of "Sandwich formula" level observable calculations requires approximately one-time investment of 0.25 FTE investments.

5.2.2 Proper Documentation of Covariances and Easy-to-access App

It is difficult for a data user to assess the quality much less the contents of a typical ENDF evaluation. For easier access, one can make use of web applications by either the IAEA or NNDC to display the data and check their consistency. The NNDC hosts a webapp called SIGMA (`https://www.nndc.bnl.gov/sigma/`) [69] which can serve this need. SIGMA presents a complete inventory of an ENDF evaluation as well as plots of cross sections, average prompt/ delayed/ total fission neutron multiplicity values and fission product yields but lacks uncertainty information. SIGMA will be modernized over the next few FY's (fiscal year's), providing an opportunity to add features of use to the UQ user community. One can build on experience gained from other tools such as EEVIEW from the Nuclear Data Section at the IAEA.

Description of Work Needed This update can build on the covariance reviews discussed above, used in the previous ENDF/B-VII.1 and ENDF/B-VIII.0 releases and built (or planned for) the ADVANCE CI/CD system. This list is very similar to the list above. Here we would expand the list by the following update: Plots of integral metrics (resonance integrals, Maxwellian-averaged cross sections, thermal values, *etc.*), with EXFOR data and covariances propagated from the evaluations. These can tell the user quickly the overall quality of an evaluation throughout the resolved resonance region. The features can be expanded as improvements to the EXFOR library and supporting infrastructure are made.

Why is it Important to Address the Issue for Users Nuclear data can be complex and opaque and the covariance data accompanying evaluations is the most complex and difficult to understand. Users are also often faced with a situation where they do not know if the evaluated uncertainties constitute a high-fidelity best estimate or merely an upper or lower bound. If they user knew whether the covariances are to be trusted, they would know if their simulated application bound is representative or might reflect rather a lower or upper bound. Not knowing this can adversely influence decisions taken based on these simulations. An easy to use tool allows users to make quick assessments of the quality of a given covariance evaluation. An integral aspect of this is a mechanism for feedback from users evaluators. If the quality of the evaluation does not meet their needs (as quality needs continually to improve), this feedback to the evaluation community would be able to trigger an updated evaluation or new measurements.

How Could this Issue be Tackled? This need can be tackled with a modest increase in scope and funding to the planned SIGMA webapp modernization project. This task is slated to begin in parallel with the winding down of the ENSDF modernization project in FY23. The present report can guide development.

Level of Funding Needed At NNDC: SIGMA modernization is already within the scope for the current NNDC base funding. Additional features to support UQ would require an additional 0.25 FTE for the web developer(s). Inclusion of "Sandwich formula" level observable calculations requires an approximately one-time investment of 0.25 FTE.

5.3 Priority 3: Improving Experimental Uncertainty Quantification Capabilities

5.3.1 Modernizing EXFOR and Storing Expert-judgment in Sister Database

Description of Work Needed The EXchange FORmat (EXFOR) library [9–12] contains experimental nuclear reaction and spontaneous decay data, such as cross sections, angular distributions, yields and spectra [9]. It is a publicly accessible data storage of experimental results. DOE requires public access to research results, see for example [21, 22], and EXFOR is one of the places where one can access the data. EXFOR's importance for the field of nuclear data evaluation cannot be overstated; it is the first place for evaluators to start an evaluation when including experimental data. EXFOR is also used by experimenters to compare their results. In addition, EXFOR contains critical information (metadata and uncertainties) that help evaluators and experimenters judge the quality of data and perform uncertainty estimates. Thus, the quality of information in EXFOR directly translates in to the quality of evaluated data and its uncertainties in our ENDF/B libraries.

Presently EXFOR does NOT store the data that are finally used for the evaluation found in any nuclear data library. Data scientists curate experimental and theoretical results (reject and accept them for evaluation purposes, cut down to reliable energy range, *etc.*), add or update uncertainties according to present-day knowledge, and even change data (*e.g.*, for new values of monitors). However, the curated data are not stored in EXFOR as its philosophy is to reproduce information true to publications and interactions with the authors of the experimental data. This represents a serious gap in archival knowledge that should be addressed.

Why is it Important to Address the Issue for Users The current gap described above represents a loss in the nuclear data pipeline as evaluators have to re-analyze experimental data again and again as past analyses of these data are lost to the community. This translates into many hours of repetitive work for a limited workforce, and process change is needed.

How Could this Issue be Tackled To resolve the nuclear data pipeline issues we propose to:

- Create a parallel, publicly accessible library to EXFOR that stores and incorporate corrections to data and uncertainties that were undertaken by evaluators.
- Store expert judgment on these data and integrate the original and derived data with the underlying nuclear bibliography [10].
- Assess published uncertainties with templates of expected uncertainties for specific measurement types developed recently by the Cross Section Evaluation Working Group (CSEWG) community [71–81].
- Use artificial-intelligence and machine-learning algorithms in conjunction with comprehensive physics models for outlier identification. EXFOR is not structured in a way that is machine learning friendly. Work is needed to develop and implement a new format that machine learning algorithms could read.
- Modernize EXFOR database using the latest computer technologies and develop a new web interface as well as a stand-alone web application.
- Ensure strong interconnectivity with other US Nuclear Data Program databases, such as NSR [23], ENSDF and ENDF, which at the moment is quite deficient due to incompatible formats.
- Collaborate with the U.S. and international nuclear data networks and incorporate the findings of the WPEC SubGroup 50. [70]

Level of Funding Needed It is a medium-sized project that can be accomplished with the help of 3 FTEs (including Postdocs and students) for three years.

5.3.2 Maintain, Update, and Extend Templates for Improved Uncertainty Quantification of Differential Reaction Observables

Description of Work Needed The templates of expected measurement uncertainties [71–81]. should not be static documents—experimental methods will continue to evolve, and our understanding of the uncertainties inherent in all measurement will grow. For this reason, the current templates should be revisited to ensure that they are up-to-date, and should be extended as needed. In addition, there are many observables of importance to the community that were not covered in the original template work, and which need to be put together by subject matter experts.

Why is it Important to Address the Issue for Users Templates to support the recording of expected measurement uncertainties are valuable tools for evaluators of nuclear data observables. Templates aid in ensuring that all experimental data sets are compared on equal footing and that no major sources of uncertainty are neglected. They can be used at the nuclear data verification and validation stage for counter-checking if evaluated uncertainties are consistent with typically achievable uncertainties. For instance, if evaluated uncertainties are significantly below typically reachable experimental uncertainties, a mistake might have happened in providing evaluated uncertainties. Standardization of the reporting of uncertainties will help in fields where the observables and measurement methods are evolving rapidly. The templates may be of use for uncertainty analysis of experiments before they are performed, however, they should be used with care in this case and treated as the absolute minimum uncertainty budget associated with a given experimental technique. Unexpected uncertainties often arise, especially in experiments deviating from prior experience.

Observables that should be assessed: charged-particle induced production cross sections (isotope production, safeguards, astrophysics), thermal scattering (nuclear energy, space reactors, NSCP), photoneutron reactions (astrophysics, isotope production). Many of these templates will overlap with the current templates, reducing the overall work effort.

How Could this Issue be Tackled? The creation of a new measurement uncertainty template for a specific observable of interest can be done with a small targeted project. Two or three subject matter experts can together review the relevant measurement types and decide where there is overlap with the currently available templates and where additional quantification is needed. Where that additional work is needed, the template should be created, reviewed by others within the field, and then published for general use. All published templates should be hosted at the NNDC so that users can access them and supply feedback. Every few years, CSEWG should take responsibility to reach out to the relevant communities and collect feedback on whether the templates are still up to date. If not, the relevant subject matter experts should be consulted and the templates should be updated.

Level of Funding Needed 0.1 FTE every year for the initial digitization of the templates and to start hosting them in a way that is accessible to the community and allows for user feedback, and from then on re-visit 2 templates/ year. If new templates are needed, 1 FTE per new observable template, split between 2-3 people, to review experimental methods, create templates, get feedback from the experimental community, and publish.

5.3.3 Quantifying Unrecognized Sources of Uncertainties in Experimental Data

Description of Work Needed Nuclear data estimates and their associated uncertainties are only as good as the statistical description of data uncertainties. Evaluators are occasionally faced with discrepant experimental data—even after accounting for all pertinent uncertainties, for instance, via templates of expected measurement uncertainties [71–81], *i.e.*, experiment uncertainties seem **collectively** too small because they do not adequately describe discrepancies "between experiments". As a consequence, nuclear data estimates are not optimal and, on top of that, their uncertainties are implausibly small.

An IAEA working group developed [82] clues how to spot these unrecognized sources of uncertainties and gave tentative algorithms how to estimate them. One of these basic fixes is to collect data uncertainties (covariances) from each experiment and then augment these with additional sources of uncertainty that encompass discrepancies between experiments. Augmented covariances need to be a fair representation of data spread both within *and* between experiments so that the corresponding statistical generative model becomes an adequate description of the entire collection of observed data across multiple experiments.

Checking statistical goodness of fit is an important but often overlooked step. This project should develop and recommend goodness of fit techniques that combine statistical rigor and appropriate subject matter input. These should be open-sourced so that every evaluator can make use of them.

Algorithms should be implemented as part of EXFOR plotting tools and/ or openly available for evaluators to automatically identify discrepancies in experimental data, and flag them for evaluators and experimenters to further explore these discrepancies. It would add benefit for the physics interpretation as to the origin of these discrepancies if metadata of the experiments could be linked to data being discrepant starting from machine learning techniques described in [83].

Why is it Important to Address the Issue for Users Identifying unrecognized uncertainties and hints towards their source in experimental data has two benefits: For experimenters, it yields important input on what measurement techniques need to be further explored. If a new measurement can resolve a discrepancy, one credibly reduces evaluated uncertainties. It is also important to know for evaluators if there are discrepancies in experimental data as that might lead to different evaluated uncertainties and mean values that might impact applications. These two benefits positively impact all down-stream users as it ultimately leads to more accurate mean values and more realistic evaluated covariances as input for application simulations.

How Could this Issue be Tackled? As a first step, one could implement the clues for finding unrecognized sources of uncertainties in an EXFOR or stand-alone open-source tool to identify quickly where are discrepancies in data. Another possibility is to perform GLS (generalized least squares)-based evaluations and applying statistical goodness-of-fit tests that combine statistical rigor and appropriate subject matter input. Lastly, one could link data being discrepant and metadata of these measurements to gain clues to the possible sources of these discrepancies.

Level of Funding Needed This is a medium project of about three years. Half a staff member (scientist) and a student or Postdoc are needed to implement prototype testing routines and explore statistic/ ML techniques. Half a staff member (programmer) is needed for implementing these tools into the EXFOR toolset. This lower estimate of the workforce rests on the assumption that one can build on WPEC SG-50 [70] format suggestions to start developing and implementing a format that renders data in EXFOR easier to use for ML algorithms.

5.4 Priority 4: UQ Training for End Users

Why is it Important to Address the Issue for Users For the improvements described above (*e.g.*, more complete covariances, covariance quality assurance and validation, more complete and accessible EXFOR [9–12]) to be impactful for application users in nuclear energy, nuclear medicine, isotope production, nuclear safeguards and security, and other applied and basic nuclear science fields, it will be essential to transfer knowledge of UQ methodologies from nuclear data experts to end users. Effective training programs can build a skilled nuclear workforce that in turn produces the greatest scientific return on the nuclear data UQ investments. A well-trained workforce can work more productively, spark future innovations, and better communicate the importance of their work to their colleagues and the public—thereby growing the field of nuclear science. And they could provide valuable feedback about their observations to the nuclear data community to inform measurement efforts or issues with the data. Most importantly, training can ensure that application users produce the highest quality results and avoid mistakes while using tools that are growing increasingly sophisticated.

Description of Work Needed By establishing a set of training programs that include both basic descriptions of UQ methodologies and modules that are customized for different user communities, the relevant skills can be most effectively transferred to users. Basic topics could include an introduction to UQ (*e.g.*, uncertainties and uncertainty propagation), the importance of correlated uncertainties (covariances), critical components of UQ analyses (*e.g.*, covariance matrices, sensitivity studies), and quality assurance (*e.g.*, benchmarking, validation and verification, adjustments). Advanced modules specific to reactors, radiation transport, space radiation protection, ion beam therapy, isotope production, and safeguards could include both details on the relevant subjects and hands-on training of specialized codes and tools to enable trainees to quickly tackle problems in their subfields. Such training exist for Whisper and SCALE codes that can serve as a blueprint for future training courses.

How Could this Issue be Tackled? Because people learn in different ways, a combination of in-person workshops, online courses, coaching/mentoring/shadowing, hack-a-thons, video training modules, well-documented case studies, code documentation, and bibliographic collections could be used to effectively train the workforce in nuclear data UQ methodologies. For example, a long-running successful series of workshops at the ICTP (Abdus Salam International Centre for Theoretical Physics, located in Trieste, Italy.) [24] that combine lectures and hands-on coached evaluation work could be adopted and modified for UQ training. These workshops could be combined with some of the other training approaches mentioned above to form the core of a new program in end-user UQ training.

Level of Funding Needed This effort could be led by a part-time staff member and a part-time Postdoc, but should involve at least four staff/professors who are experts in different application areas to help design the modules and to teach at the workshops. An approximate cost would be one-time funding of 0.5 FTE to develop the course, and additional funding (0.5-0.75 FTE split between 2–3 people) on a continuing basis to teach and update it.

5.5 Priority 5: Adjustment Tools for General Users

Description of Work Needed If general purpose libraries are adjusted with respect to integral experiments, evaluated covariances can often be greatly reduced [15, 39, 86] leading to tighter bounds on application simulations [68] as was also shown by means of example for Sects. 4.2. This can often be translated into cost savings by having plausibly reduced safety constraints for instance when defining the upper sub-critical limit (see example in Sect. 4.4). However, adjustments can be very complex and experiment and target nuclear data selection for adjustment need to be done with care if others are to use the adjusted values. For some subject areas, like Nuclear Criticality Safety and reactor physics, adjustment has been frequently used, and tools exist for these communities. However, these tools are not openly available, and are also limited to specific subject areas. And, it should be emphasized that the adjusted libraries obtained are always tied to the subject areas represented by the experiments adjusted to and should not be used to simulate applications beyond their scope. Therefore, we state as priority 5 that open-source tools for adjustment for general users should be developed.

Why is it Important to Address the Issue for Users Several user communities (nuclear medicine, safeguards, aerospace, *etc.*) do not currently have the capability to adjust nuclear data mean values and covariances for their application area. Due to this, they do not have the capability to plausibly reduce evaluated uncertainties by the knowledge they have from application specific experiments. This might be especially problematic for users of nuclear data where experimental data are scarce defining the nuclear data. In this case, nuclear data are likely very uncertain and folding in knowledge from application specific experiments would be of high value.

This tool would not only benefit users but also the nuclear data producers. Evaluators could use the tool to explore possible areas of weakness within the library as adjustment points us to changes needed in nuclear data to better predict integral experiments. If this project would be done in tandem with the one on re-evaluating cross-cutting integral data in Sect. 5.13, one could gain additional insight into changes indicated to be beneficial to our libraries that are usually less explored within the current CSEWG validation effort.

How Could this Issue be Tackled? Open-source tools for adjustment need to be developed. These can be based on knowledge gained from tools used by NCSP or WPEC subgroups focused on adjustment. However, one needs to acknowledge that integral experiments and sensitivities of other subject areas might be affected by biases larger than nuclear data producers are used to in, for instance, criticality experiments, and may have large uncertainties. Hence, these adjustment tools need to be developed to be robust to large sensitivity uncertainties and biases in experimental data.

Another challenge to address is the sheer amount of nuclear data mean values and covariances that need to be loaded and processed before-hand. That requires the implementation of processing tools to get the input data. But also, the capability needs to be developed to either select partial datasets for adjustment, or dimension-reduction algorithms need to be applied.

The one question that remains open is the development of tools that produce sensitivities. This is a separate medium-tier project detailed in Sect. 5.6. Experimental data for given application areas will need to come from the users.

Level of Funding Needed This is a medium-sized project, requiring a staff for coding and testing, a student and Postdoc for exploring statistic techniques.

5.6 Medium-tier Need: Expanded and Improved Sensitivity Calculation Capabilities

Description of Work Needed Review and thorough verification of existing approaches, and development of new approaches are needed in sensitivity calculations. Initially, a comprehensive list of the sensitivity calculation capabilities available in radiation transport codes is required. The resulting sensitivities would be a matrix of output responses (*e.g.*: k_{eff}, reaction rates, Rossi-alpha, *etc.*) with respect to a list of input nuclear data (*e.g.*: energy-dependent-angle-integrated cross sections, angular distributions, TSL, PFNS, *etc.*). For some of those, ready-made tools are available like the "ksen" card for k_{eff} in MCNP [2], while others were obtained in an one-off effort [67]. In order to assess the availability of sensitivity tools for various responses, an in-depth review of existing tools should be made as the very first step. This review should bring to light whether this is available for criticality calculations, source-driven calculations, or neutron noise analysis methods and for deterministic and/or Monte Carlo methods. When more than 1 code is identified for the same response time, code-to-code verification should be establish based on previous literature unless providing sensitivities is well-established for that particular response (*e.g.*, as for k_{eff}). Afterwards, resources should be dedicated to filling in the identified gaps, where there either are no existing capabilities and those where only 1 code capability exists. It is of high importance that these tools should be made available in a way that users can easily request access to it or may even be open-sourced to begin with to reach a large community.

Why is it Important to Address the Issue for Users Calculated sensitivities are the cornerstone of first-order propagation of uncertainty methods as detailed in Section 3. While Monte Carlo propagation of uncertainty methods are capable, there are certain advantages of first-order propagation of uncertainty methods, namely the ability to decompose the propagated uncertainty into sources, rapid calculations, and enabling of adjustment/assimilation methods. Sensitivity calculation capabilities are an irreplaceable part of the nuclear data pipeline and must evolve in-pace with the expansion of the measured responses in integral experiments (*e.g.*: subcritical integral experiments measuring Rossi-alpha) and the expansion of the available covariance data in ENDF (*e.g.*: TSL covariance data). Expansion of the sensitivity calculation capabilities along the input nuclear data dimension, will support multiple users/programs (*e.g.*: the ability to propagate TSL covariance data). Expansion along the output responses dimension will support users/programs with interest in those responses (*e.g.*: detector count rate for safeguards) but will also benefit a broad spectrum of users by enabling the methods for the assimilation of an expanded set of integral measurements. Sensitivity tools will likely reach users first that already use adjustment tools. It is important to tackle the projects answering the need for adjustment tools in Sect. 5.5 for those users that do not have easy access to one right now.

How Could this Issue be Tackled? A review of the current methods can be done through the literature as well as through compilation of published/presented code-to-code verification. Projects implementing new sensitivity capabilities connecting output responses with input nuclear data can be done independently and in parallel. These latter projects will naturally flow from the in-depth literature review which could be seen as a scoping study as they will reveal what methods already exist for calculating sensitivities for various responses. Right now, it was assumed by the committee that in a second step, after the review, sensitivities for reaction rates, spectra, sub-crit FeynmannY, Rossi-alpha, and count rates should be provided. These would begin answering needs of several communities, *e.g.*, neutron dosimetry, general validation, NCSP, *etc.* Of secondary priority would be an extension of providing sensitivities for pulsed-sphere neutron-leakage spectra (fixed-source), and reactivity coefficients. This ranking might change with the outcomes of the scoping study.

Level of Funding Needed The literature review is likely to be a small project, 0.75 FTE for 1 year. Implementing new sensitivity capabilities can be independent small projects on the order of 0.75 FTE over 1–2 years and may involve students and Postdocs.

5.7 Medium-tier Need: Sampling Replica Data from Covariances

Description of Work Needed While the so-called "sandwich rule" based on linear perturbation theory using computed sensitivities and covariance matrices has been shown to be an effective means of propagating uncertainties for a wide array of applications, it is sometimes desired to expand beyond this approach. One can rely on sensitivity coefficients if the parameters they consider are very well specified or the system is linear. However, most complex systems have some non-linearities. or would benefit from MC approaches if their overall simulation could run faster. One solution is to sample suites of replica data based on the covariance data using Monte Carlo approaches that incorporate uncertainty quantification as is introduced in Sect.3. The SCALE code contains the SAMPLER package [84] that provides such samples, and LLNL's EMU code does too, but none are open source.

Why is it Important to Address the Issue for Users This may be necessary if one is interested in nonlinear systems (often in a multi-physics context), if one is sensitive to the tails of a distribution rather than higher probability realizations, or in certain approaches to using outside constraints on the distributions. This effort also become importantwhen the uncertainty on any piece of the nuclear data is relatively large, *i.e.* when the standard deviation is beyond the validity of the first order Taylor expansion to the quantity of interest.

How Could this Issue be Tackled? To do this effectively, there are various considerations that should be addressed:

- The most common approach to sampling uses an eigenvalue decomposition of the covariance matrix and generating random distances along the eigenvectors. Unlike the sandwich rule, this approach is very sensitive to deficiencies in the covariance matrices, including small negative eigenvalues which can arise from finite precision. Approaches to correcting these deficiencies are needed.

- Because they only have covariances as represented in evaluations, users are left to assume a distribution. Typically, a multivariate normal distribution is assumed, both because of its ubiquity and the ease of use. However, this can lead to sampling unphysical values (*e.g.*, negative cross sections or scattering cosines greater than unity). An understanding of the possible means of handling these unphysical values is necessary. At the simplest, one could ignore unphysical values, but this biases the distribution. Other options include using other distributions such as the lognormal distribution, but this can violate extreme linear constraints.

- Building upon the previous point, a proper uncertainty quantification for the difficult systems considered here may require more probability distribution information than what is captured by current characterization of the covariance data. A study driven from evaluators should identify how much information is lost with this first-order approximation. While specifying general distributions is not trivial, one could explore opening up a variety of well-behaved distributions to evaluators.

- The ultimate way to avoid loss of information in creating replica data is to sample model parameters, in the style of the "Total Monte Carlo" method championed by the developers of the TALYS model code. However, to use this approach more generally, an ability to impose constraints based on differential data is needed, along with extensions to quantities and energy regimes not covered by current approaches.

- Monte Carlo uncertainty propagation typically requires an enormous number of runs of a potentially very expensive application code. As such, this approach may require the use of statistical emulators and dimension reduction techniques.

- Robust and user-friendly tools to perform sampling and applying outside constraints are needed. While many single-institution solutions exist in varying levels of maturity, the field could benefit from additional cross-code and cross-organization comparisons and an accepted industry-standard tool, preferably using open-source codes.

Level of Funding Needed This would be a medium-sized project at 2 FTEs for 3 years with the potential to involve students and Postdocs on the science and tool development side (*e.g.*, building emulators, building robust sampling tools).

5.8 Medium-tier Need: TSL Covariance Data

Description of Work Needed A medium-tier priority effort is the addition of covariance data for the thermal neutron scattering cross sections. This would close a gap in missing uncertainty data for an important set of data in application areas such as criticality safety and reactor physics. Covariance data for the most relevant moderator materials need to be generated. A covariance data format for TSL needs to be developed. And, then processing and application tools need to be extended to be able to make use of these new data. Currently, a joint ORNL/ University of Michigan project develops a GNDS format, while MIT is developing a sampling approach. These projects can serve as starting points for providing TSL covariances for the most important TSL nuclear data for applications.

Why is it Important to Address the Issue for Users In thermal-spectrum reactors and critical assemblies, neutrons are born at high energies (approximately 2 MeV) and slowed down through elastic scattering with the moderator to thermal energies (around 0.025 eV). In this energy range, neutrons achieve a state of pseudo-equilibrium by exchanging energy with the atoms and molecules of the moderating medium (*e.g.*, water, graphite, *etc.*). The double differential cross sections in energy and angle of the moderator are proportional to a quantity known as the thermal scattering law (TSL) $S(\alpha,\beta)$ which is a probability distribution function of the momentum and energy transfer in the material and used to calculate incoherent scattering. For coherent scattering in crystaline materials such as in graphite, information about Bragg edges is needed which determine how the neutrons scatter to discrete angles. Only with the consideration of TSL data, an accurate prediction of the neutron flux—the basis for all other quantities of interest—can be obtained. The current ENDF/B library (ENDF/B-VIII.0) release does not include covariance data for the provided TSL data. Therefore, uncertainties in these data cannot be considered when quantifying nuclear data induced uncertainties in key metrics for criticality and reactor physics analysis. An accurate prediction of the nuclear data induced uncertainty of any output quantity requires the consideration of all uncertainties and correlations for the data used in the simulation of the model. Missing uncertainties and missing correlations can cause over-/underprediction of uncertainty as is highlighted in Section 4.3. To close this gap, the ENDF/B thermal scattering library must include TSL covariance data and these data must be considered in uncertainty quantification studies.

How Could this Issue be Tackled Previous efforts to quantify covariances in thermal neutron scattering have involved Monte Carlo sampling from a phonon density of states [25, 26], analytical fitting of LEAPR (a module in the processing code NJOY that translates TSL data from ENDF-6 to other formats) [5] parameters to data [27,28], or analytical fitting of molecular dynamics (MD) model parameters to data [29]. The methods come with different trade-offs, in particular in terms of the processing time and the required disk space for the data.

In a potential project, efforts should be undertaken to evaluate which of these methods should be used in a more extensive TSL covariance data generation, considering the different trade-offs. Then, this method is used to generate complete sets of TSL covariance data for a set of major moderators (including at least light water, heavy water, and graphite). While the GNDS format for ENDF/B data can already consider TSL covariance data, common US nuclear data processing codes such as AMPX [4] cannot yet process these data. Furthermore, the covariance library formats in which the processed data is stored for use with application tools need to be extended to be able to handle these additional data, and the application tools (*e.g.*, sampling routines to support sampling-based uncertainty propagation) need to be extended correspondingly to be able to handle these data in the new formatted libraries.

The most efficient application and therefore testing of the TSL covariance data would rely on sensitivity coefficients to TSL data. Given that such sensitivity coefficients are not calculated by any known simulation code, related developments (see Sect. 5.6) should be supported simultaneously.

Level of Funding Needed This would be a medium-sized project of 3 years with 1–3 staff / year including Postdocs and students.

5.9 Medium-tier Need: Fission Yield Covariance Data

Why is it Important to Address the Issue for Users Precise knowledge of fission yields impacts many applications encompassing both pure and applied areas, such as nuclear reactor operations, nuclear waste disposal, decay heat and nuclear reactor antineutrinos.

Description of Work Needed The current libraries give recommended independent and cumulative fission yields for ground state levels and long-lived isomers, approximately 1,000 of them, per incident neutron energy. Independent fission yields are defined as the probability that a given nuclear level is populated following a fission event, while the corresponding cumulative yield is defined recursively as its independent fission yield plus the sum of the cumulative fission yields of the parent nuclides weighted by the corresponding decay probability.

Three main libraries contain fission yield data currently, ENDF/B-VIII.0 [1], JEFF-3.3 [32] and JENDL-5 [33]. The ENDF/B fission yield data were released in 1993, except for the 2 MeV ^{239}Pu data that were released in 2011. The JEFF-3.3 data were released in 2017, and JENDL in 2020. Ideally, these libraries should be consistent with the corresponding decay data sub-libraries, which contain the decay data for those ground state levels and isomers, which allow users to convert between independent and cumulative yields [36]. Following a 2018 Funding Opportunity Announcement, NA-22 is currently funding a 5-year multi-lab fission yield evaluation effort led by LANL, which includes a much-needed modeling on the dependence of fission yields with incident neutron energy. Additionally, the Nuclear Data Section at the International Atomic Energy Agency has setup a Coordinated Research Project on fission yields [35] to promote and coordinate this type of research worldwide.

A deeply disquieting issue among the current yield libraries is the lack of agreement in the yield uncertainty, which not only reflect distinct numerical approaches arising from the libraries' diverse vintages, but also the weight given to individual datasets. This is exemplified in Fig. 5.1 for the ^{235}U thermal neutron fission cumulative yields that is different between ENDF/B-VIII.0 and Jeff-3.3. ENDF/B relies heavily on the cumulative fission yields measured by W. Maeck's group at INL in the 1970s [37], while JEFF does not. As a further example, the ^{137}Cs fission yield for the above mentioned fission reaction has a 0.5% uncertainty in ENDF/B-VIII.0, but a 1.9% uncertainty in JEFF-3.3.

The lack of correlation matrices between different fission products in the current libraries is another troubling issue since uncertainty propagation in quantities that use fission yields are likely to be incomplete. These correlations would include model correlations as well as those arising from the fit to all experimental data that lead to the recommended fission yield values. From the modeling point of view, the path from saddle to scission can be succinctly understood as the competition of three fission modes, the symmetric SL, and the asymmetric S1 and S2 ones, which will lead to independent fission yields following the emission of neutrons from the excited fission products. At thermal energies, the SL contribution is very weak, therefore most independent fission yields will be positively correlated with members of the same mode and anti-correlated with those in the competing mode. The model correlations among cumulative fission yields get somewhat spread by the mixing of the S1 and S2 modes through beta decay. Correlations arising from experimental data is a topic that has yet to be fully explored. Templates of uncertainties for fission yields have been developed [80] to provide some guidelines as to those experimental correlations but have yet to be applied. While the LANL-led project aims to provide a covariance format and some covariances, more targeted funding would be needed to provide all relevant covariances starting from experimental correlations.

How Could this Issue be Tackled Future developments would require fully documented experimental libraries, with uncertainties that have been critically reviewed against the relevant templates, and in a modern numerical format that would allow easy interface with the associated decay data. Additionally, we would need data that are very sensitive to fission yields data, such as delayed neutron multiplicities and activities. These data, in conjunction with advanced fission modeling tools, would

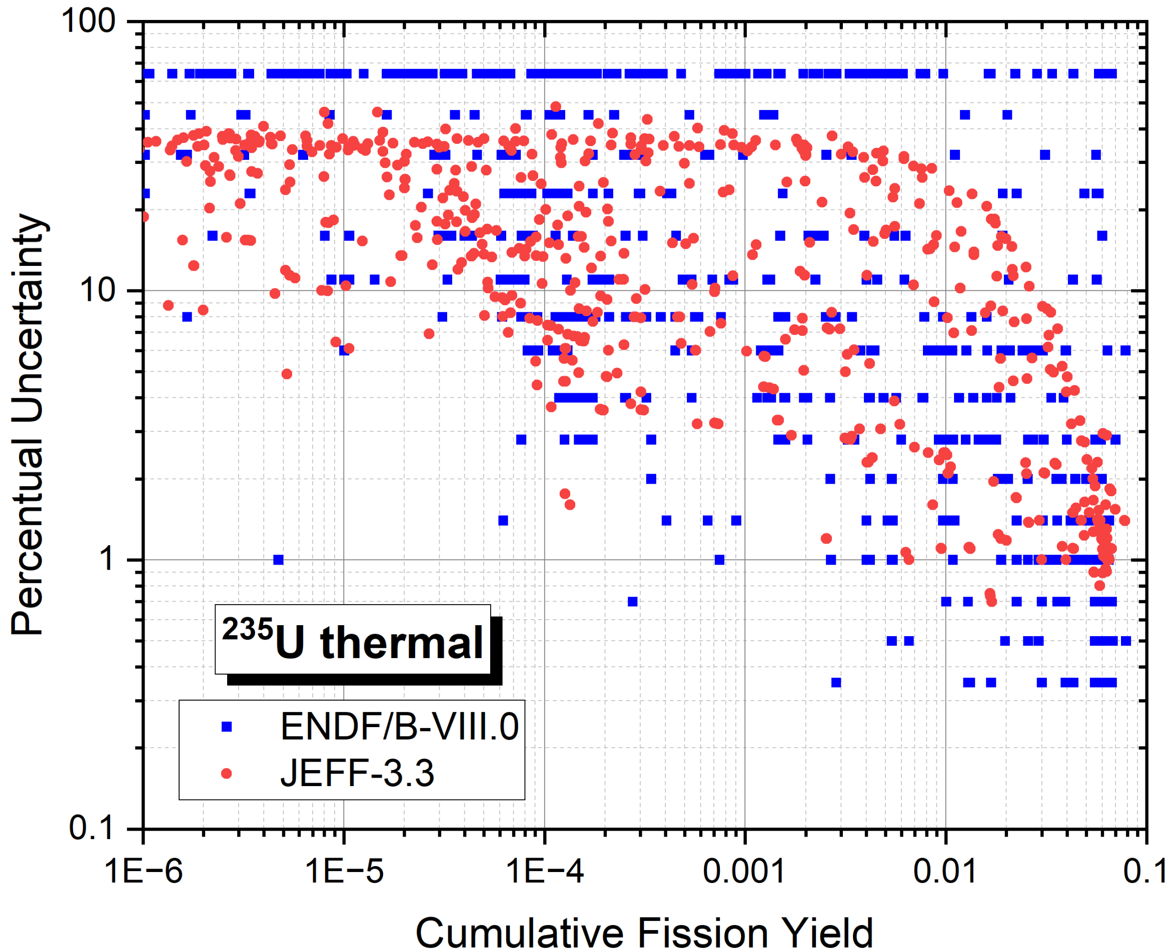


Figure 5.1: Comparison of cumulative fission yields relative uncertainties as function of cumulative fission yield between the ENDF/B-VII.0 and JEFF libraries for the ^{235}U thermal neutron yields.

be used in ML/AI uncertainty quantification algorithms to derive recommended fission yield data with covariance matrices. Due to the impact of the Maeck data [37], a campaign to repeat these measurements taking advantage of modern Atomic Mass Spectrometry techniques as well as other novel experimental approaches such as the use of X-ray Fluorescence at light sources could further improve the accuracy of the stable or long-lived cumulative yields.

Level of Funding Needed We estimate that we would need about 5 years and a multi-million-dollar investment to complete this effort.

5.10 Medium-tier Need: Decay Constants & Branching Ratio Covariance Data

Description of Work Needed The decay data for many nuclides of high relevance in applications are surprisingly not as accurate as they could be. As a representative example, the half-life of ^{236}U in ENSDF is given with a 0.17% uncertainty, but it is derived from just three measurements performed in the early 1950s. Spontaneous fission branching ratios are also in a similar situation. Another issue affecting the decay data in actinide nuclides is that gamma transitions are typically below 150 keV and are, as a consequence, heavily converted, leading to large X-ray yields. These X-rays and the competing Auger electrons are calculated by propagating outwards the vacancies created by electron conversion. Our best tool for that purpose is the EADL data, itself a sub-library in ENDF/B, which lack uncertainty and correlation information.

However, decay radiation intensities are often highly correlated, for instance, positively if two gamma rays are in a cascade, or negatively for instance the intensities of alpha particles. Similarly, all the K X-ray intensities are anticorrelated. Accurate and properly documented uncertainty values are often not found due to limitations of the current format, and correlation matrices are not available.

Why is it Important to Address the Issue for Users The need to address the electron conversion process with an updated EADL data [1] has been identified as a top priority in other forums due to its relevance to calculate Auger electrons of interest in nuclear medicine.

How Could this Issue be Tackled We currently use much improved tools to calculate the electron vacancies which are created following electron capture and electron conversion using the Beta-shape [40] and BRICC [41] codes, but we lack the data, fluorescence yields and vacancy transfer probabilities, to precisely calculate the atomic radiation produced as these vacancies are filled. Recent advances in micro-calorimeter detector systems with much improved resolution over Germanium detectors would make the need for an improved EADL even greater.

The usefulness of Total Absorption Gamma Spectroscopy (TAGS) measurements [42,43] for fission products to better predict decay heat and the antineutrino spectrum generated by nuclear reactors has been widely demonstrated. The early detectors consisted of a single scintillator crystal that measured the gamma spectrum following beta-minus decay in perfect summing conditions. Recently, more segmented detector systems have been deployed. From these measurements the beta intensities and mean electron and gamma energies following beta-minus decay can be determined. However, the singles gamma spectra free of summing has not been reported, creating an inconsistency in the databases and the inability to predict the beta-delayed gamma spectrum at short times, less than 200 seconds, after fission.

These new measurements form the basis for more realistic evaluated uncertainties. These data need to be compiled and then evaluated, including of course covariances, which entails calculation tool development. The resulting database needs to be provided to the community in a processable format.

Level of Funding Needed A coordinated set of experimental campaigns as well as the engagement of atomic physicists to work on EADL would be needed to tackle these issues. The effort may possibly span up to 5 years requiring funds totaling several FTEs.

5.11 Medium-tier Need: Stopping Power Covariance Data

Why is it Important to Address the Issue for Users Well-benchmarked charged-particle stopping powers (*e.g.*, dE/dx) are critical for a wide variety of applications: from modeling single event effects (SEE) and human dosimetry calculations for space exploration; fission and fusion materials damage; Ion Beam Therapy (IBT) and optimized isotope production; and the modeling of detectors for basic science, national security, nuclear nonproliferation. These needs have been well-documented at a number of Workshops for Applied Nuclear Data Activities (WANDA) including the materials damage session at WANDA 2019 [53]; the detector modeling session at WANDA 2020 [54]; the space applications session at WANDA 2021 [55], and most recently in a dedicated stopping power session at WANDA 2022 [56].

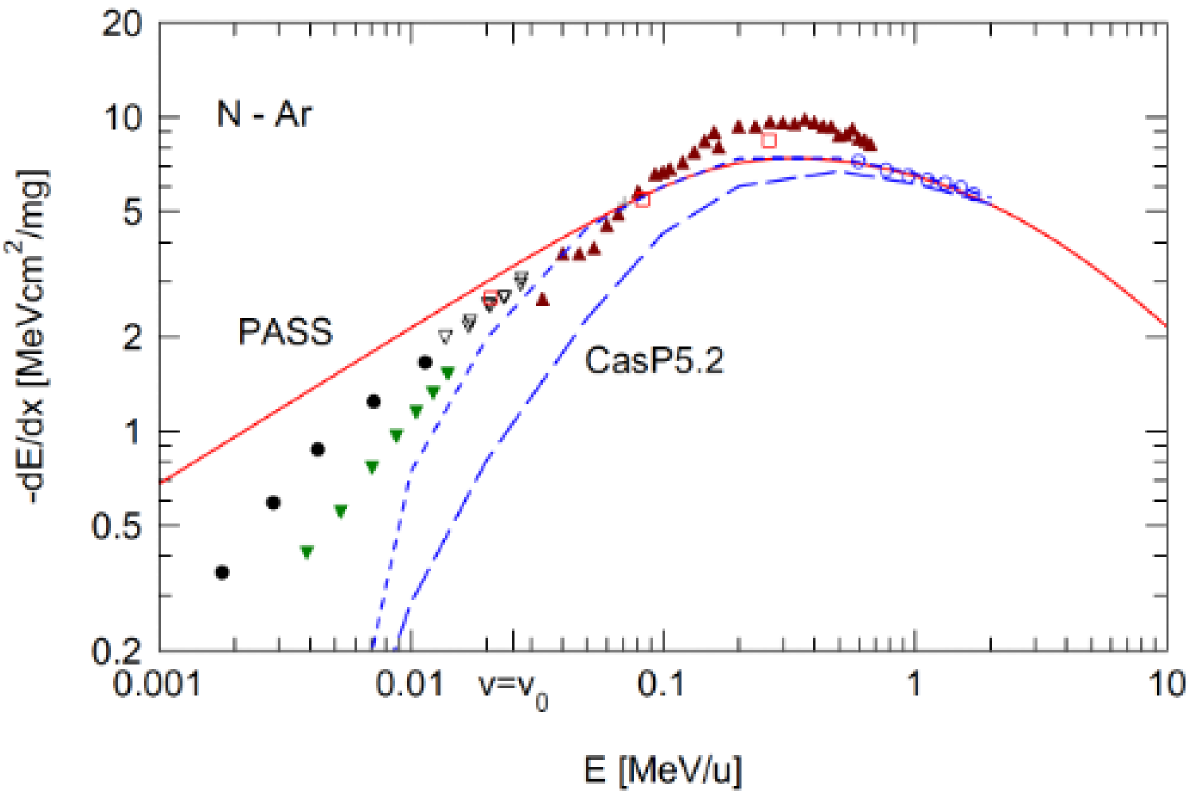


Figure 5.2: Stopping powers for N in Ar including experimental data and the predictions of the PASS and CasP5.2 model codes.

Description of Work Needed Stopping powers themselves introduce covariances into the measured and modeled nuclear data quantities that are most relevant to these applications, but this document will concentrate only on the quantities that introduce uncertainties into calculations of stopping powers themselves. In general, the largest uncertainties in dE/dx are at the lowest relative velocity of the ion referred to as the Bragg Peak where the two different theoretical models from Bohr and Bethe show the greatest difference, and guidance from experiment is often most lacking. Modern dE/dx models introduce missing physics, including atomic excitation of both the beam and the material, but require experimental data for adjustment. An example from [57] for nitrogen ions in argon for two modern models, Binary Theory [58] and PCA/UCA [59] together with the experimental data available for the system is shown in Fig. 5.2. Any optimization of these model parameters clearly requires guidance from experiment at low energy/nucleon.

The need for improved experimental data is particularly evident for SEE (single event effects) and IBT (ion beam therapy) where high dose density is of the greatest concern, alteration of stopping powers can cause huge changes in the location of the Bragg peak near the end of particle trajectory where the largest Linear Energy Transfer (LET) occurs. In the case of materials damage for fission and fusion power systems, a wider range of stopping powers is of interest since reaction channels covering a wide range of recoil and ejectile energies contribute to the total cross section for displacements per atom (σ_{dpa}) and gas production in reactor pressure vessels and tokamaks and energy deposition in inertial confinement fusion plasmas.

A common theme from all of these applications is a paucity of measurements, particularly at low energies near the Bragg Peak. This lack of data was well summarized in the talk given by Claudia Montanari at WANDA 2022. Figure 5.3 shows a figure from that talk showing how many proton stopping power data sets exist for elements across the periodic table.

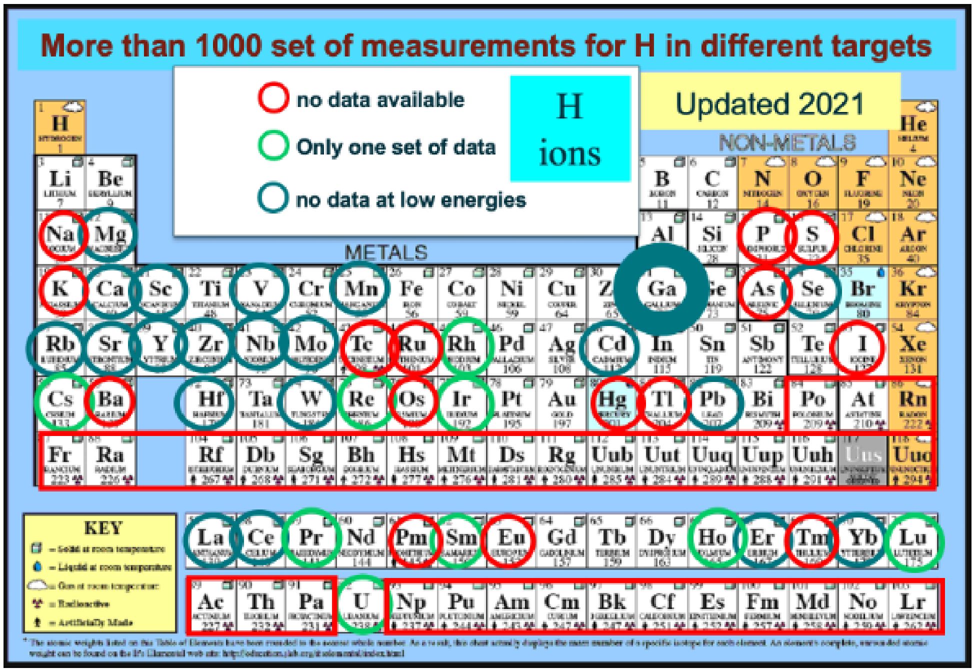


Figure 5.3: Stopping power data sets for protons in different elements from the talk by Montanari at WANDA 2022. Limited-to-no data exists for a number of elements used in semiconductors (Ga, As and Se), detectors (Ba, I, K, Na) and shielding (Pb) and isotope production (Tl), and both fission (Zr) and fusion (Nb) applications.

How Could this Issue be Tackled The top priority to address this need is to perform measurements of light- and heavy-ion stopping powers, covering the entire range from multi-MeV/nucleon down to the Bragg peak. One potential path for performing these measurements would involve performing target thickness differential time-of-flight measurements using heavy-ion "cocktail" beams used for SEE testing. These cocktail beams include multiple ions with similar energy/nucleon, enabling measurement campaigns that would cover multiple ions in a single run with common, well-defined systematic uncertainties.

Figure 5.4 shows one potential experimental set-up for performing stopping power measurements using the Berkeley Accelerator Space Effects (BASE) Facility at the LBNL 88-Inch Cyclotron. Cocktail beams [87] with E/A of 4.5, 10, 16, 20 and 30 MeV/nucleon, $5 \leq Z \leq 79$ and $10 \leq A \leq 197$ would be extracted from the cyclotron and sent along a fixed path length between two sensors located at positions t_1 and t_2 with a differential thickness degrader located immediately after position t1 at the location labeled "Foil". It is critically important that all of the sources of uncertainty in these TOF measurements be carefully recorded for use in optimizing stopping powers model parameters. This would include accuracy of absolute and relative timing and beam energy measurements. This facility is given as one representative example; other facilities should also be considered for such a project.

Lastly, it is important to note that the International Atomic Energy Agency (IAEA) hosts a database of stopping power data sets that can serve as a central repository for improvements in modeling the atomic physics [88]. Maintenance of this database is essential, including the regular incorporation of new data is of foundational importance.

Level of Funding Needed This project at various facilities would be both modest in expense and extensible in scope, with initial measurements focused on the needs of specific sponsors and utilizing specific cocktail ions that are close to isotopes of interest (*e.g.*, Y as a surrogate for Zr for materials damage; P and S for reactions on Si for SEE *etc.*). Later efforts could include the development of

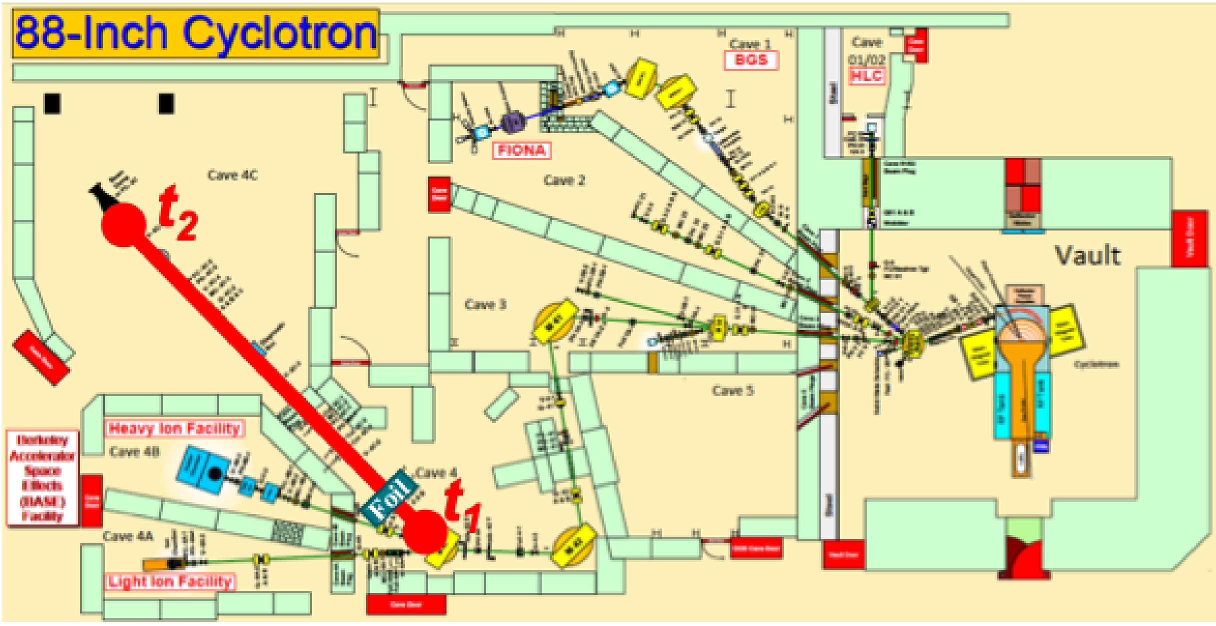


Figure 5.4: Experimental set-up for performing stopping power measurements at the Berkeley Accelerator Space Effects Facility at the 88-Inch cyclotron. The variation in the time-of-flight for ions from a "cocktail" beam as a function of foil thickness allows for multiple measurements in a single experimental campaign.

other, more targeted cocktail beam components. Furthermore, the measurements are well-suited for an engineering Ph.D. project. Establishing an initial capability would require approximately 0.75 FTE per year each for a researcher and a Ph.D. student, with stopping powers for 3 nuclides/year being measured starting in year 2. A three year program could cover approximately 6 nuclides of interest.

5.12 Medium-tier Need: Delayed-neutron Covariance Data

After the fission of actinides nuclides, neutrons can be produced following the beta-decay of nuclides whose beta-minus Q-value exceeds the separation neutron energy in the daughter. These delayed neutrons were first discovered by Fermi's group in Chicago and their crucial importance in the safe operation of nuclear reactors was soon understood.

Delayed neutron data includes the delayed neutron multiplicity, known in technical parlance as delayed nu-bar, ν_d, and the delayed decay constants λ_i with corresponding probabilities a_i, so that the delayed neutron activity is parametrized as

$$DNA(t) = \nu_d \sum a_i exp(-\lambda_i t), \tag{5.1}$$

Description of Work Needed In the ENDF/B-VIII.0 library, 6 pairs of (λ_i,a_i) are given, with the λ_i decay constants slightly different for each fissioning system. In JEFF-3.3 8 pairs are used, with the λ_is maintained constant for all systems. Unfortunately, uncertainties in these parameters and correlations among them are not given, making it impossible to support any uncertainty calculation that involves them. Moreover, the ENDF/B derived DNA values differ by as much as 20% from the seminal measurements performed by G.R Keepin's group at LANL [44], as shown in Fig. 5.5.

Why is it Important to Address the Issue for Users The 6-group parameters are highly correlated and can be related to a particular set of fission products fission yields and decay constants.

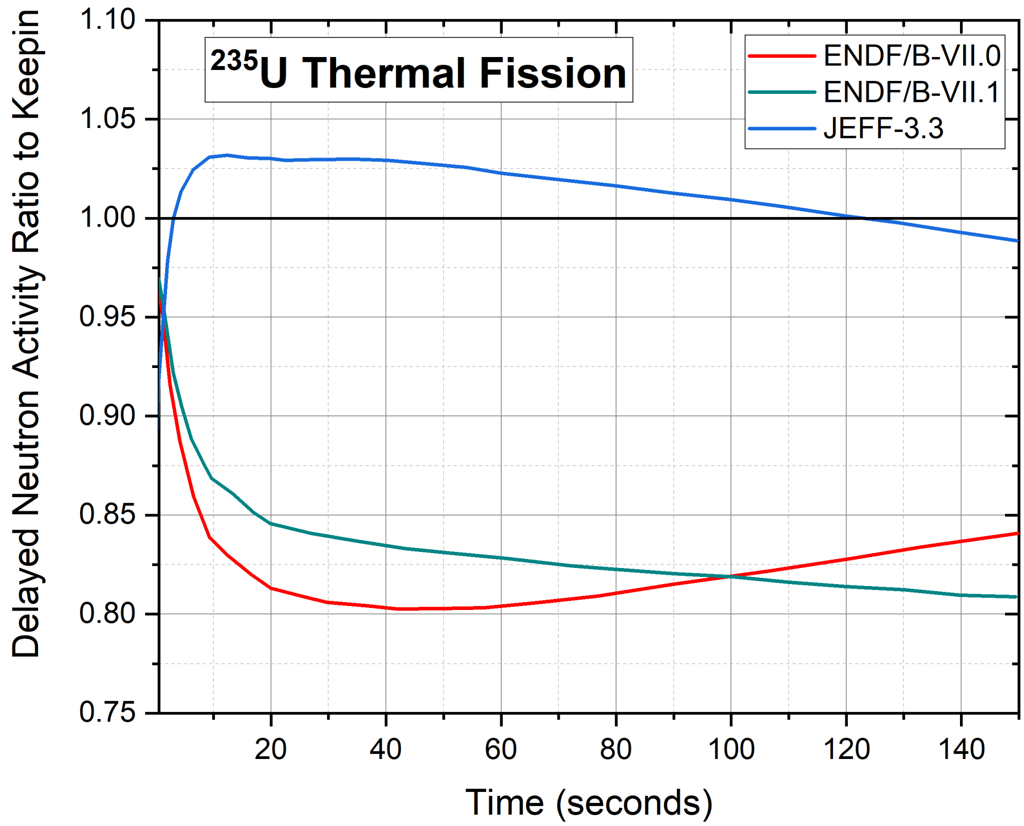


Figure 5.5: Ratio of the calculated delayed neutron activity from JEFF-3.3 and ENDF/B-VIII.0 to that measured by Keepin.

Their uncertainties and correlation matrices are needed to properly quantify uncertainties in reactor analysis.

How Could this Issue be Tackled There has been a recent Coordinated Research Project at the IAEA Nuclear Data Section on this topic [45], plenty of the data needed to update ENDF/B can be obtained from this work. Additional synergy with the current fission yield evaluation can be exploited to obtain the DNA parameters covariance matrices.

Level of Funding Needed We estimate that this work would require about two years with an investment of approximately 1 FTE per year.

5.13 Medium-tier Need: Re-evaluation of Cross-Cutting Integral Data Covariances for Validation and Adjustment

Description of Work Needed Adjustment with integral data beyond k_{eff} has been shown to cause significant changes in major actinide cross sections [15, 39, 86], indicating either a problem in actinide evaluations or in the integral data covariances. To justify using these integral data for future validation or adjustment, covariances of these data must be re-evaluated. Despite the extraordinary value these historical data represent a down-select for the most cross-cutting integral data must be made. A feasibility study should be performed for impactful examples with minimal cross-material correlations;

for example the ^{239}Pu(n,f)/^{235}U(n,f) ratio measured in a ^{252}Cf(sf) neutron spectrum as used, for instance for validating ENDF/B-VIII.0 [1].

Why is it Important to Address the Issue for Users Many application spaces rely on accurate actinide nuclear data, including Stockpile Stewardship, Nuclear Energy, Nuclear Criticality Safety, and Global Security applications in non-proliferation, counterterrorism, and nuclear forensics. Integral data measurements have lower uncertainties than differential, and can be used for some range of applications to adjust data to increase accuracy. Adjusted data can lead to reduced uncertainties, if appropriate experimental data are carefully chosen, as shown in the examples in Chapter 4 for application metrics, with significant impacts on costs, time, and/or safety. We currently rely heavily on critical assemblies, but alternate data sources, such as activation ratios and pulsed spheres, are available. However, these integral experiments need to be re-evaluated to ensure proper uncertainty propagation and realistic data uncertainties.

How Could this Issue be Tackled? A survey of available integral data and application sensitivities would be performed to identify the highest impact integral data to be re-evaluated. Integral data with high spectral sensitivity and those involving actinides are expected to be the most cross-cutting, as ENDF actinide validation concerns have already been identified and spectral sensitivity provides information beyond k_{eff}.

Feasibility studies re-evaluating a few high-priority examples would be performed. Information in past reports and log books would be used to approximate the analysis path taken for each integral experiment. In cases where corrections were made using past transport codes and evaluations, these corrections would be recalculated using modern codes and libraries. Such corrections could include room return, sample scattering, and detector response. Relevant uncertainties in our understanding of the experiment geometry should be forward propagated. Modern lessons learned about unidentified sources of uncertainty for given detector types would also be employed, likely leading to increased uncertainties. The goal would be to produce a more realistic uncertainty for the integral quantity, but the mean value may change as well.

Level of Funding Needed 2 FTE for two years. The project may be suitable for student involvement. HPC would be useful for transport simulations and UQ.

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Appendix

The agenda of the NDUQWM is shown on the next few pages.

Tuesday Oct. 11, 2022				
EDT	MDT	PDT	Speaker/ Discussion	Title/ Topic
Introduction to Nuclear Data Uncertainty Quantification Working Meeting (NDUQWM)				
10:00 AM	8:00 AM	7:00 AM	Denise Neudecker	Welcome and administrative
10:05 AM	8:05 AM	7:05 AM	Keith Jankowski	Welcome adress and motivation for this meeting
10:15 AM	8:15 AM	7:15 AM	Discussion	Questions
10:20 AM	8:20 AM	7:20 AM	Denise Neudecker	Introduction to nuclear data covariances and uncertainty quantification
11:05 AM	9:05 AM	8:05 AM	Discussion	
Examples of the impact of Nuclear Data Uncertainty Covariances and UQ on Applications				
11:10 AM	9:10 AM	8:10 AM	Rike Bostelman	Impact of nuclear data uncertainties on non-LWR reactivity analysis
11:25 AM	9:25 AM	8:25 AM	Discussion	
11:30 AM	9:30 AM	8:30 AM	Bob Little	Nuclear data covariances are critical input to determine upper sub-critical limits and to design experiments to increase it
11:45 AM	9:45 AM	8:45 AM	Discussion	
11:50 AM	9:50 AM	8:50 AM	Break	
Feedback on nuclear data covariances & UQ needs from previous meetings				
12:10 PM	10:10 AM	9:10 AM	Cathy Romano	Feedback from WANDA meetings on covariances and UQ
12:20 PM	10:20 AM	9:20 AM	Pat Griffin	User challenges with covariance data and feedback from CW2022
12:35 PM	10:35 AM	9:35 AM	Discussion	
Evaluation input covariance and UQ needs				
12:45 PM	10:45 AM	9:45 AM	Amanda Lewis	Improving estimates of experimental data uncertainties
12:55 PM	10:55 AM	9:55 AM	Discussion	
1:00 PM	11:00 AM	10:00 AM	Marco Pigni	Theoretical and calculable dependent variables and their covariance in nuclear data libraries
1:10 PM	11:10 AM	10:10 AM	Discussion	
1:15 PM	11:15 AM	10:15 AM	Bob Little	LANL UQ priorities
1:25 PM	11:25 AM	10:25 AM	Kyle Wendt	LLNL UQ priorities for nuclear data evaluation
1:35 PM	11:35 AM	10:35 AM	Dave Brown	NNDC UQ priorities
1:45 PM	11:45 AM	10:45 AM	Discussion	
1:55 PM	11:55 AM	10:55 AM	Break	
Nuclear data covariances & UQ needs from safeguards, aerospace, and nuclear medicine				
2:15 PM	12:15 PM	11:15 AM	Stephen Croft	Safeguard needs
2:25 PM	12:25 PM	11:25 AM	Discussion	

2:30 PM	12:30 PM	11:30 AM	Cathy Romano	Safeguard and space application needs
2:40 PM	12:40 PM	11:40 AM	Brad Rearden	Covariance Data Needs for Space Nuclear Power and Propulsion Applications
2:50 PM	12:50 PM	11:50 AM	Shaheen Dewji	Nuclear data needs from nuclear medicine and radiation protection dosimetry applications
3:00 PM	1:00 PM	12:00 PM	Discussion	
Nuclear data covariance needs for various subject areas				
3:10 PM	1:10 PM	12:10 PM	Michael Smith	Nuclear Data UQ for nuclear astrophysics
3:20 PM	1:20 PM	12:20 PM	Discussion	
3:25 PM	1:25 PM	12:25 PM	Vlad Sobes	A vast, empty space in nuclear data uncertainty
3:35 PM	1:35 PM	12:35 PM	Rike Bostelman	ORNL needs
3:45 PM	1:45 PM	12:45 PM	Discussion	
3:55 PM	1:55 PM	12:55 PM	Jo Ressler	LLNL UQ priorities for nuclear data
4:05 PM	2:05 PM	1:05 PM	Discussion	
4:10 PM	2:10 PM	1:10 PM	Break	
Adjustment, Forward-propagation, and user UQ needs				
4:15 PM	2:15 PM	1:15 PM	Larry Greenwood	Nuclear data uncertainties and covariances for neutron spectral adjustments
4:25 PM	2:25 PM	1:25 PM	Discussion	
4:30 PM	2:30 PM	1:30 PM	Robert Casperson	LLNL UQ priorities for nuclear data adjustment
4:40 PM	2:40 PM	1:40 PM	Discussion	
4:45 PM	2:45 PM	1:45 PM	Nathan Gibson	LANL's needs along the covariance pipeline
4:55 PM	2:55 PM	1:55 PM	Discussion	
5:00 PM	3:00 PM	2:00 PM	End of the day	

Wednesday Oct. 12, 2022				
EDT	MDT	PDT	Speaker/ Discussion	Title/ Topic
Various Nuclear Data Covariance and UQ needs				
10:00 AM	8:00 AM	7:00 AM	Alejandro Sonzogni	Fission yield covariances
10:10 AM	8:10 AM	7:10 AM	Discussion	
10:15 AM	8:15 AM	7:15 AM	Boris Pritychenko	Uncertainties in EXFOR
10:25 AM	8:25 AM	7:25 AM	Discussion	
10:30 AM	8:30 AM	7:30 AM	Lucas Kyriazidis	Nuclear Data at the US NRC
10:40 AM	8:40 AM	7:40 AM	Discussion	
10:45 AM	8:45 AM	7:45 AM	Andrew Voyles	Isotope production needs for uncertainty quantification
10:55 AM	8:55 AM	7:55 AM	Discussion	
11:00 AM	9:00 AM	8:00 AM	Nicole Vassh	The Need for Nuclear Data UQ for Heavy Element Synthesis Studies
11:10 AM	9:10 AM	8:10 AM	Discussion + Back-up time	
11:30 AM	9:30 AM	8:30 AM	Break	
Discussion on which needs are of highest priority				
11:50 AM	9:50 AM	8:50 AM	Discussion	Ordering of priority of needs
2:50 PM	12:50 PM	11:50 AM	Discussion	Assignment of writing of whitepaper
3:00 PM	1:00 PM	12:00 PM	Break	
Writing of whitepaper (online and offline as preferred)				
3:20 PM	1:20 PM	12:20 PM	Writing and assembling whitepaper	
5:00 PM	3:00 PM	2:00 PM	End of the day	

Thursday Oct. 13, 2022				
EDT	MDT	PDT	Speaker/ Discussion	
Assembling and follow-up discussions on the draft				
10:00 AM	8:00 AM	7:00 AM	Discussion on submitted text	
12:00 PM	10:00 AM	9:00 AM	Break + last edits	
Last go-through				
12:30 PM	10:30 AM	9:30 AM	Last go-through	
1:30 PM	11:30 AM	10:30 AM	**End of the meeting**	