Status of the US Nuclear Data Program
Report from the
Nuclear Data Charge Subcommittee of the Nuclear Science Advisory Committee
(NSAC-ND)

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1 Introduction

1.1 Executive Summary

Accurate, reliable nuclear data is essential for the success of Federal missions such as nonproliferation, nuclear forensics, homeland security, national defense, space exploration, clean energy generation, and scientific research. Data access is also key to innovative commercial developments such as new medicines, automated industrial controls, energy exploration, energy security, nuclear reactor design, and isotope production. The United States Nuclear Data Program (USNDP) is the domestic custodian of nuclear data. In its April 2022 meeting, the DOE/NSF Nuclear Science Advisory Committee was charged with preparing two reports on nuclear data. In this first report, we review recent accomplishments of the USNDP and discuss complementary and collaborative international efforts. Detailed descriptions of nuclear data needs for basic science, nonproliferation, national security, nuclear energy together with medical and space applications are also presented. Lastly, a set of specific cross-cutting nuclear data needs with relevance for multiple applications areas are also identified for further discussion in a follow-on report planned for release at the end of January 2023.

1.2 Historical Context

From its birth early in the 20th century in the laboratories of Curie, Lawrence and Seaborg and the Manhattan project to the development of next generation small modular reactors and novel radiopharmaceuticals in the 21st century humanity's study of the atomic nucleus has provided both insight into the workings of nature and also a wealth of opportunities and challenges for society. However, even 120 years after its founding, a quantitatively predictive theory of nuclear properties and interactions remains elusive. As a result, a combination of quantitative modeling informed by carefully performed and documented measurements referred to as nuclear data remains essential for harnessing the promise of nuclear science to address many of the greatest challenges facing the 21st century including climate change, the diagnosis and treatment of disease, and evolving threats to national and international security.

The international community understands the importance of nuclear data, and several organizations have been formed to act as custodians. The leading organization in the US is the United States Nuclear Data Program (USNDP), managed by the Department of Energy (DOE) Office of Nuclear Physics (NP). The mission of the USNDP is to provide current, accurate, and authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through compiling, evaluating, disseminating, and archiving nuclear datasets. USNDP also addresses gaps in nuclear data through targeted experimental studies and the use of theoretical models. The USNDP collaborates with other domestic and international organizations including the Cross Section Evaluation Working Group (CSEWG), the Nuclear Energy Agency in the Organization for Economic Cooperation and Development (OECD-NEA) and the Nuclear Data Section of the International Atomic Energy Agency (NDS-IAEA). A 2019 review article [Ber19b] describes the nuclear data compilation → evaluation → dissemination process and lists a set of specific data needs for a range of applications.

In July 2014, the first review of the US Nuclear Data Program in more than 20 years recommended that the USNDP increase its outreach efforts to nuclear data users in the energy, national security/nuclear nonproliferation and isotope production communities. The first step in this process was the Nuclear Data Needs and Capabilities for Applications (NDNCA) Workshop that was held in Berkeley, CA in May 2015 [Ber15]. NDNCA served as a watershed moment for nuclear data, raising awareness of the importance of nuclear data to these user communities and providing impetus to the members of the USNDP to work collaboratively with non-USNDP partners to address nuclear data needs relevant to all users in areas such as fission, neutron scattering, decay data and uncertainty quantification.

The NDNCA meeting started a series of nuclear-data-related meetings in the US to identify nuclear data needs and develop a mission-centric actionable plan or “roadmap” to address them. These included the 2016 Nuclear Data Needs and Capabilities for Basic Science (NDNCBS) [Kon16], the 2018 Nuclear Data Roadmapping Enhancement Workshop (NDREW) centered on nonproliferation [Rom18], and finally the annual Workshop for Applied Nuclear Data Activities (WANDA) in 2019 [Ber19a], 2020 [Rom20a], 2021 [Kol22] and 2022. These meetings have grown in both size and scope with the inclusion of new topics such as nuclear data in support of space applications. Participants are drawn from programs across DOE, NNSA, DOD and DHS, together with significant participation from the nuclear energy industry, national laboratories, universities and international partners.

The overarching picture emerging from these workshops is the extreme degree of interconnection between the facilities and capabilities needed to perform nuclear science and engineering measurements, the nuclear data they generate, the modeling codes they inform, and the applications they serve. This web of interdependencies is expressed in Figure 1.1. Certain capabilities and nuclear data classes, indicated in **bold face** are highly-connected indicating the important role they play in nuclear applications. While many users from these application communities contribute to the process of nuclear data generation, curation, and dissemination, the organizational role played by the USNDP within the DOE-NP office is essential to the orderly transfer of data to applied users.

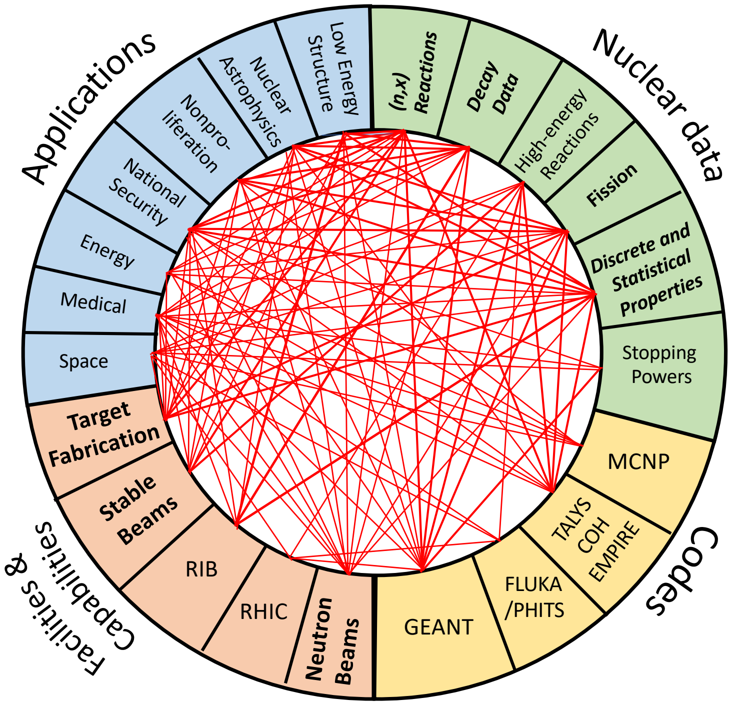

Figure 1.1: Connections between Nuclear Data, Facilities & Capabilities, Codes and Applications. Highly interconnected capabilities and nuclear data classes are indicated by **bold face**.

DOE-NP recognizes the leading role played by the USNDP and the responsibility that comes with it. Therefore, the most recent chapter in the evolving nuclear data picture was initiated in April 2022 when the Nuclear Science Advisory Committee (NSAC) for the Department of Energy and the National Science Foundation was asked to prepare two reports addressing Nuclear Data. This document is the first of those reports, and its goal is to:

1) *Assess USNDP Status, which would include the following actions:*
    a. *Assess and document recent achievements in nuclear data and their impact.*
    b. *Survey current and future federal and non-federal needs for reliable, accurate, secure, accessible nuclear data.*
    c. *Assess the role, competitiveness, and importance of the USNDP in an international context.*

The second report will use the input from this status report to provide recommendations for *maintaining effective stewardship of nuclear data, including the following actions:*

- a) *Identify challenges for nuclear data stewardship in the future, including identifying and prioritizing the most compelling opportunities to enhance and advance NP stewardship of nuclear data and the impact if those opportunities can be realized.*
- b) *Describe possible ways the Nuclear Data (ND) community can work to train and retain a diverse, equitable, and inclusive workforce capable of sustaining the US ND enterprise.*
- c) *Identify access needs for facilities and instrumentation, crosscutting opportunities with other federal programs, and potentially mutually beneficial interactions with other domestic and international stakeholders.*

This second report is due in early 2023.

NSAC responded with the formation of a new Nuclear Data subcommittee (NSAC-ND), chaired by NSAC member Lee Bernstein from the University of California – Berkeley and Lawrence Berkeley National Laboratory (UC Berkeley/LBNL) to address these charges. Prof. Bernstein recruited a committee comprised of subject matter experts in topical areas dependent on nuclear data without regard to institutional or programmatic affiliation to aid in the generation of these two reports. The NSAC-ND members include:

- National Security and Nonproliferation – Mark Chadwick (LANL); Jennifer Jo Ressler (LLNL); Catherine Romano (Aerospace Corp.); Ramona Vogt (LLNL/UC Davis);
- Medical Applications – Cynthia Keppel (JLab); Syed Qaim (Jülich); Cristiaan Vermeulen (LANL);
- Nuclear Energy – Fredrike Bostelmann (ORNL); Massimiliano Fratoni (UCB); Ayman Hawari (NCSU);
- Basic Science - Michael Carpenter (ANL); Calvin Howell (Duke); Caroline Nesaraja (ORNL); Artemis Spyrou (MSU);
- Space Applications – Lawrence Heilbronn (University of Tennessee - Knoxville); Kenneth LaBel (NASA); Thomas Turflinger (Aerospace Corp.);

- Nuclear Databases and International Collaboration – Arjan Koning (IAEA-NDS); Sunniva Siem (University of Oslo).

Most of the NSAC-ND subcommittee members participated in multiple subgroups, providing an opportunity to identify crosscutting nuclear data topics. Input from the two reports will also help craft the 2023 Nuclear Science Long Plan, which commenced its mission at the July NSAC meeting.

The first part of this report covers notable recent (≤ 5 years) accomplishments of the USNDP as well as collaborative efforts with other sponsors and international agencies. The second part of the report includes specific nuclear data needs on the topic areas covered by the NSAC-ND committee. Lastly, a discussion of several crosscutting nuclear data needs topics is presented, which will be expanded upon in the second report.

2 Accomplishments

The US Nuclear Data Program is comprised of subject matter experts with experience in low energy nuclear physics measurements, modeling, and theory. Most programs in DOE Nuclear Physics feature flagship experimental or computational facilities, such as FRIB, ATLAS, RHIC, or NERSC. In contrast, the USNDP's principal value arises from the unique combination of the specific skills, knowledge and abilities of its members and the roles they play in providing authoritative nuclear physics data for a wide range of applications. This includes nonproliferation, nuclear forensics, homeland security, national defense, space exploration, clean energy generation, and scientific research. The USNDP is also key to innovative commercial developments such as new medicines, automated industrial controls, energy exploration, energy security, nuclear reactor design, and isotope production. While some of this work is performed using a mix of USNDP and non-USNDP funding, all of it is made possible by the core competencies of the personnel supported by the NP office.

The single largest effort funded solely by the USNDP involves low-energy nuclear structure data. The primary nuclear structure databases include the Experimental Unevaluated Nuclear Data Library (XUNDL) and the Evaluated Nuclear Structure Data file (ENSDF). ENSDF contains only data for *known discrete* nuclear levels, which are overwhelmingly located at low energies, making it purposefully incomplete at excitation energies above a few MeV. Nuclear structure evaluation is a painstaking process, requiring specialized training that typically takes place over the course of several years. Evaluation is usually performed for common isobars (e.g., an "*A*-chain") that reflects the interconnection between elements with the same number of nucleons due to β-decay. *A*-chains vary greatly in complexity depending on the number of stable isotopes with published data and take anywhere from several months to more than a year to be processed. The center of nuclear structure evaluation activity is at the National Nuclear Data Center at Brookhaven National Laboratory (BNL) with contributions from Data Centers at Argonne National Laboratory (ANL); Lawrence Berkeley National Laboratory (LBNL); Oak Ridge National Laboratory (ORNL); Texas A&M University (TAMU), North Carolina State University (NCSU)) and the Facility for Rare Isotope Beams (FRIB). ENSDF is continuously updated as new *A*-chains are published in Nuclear Data Sheets. In the past 5 years a total of

1596 publications have been compiled into XUNDL and 1071 nuclides have been updated in ENSDF.

In contrast, evaluated nuclear reaction data, which resides in the Evaluated Nuclear Data File (ENDF), is updated more infrequently, reflecting the direct dependence of the application community on cross sections and related information and the impact of a change in cross section on end users. While the USNDP is a significant contributor to ENDF, most evaluations in ENDF are performed by non-USNDP evaluators that make up the Cross Section Evaluation Working Group (CSEWG). However, the NNDC does play the central organizational role in the production and dissemination of ENDF, with the head of the USNDP also serving as the head of CSEWG. In 2020 the USNDP spearheaded the roll out of the 8th edition of ENDF, contributing 175 reactions to its publication over the last 5 years.

Additionally, the USNDP, working collaboratively with members of the IAEA-NDS provides two other critically important databases. The first is Nuclear Science References (NSR), which provides a keyworded index of published and unpublished articles. The second is the Experimental Nuclear Reaction Data (EXFOR) database, a compilation of published nuclear reaction data used to generate ENDF. In the last 5 years the USNDP compiled 18,021 and 1,001 datasets into NSR and EXFOR respectively.

Lastly, it should be noted that the USNDP workforce is a vital and productive scientific research community that produces publications in virtually every major peer-reviewed nuclear-related journal. In the past 5 years this included a total of 375 peer-reviewed articles and 277 invited talks.

In addition to its core functions, the USNDP has contributed to a wide variety of bespoke nuclear databases as well as performing targeted high-priority measurements. In the rest of this portion of the report we include a summary of recent accomplishments by the USNDP and its members over the last four years organized by the major functions of the data program: compilation/evaluation, dissemination and measurements/modeling. Contributions came from the NSAC Nuclear Data Charge subcommittee members themselves and were also solicited from the leaders of the various USNDP centers.

2.1 USNDP Accomplishments

The accomplishments below are listed first by the year they were achieved and then a descriptor such as a library name, a publication or other identifier.

2.1.1 2018 ENDF/B-VIII.0

The ENDF library is the United States primary source of nuclear reaction data in simulations of nuclear systems and underpins codes such as MCNP and GEANT. On Feb. 2, 2018, the latest major release of the ENDF nuclear reaction data library, ENDF/B-VIII.0, was announced. This marked the 50th anniversary of the ENDF library (ENDF/B-I was released over the summer of 1968). ENDF/B-VIII.0 fully incorporates the new Neutron Data Standards, includes improved thermal neutron scattering data and uses new evaluated data from the Coordinated International

Evaluation Library Organization (CIELO) pilot project for neutron reactions on ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. The evaluations benefit from recent experimental data obtained in the US and Europe, and improvements in theory and simulation, notably input from members of the USNDP who develop the EMPIRE (https://www.sciencedirect.com/science/article/pii/S0090375207000981), CoH and FRESCO (http://www.fresco.org.uk) reaction codes. Key advances include updated evaluated data for light nuclei, structural materials, actinides, fission energy release, prompt fission neutron and gamma-ray spectra, thermal neutron scattering data, and charged-particle reactions. The library is detailed in a series of articles in the March 2018 issue of Nuclear Data Sheets [Bro18]. In recognition of this achievement the ENDF database manager and USNDP Head Dave Brown was awarded a LANL Challenge Coin by Mark Chadwick.

2.1.2 2020-2022 XUNDL Pre-publication review

The eXperimental Unevaluated Nuclear Data List (XUNDL) was initiated in the late 1990s to serve as a compilation database for nuclear structure and decay articles. The traditional workflow for compilation is shown in the figure below; following publication a compiler would extract data from the publication, convert it to ENSDF format and run a suite of analysis and checking codes on the data. If issues or deficiencies were identified in the data, the compiler would attempt to contact the authors for clarification or additional data. There are several disadvantages to this workflow, including possible discrepancies between data in the database and in the publication, and authors not responding to compiler requests. To improve on this workflow, around 2019 the NNDC began a pilot project with Physical Review C to embed the data compilation step into the publication process, as shown in Fig. 2.1. Following submission, manuscripts are sent to the Nuclear Data Review Group, where data are checked for consistency and completeness. At this stage, any issues with the data are resolved, ensuring that the data in the databases and in the publication are identical. In addition, the data review group can make requests for additional numerical data, which are usually then made available through the supplemental material section of the journal. This new workflow has been very well received by nuclear structure researchers and serves as a steppingstone for increased collaboration between the data and experimental communities.

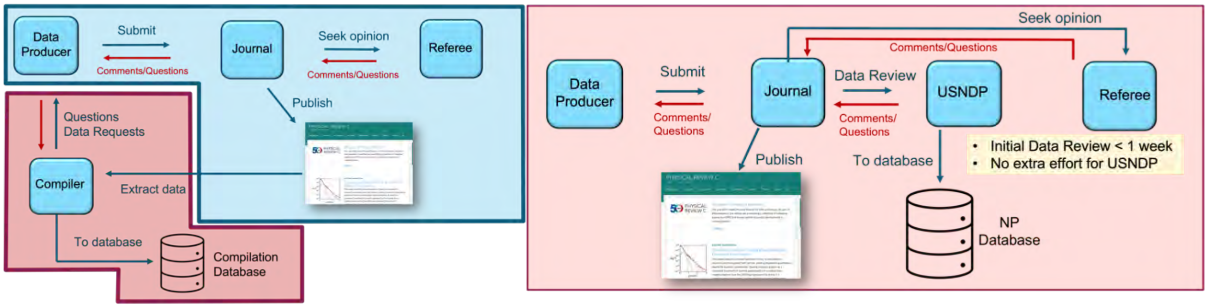

Figure 2.1: Workflow of XUNDL compilations prior to 2019 (left) and after 2019 (right). In the new workflow, compilations and data vetting are embedded into the publication process of Physical Review C and European Physical Journal A.

2.1.3 2020, 2022 GNDS-1.9 & GNDS-2.0 & ENDF modernization

In FY20, the first official release of the Generalized Nuclear Database Structure (GNDS) version 1.9 specifications were published by the OECD/NEA [Bro20] (the book cover is shown to the right)[1]. The GNDS format is part of a larger, community-wide, nuclear reaction data modernization effort. The ENDF/B-VIII.0 library was released simultaneously in both the legacy ENDF-6 format and the new GNDS-1.9 format. Newer GNDS format versions will likely be incompatible with the legacy ENDF-6 format. The GNDS Expert Group is chaired by D. Brown (BNL) with collaborators at LLNL, LANL, ORNL and elsewhere.

Specifications for the Generalised Nuclear Database Structure (GNDS)

2.1.4 2022 EXFOR-NSR PDF database, published in Journal of Instrumentation

The first step in the production of authoritative nuclear data is the compilation of published bibliographic and experimental reaction data into a database accessible to the nuclear science and evaluation community. The experimental nuclear reaction data (EXFOR) and Nuclear Science References (NSR) databases contain compilations based on primary (journals) and secondary (conference proceedings, theses, preprints, etc.) publications, and data received from authors via private communications. In addition to the primary information compiled into these databases, supporting library materials and private communications are often needed for nuclear data verification, compilation, evaluation, and dissemination activities. To address this issue, bibliographic materials were scanned into PDF (Portable Document Format) files and uploaded to a relational database. The Web interfaces for authorized and public access to the EXFOR-NSR nuclear publications database were implemented at the US NNDC and the IAEA NDS, https://www-nds.iaea.org/.

2.1.5 2020 AME 2020, NUBASE 2020

USNDP member Filip Kondev (Argonne National Laboratory), in collaboration with scientists from the Institute of Modern Physics of the Chinese Academy of Sciences (China), Universite Paris-Saclay, IJCLab (France), Max-Plank Institute (Germany) and RIKEN Nishina Center (Japan) recently produced new evaluations of atomic masses (AME2020) and basic nuclear physics properties for ground states and isomers (NUBASE2020) that were published in March 2021 [Kon21].

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[1] https://oecdnea.org/download/wpec/documents/7519-GNDS.pdf

The mass of the nucleus provides the nuclear binding energy, a fundamental property that is indispensable for the study of nuclear structure, stellar nucleosynthesis and neutron-star composition, as well as atomic and weak-interaction physics. Together with other basic nuclear properties for the ground and isomeric states, such as excitation energies (for excited isomers), quantum numbers, half-lives, decay branches and their intensities, these carefully crafted nuclear data are important to both the basic nuclear science program and to many practical applications. They are also crucial input to the main USNDP databases, such as ENSDF and ENDF, which is excellent testimony to their relevance. One of several images available on the web from AME 2002 displaying the mass-excess uncertainties for all (3340) nuclei in their ground state.
is shown in Figure 2.2.

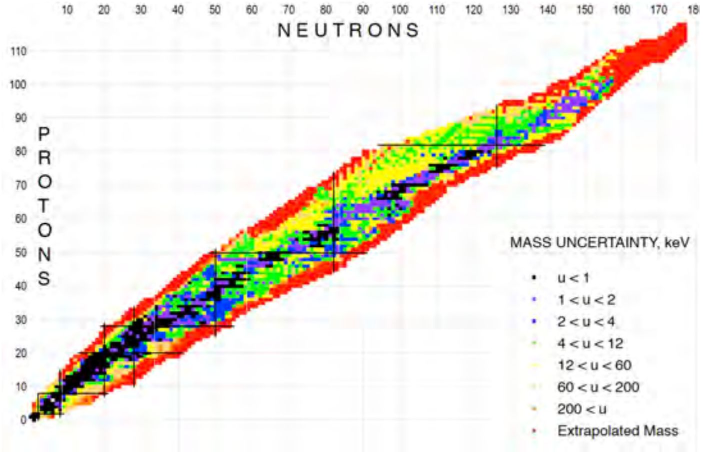

Figure 2.2: Nuclear chart displaying the mass-excess uncertainties for all (3340) nuclei in their ground

2.1.6 2021 ENSDF Code Modernization

The ENSDF utility and analysis codes are indispensable and play a critical role in every step of data compilation, evaluation, validation and dissemination; the modernization of codes has enabled evaluators to produce results while often improving efficiency and ensuring the quality of compilations and evaluations. The codes are essential tools for the USNDP as well as the international network of Nuclear Structure and Decay Data (NSDD) evaluators' work. The legacy ENSDF codes had been reported to have longstanding issues that were not resolved because of lack of maintenance for many years; the codes were also outdated in comparison with modern computer technology. Beginning in 2015 coordinated work began to modernize most ENSDF utility and analysis codes. Significant progress has been made. New codes have been released that have solved issues in the legacy codes and they have greatly helped evaluators facilitate XUNDL compilations and ENSDF evaluations. Meetings to develop the codes have been coordinated by the IAEA and held under the framework of USNDP and NSDD to bring together code developers and evaluators to discuss needs for development, improvement and extension of these codes. The new codes are maintained by USNDP and NSDD evaluators and new recommendations are quickly implemented and disseminated to evaluators and users via the IAEA ENSDF codes webpage[2]. At present nearly all legacy ENSDF codes have been updated or replaced with new codes in Java. The figure on the right shows how these codes fit into the nuclear structure data pipeline from compilation to evaluation to validation to dissemination. This project was awarded as part of the FY2019 Nuclear Data InterAgency Working Group (NDIAWG) Funding Opportunity Announcement.

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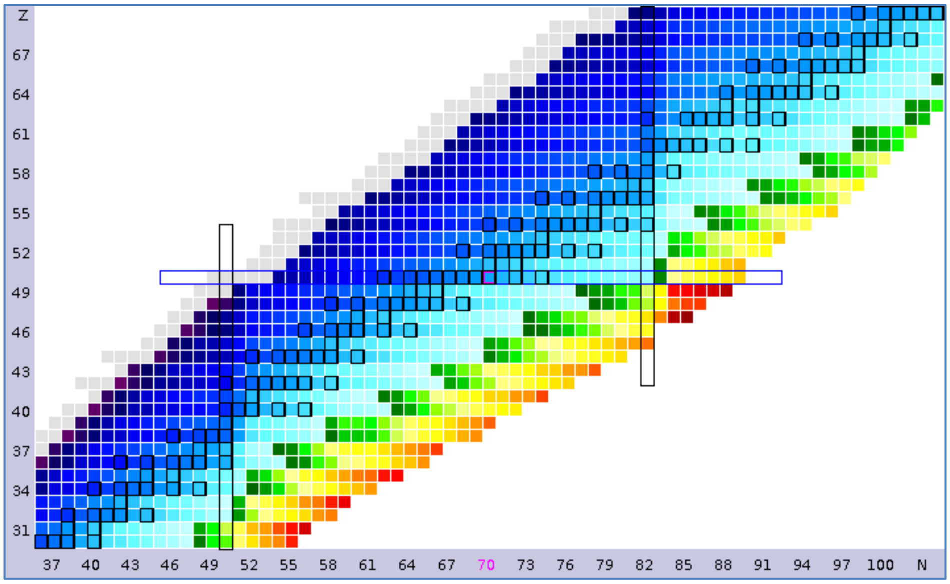
[2] https://www-nds.iaea.org/public/ensdf_pgm/

2.1.7 2020 Beta delayed neutron emitters CRP (published 2021)

The emission of neutrons following beta-minus decay is a phenomenon that happens for neutron-rich nuclides, when the beta-minus Q-value is larger than the neutron separation energy of the daughter. The difference between these two parameters is known as Qβ-n, which colors the chart on the right. As can be seen, odd-Z nuclides are energetically more favored to show this decay mode. In particular, Br, Rb, I and Cs fission products are the main contributors to the delayed-neutron multiplicity, a fundamental parameter in nuclear reactor operations. Additionally, this decay mode is of interest in nuclear astrophysics to compare natural abundances to those generated in the r process.



Due to the relevance of this topic, the IAEA NDS organized a Coordinated Research Project with goals including the compilation and evaluation of half-lives as well as 1- and 2-neutron emission probabilities following β^- decay. Balraj Singh, Elizabeth McCutchan and Alejandro Sonzogni were the USNDP members involved in this project. The results were published in Nuclear Data Sheets in 2021 [Dim21].

2.1.8 2021 Baghdad Atlas compilation/publication

Gamma-ray production following the inelastic scattering of fast neutrons is becoming increasingly important for national security and nonproliferation applications and offers a valuable tool for the development of improved shielding for fast neutrons relevant to the design of both fast reactors and space applications. In recognition of this fact the Berkeley Group working in collaboration with the Nuclear Science and Security Consortium (NSSC) funded by the NNSA office of Nonproliferation Research and Development (NA-22) developed a relational database based on the original (*n,n'γ*) work carried out by A.M. Demidov *et al*. at the Nuclear Research Institute in Baghdad, Iraq [Dem78]. A summary providing an overview of the project was published in 2021 [Hur21] and is available for download from the Berkeley group website.[3]

The information in the ATLAS includes:

- γ-ray energies and intensities;
- Nuclide and level information from which the γ-ray originated;
- Target (sample) experimental measurement information.

Taken together, this information allows for the extraction of the flux-weighted ($n,n'\gamma$) cross sections for a given transition relative to a defined value. In the examples presented here, we are currently using the fast-neutron flux-weighted partial cross section for the production of the 847-keV $2^+_1 \rightarrow 0^+_{gs}$ transition in ^{56}Fe, σ_γ=329.46 mb. This value can be changed to accommodate the user preference.

The ($n,n'\gamma$) data has been compiled into a series of ASCII comma separated value tables and can also be interacted with directly via the SQLite engine. A suite of Structured Query Language (SQL) scripts in the sql_codes directory illustrating various methods for querying the data was also provided. The database can also be accessed via the Jupyter Notebook Python-browser interface. A figure from the original publication and a gamma-ray spectrum from the database are shown in figure 2.3.

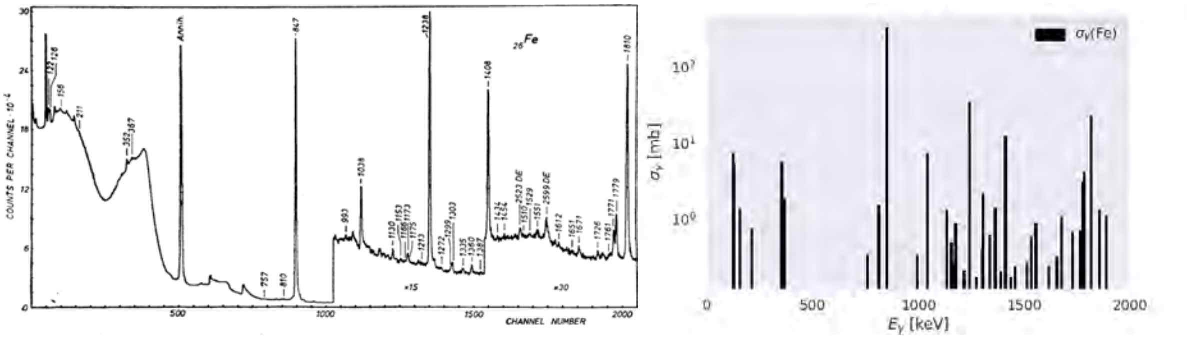


Figure 2.3: Gamma-ray spectra from the original work by *Demidov* and the 2020 relational database.

2.1.9 2022 Natural Language Modernization of Nuclear Science References

The first step in nuclear data evaluation, as with all scientific research is a comprehensive review of the existing peer- and non-peer-reviewed literature. However, there is a constant torrent of new articles published in over 80 mainstream journals that makes this sort of review extremely challenging. For example, in 2020 there were over 4000 papers published in the top nine nuclear science journals alone. Currently, the search, categorization, and tabulation of these articles into the Nuclear Science References (NSR) Database [Pri11] is a manual and laborious process, which only incorporates data from a limited number of peer-reviewed journals. Assuming 30 minutes per paper of processing time (used to read the paper, categorize it, and extract all

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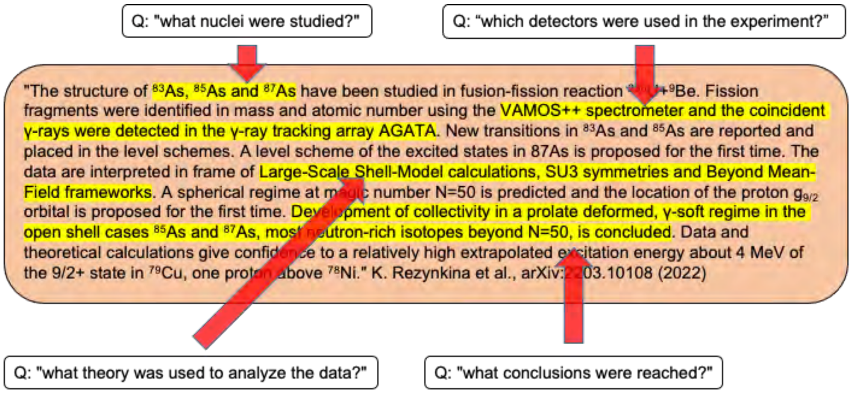
[3] https://nucleardata.berkeley.edu/atlas/download.html

relevant data), the amount of effort needed to simply keep up with new literature corresponds to roughly one full-time PhD-scientist. **Automation is not just desirable, it's a requirement.**

To address this need, a team of Berkeley scientists and students led by Drs. Bethany Goldblum and Walid Younes and Prof. Juan Manfredi from the Air Force Institute of Technology consulted with expert nuclear data evaluators at the various US Nuclear Data Program centers to understand the needs of the community, establish priorities, and develop software requirements for NucScholar. NucScholar automates the retrieval, categorization, and search of nuclear science literature using recent developments in natural language processing *(NLP)* that are available through open-source libraries, such as PDFMiner, Gensim, and the Bidirectional Encoder Representations from Transformers (BERT) [Dev19]. The goal of this project is to provide a "Google-like" search capability tailored for use by nuclear science researchers. An example of the interaction between a natural language query and a portion of a nuclear science publication is shown in Figure 2.4.

To date, the NucScholar team has converted all NSR entries into JSON format for use in NLP model training/benchmarking and demonstrated categorization of nuclear physics literature based on experiment versus theory and into the 7 NSR topical areas (Atomic Masses, Atomic Physics, Compilation, Nuclear Moments, Nuclear Reactions, Nuclear Structure, and Radioactivity). The team is in the process of generating a large database of nuclear science literature in text format for training and NLP queries.

NucScholar can be found on the web at https://nucscholar.lbl.gov. It was made available to the nuclear data evaluation community in August 2022 as a tool to generate nuclear science specific training data. As training data are generated and the model is fine-tuned, this tool will develop into a full-fledged nuclear-science-specific search engine. More information about the project can be found at https://nucscholar.berkeley.edu/.



"The structure of ^{83}As, ^{85}As and ^{87}As have been studied in fusion-fission reaction [illegible]U+^{9}Be. Fission fragments were identified in mass and atomic number using the VAMOS++ spectrometer and the coincident γ-rays were detected in the γ-ray tracking array AGATA. New transitions in ^{83}As and ^{85}As are reported and placed in the level schemes. A level scheme of the excited states in 87As is proposed for the first time. The data are interpreted in frame of Large-Scale Shell-Model calculations, SU3 symmetries and Beyond Mean-Field frameworks. A spherical regime at magic number N=50 is predicted and the location of the proton $g_{9/2}$ orbital is proposed for the first time. Development of collectivity in a prolate deformed, γ-soft regime in the open shell cases ^{85}As and ^{87}As, most neutron-rich isotopes beyond N=50, is concluded. Data and theoretical calculations give confidence to a relatively high extrapolated excitation energy about 4 MeV of the 9/2+ state in ^{79}Cu, one proton above ^{78}Ni." K. Rezynkina et al., arXiv:2203.10108 (2022)

Figure 2.4. Nuclear science literature excerpt showcasing natural language queries, with the model response highlighted in gold.

2.1.10 2021 PuRe Designation

In April 2021, the NNDC was designated by DOE as a PuRe Data Resource. PuRe is a designation for key data repositories, knowledge bases, analysis platforms, and other activities that strive to make data publicly available to advance scientific or technical knowledge. By designating the NNDC as a PuRe Data Resource, the DOE recognizes the importance of this designation, and it carries the weight of scientific data stewardship. The DOE Office of Science manages these resources under an oversight model with high standards for data management, resource operations, and scientific impact. The inaugural list of PuRe Data Resources can be found here[4].

As a requirement of the PuRe designation, the NNDC must abide by several conditions, including adding Document Object Identifiers (DOIs) to all datasets for which they are appropriate, including ENSDF, ENDF and EXFOR data, and developing robust data preservation and backup systems. To support the PuRe designation, the NNDC has made several computer infrastructural improvements:

- NNDC Cloud-Based Backup and Disaster Recovery: continuous backup three mission-critical servers, enabling quick recovery within 2 hours in case BNL computer services are compromised by a disaster. This is one of the operational requirements for NNDC to be declared by DOE as a PuRe data resource center.
- GitLab upgrade from the Starter Edition to the Premium Edition and standing up a Kubernetes Cluster of Docker containers.
- To be able to perform continuous integration and deployment using GitLab and the Kubernetes cluster as a platform. This is also a key step in automating the nuclear data pipeline.

Figure 2.5 shows a screenshot of the DOI landing page for the ENSDF library.

Figure 2.5: Screenshot of the ENSDF Library DOI landing page. ENSDF was the first NNDC library assigned a DOI, followed by XUNDL and NSR

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[4] https://www.energy.gov/science/office-science-pure-data-resources

2.1.11 2022 Global Charged Particle Emission Database

The successful commissioning of the Facility for Rare Isotope Beams (FRIB) heralds a new source of decay data for nuclei far from stability. The decay of these nuclei reveals properties of nuclear structure phenomena at an extreme imbalance of the number of neutrons and protons with respect to stable nuclei, allowing a better understanding of fundamental nuclear interactions. In most cases, the study of heavy charged particle decay modes is the only method available to populate the nuclear states necessary to obtain this information. Nuclei near the proton drip line with large Q values for β^+ decay often β decay to excited states that subsequently decay by the emission of a proton (or alpha particle). This beta-delayed proton (or alpha) emission (β^+p or $\beta^+\alpha$) provides valuable information on the ground state in the precursor, such as β^+ branching, half-lives, spin, and parity. Nuclei even farther from stability can emit a proton (or alpha) directly from its ground state. The properties of protons and alphas feeding a known state in the daughter nuclide provides information on the structure of the proton-unbound states and gives information on the structure and mass of the parent nucleus. These decay modes are illustrated in Figure 2.6 for a precursor nucleus unbound to direct and β^+-delayed particle emission.

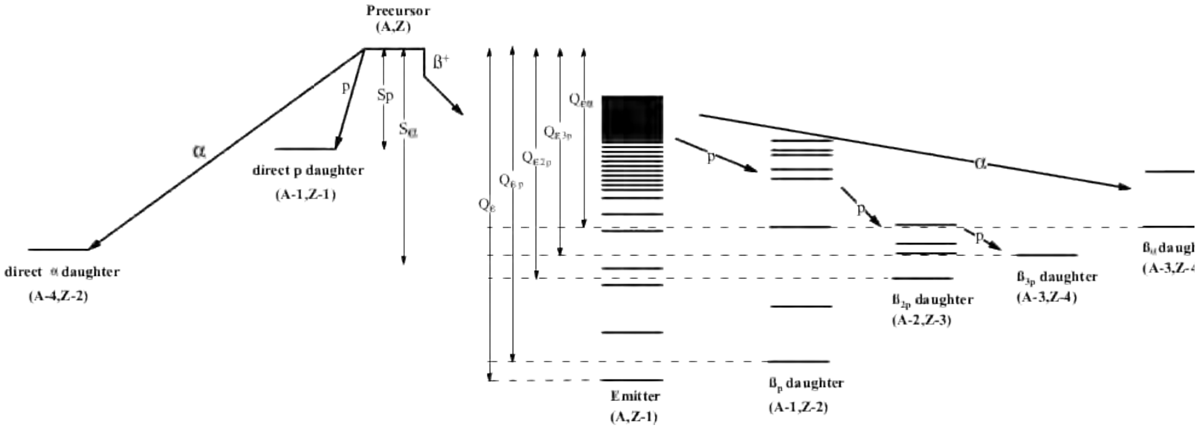

Figure 2.6: Schematic representation of the decay modes covered in the new Heavy Charged-Particle Decay Database produced by the Berkeley Group.

In recognition of the importance of this data Jon Batchelder from the Berkeley nuclear data group, working with Aaron Hurst and undergraduate Yun-Hsuan (Abby) Lee, built on the effort put into producing the "*Recommended values for β^+-delayed proton and α emission*" published in 2020 [Bat20] to prepare a new Global Heavy Charged-Particle Decay Database[5] of all known delayed and direct heavy charged particle emitters (p, α). This database includes branching ratios, half-lives, and all relevant Q and S energies (taken or calculated from Ref. [Wan21b]) for those nuclei where these decays are energetically possible. In addition, for those nuclei with known resolved proton and alpha transitions, particle energies, intensities, and the energies of the particle-emitting states are compiled and evaluated. A list of experimental references for each precursor is also given. The nuclei are organized by their isospin projection (T_z) in this evaluation. In the early version of the database complete compilations from T_z = -4 to T_z = +4 are included, with additional T_z groups still to be included up to the heaviest nuclei known (T_z =

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[5] https://nucleardata.berkeley.edu/research/betap.html

+32). This database will be updated as new papers are published. Information from this database can currently be downloaded as a pdf document.

2.1.12 2021 Solar r-process Abundances using Nuclear Data

The recent observation of neutron stars merger (GW170817) by the Laser Interferometer Gravitational-Wave Observatory (LIGO) collaboration and the measurements of the electromagnetic emission spectrum as a function of time for different wavelengths have profoundly transformed our understanding of *r*-process sites as well as considerably energized nuclear astrophysics research and computer modeling efforts. Solar system *r*-process abundances are observables in *r*-process simulations, as calculations rely on astrophysical models and high-quality nuclear data to emulate these abundances in the final debris of a stellar cataclysmic event.

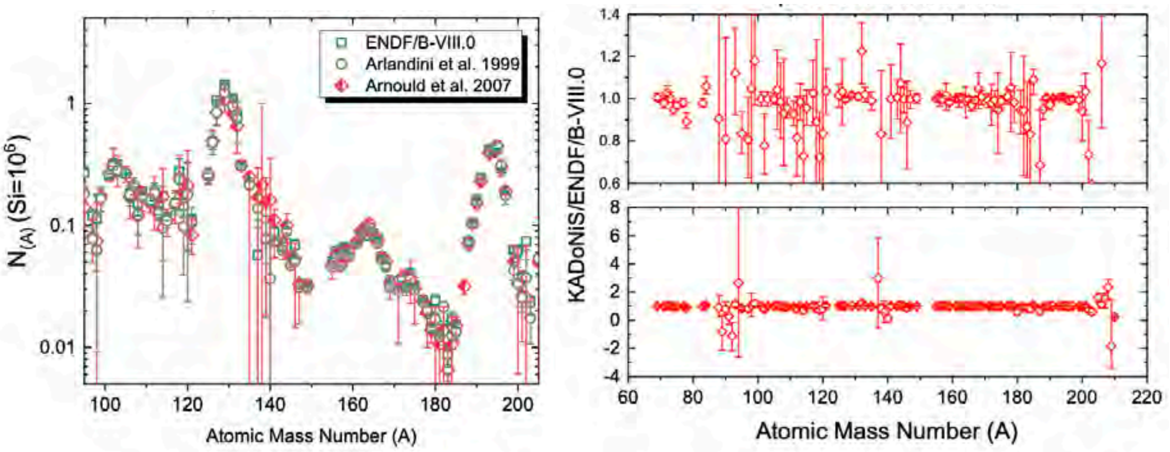


Figure 2.7: (Left) Solar r-process abundances for nuclides that are produced by both the s- and r-processes derived from ENDF /B-VIII.0 (squares) compared with those obtained by Arlandini et al. [Arl99] (circles) and Arnould et al. [Gor99, Arn07, Pal93] (diamonds). (Right) The ratio of KADoNiS 0.3 [11] to ENDF /B-VIII.O solar r-process abundances. Upper panel: Zoomed view. Lower panel: Complete view. The imperfectly subtracted residuals or s-process overproduction cases are depicted as negative ratios.

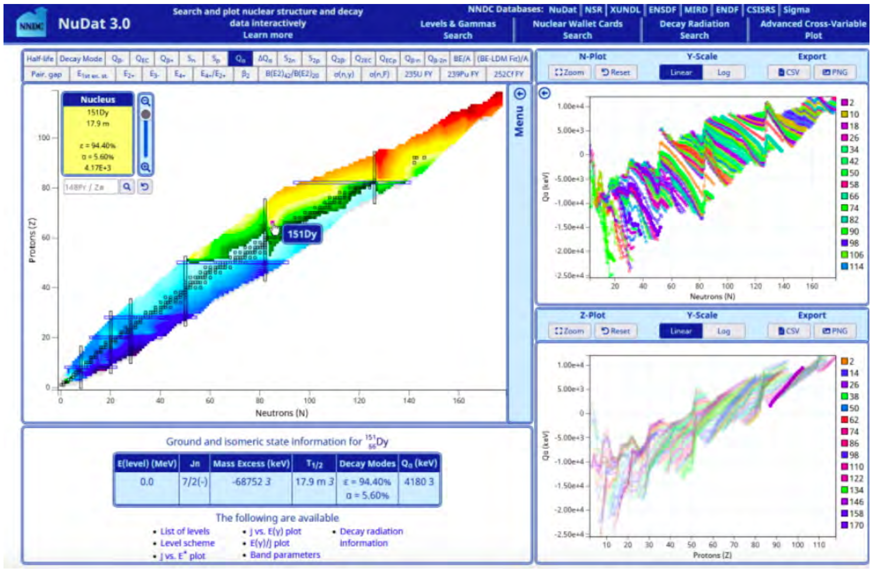
A recent reanalysis of the Karlsruhe Astrophysical Database of Nucleosynthesis in Stars (KADoNiS) reveals multiple issues with the Karlsruhe neutron cross sections and a strong need for complementary data. The release of the ENDF/B-VIII.0 library provided comprehensive neutron data sets for nuclear science and technology and basic science applications. The Maxwellian-averaged (n,γ) cross sections for 553 ENDF/B-VIII.0 library target nuclides have been computed and used in slow neutron capture (*s*-process) simulation. Solar system *r*-process abundances were extracted and compared with the previous values. An example of the data is shown in figure 2.7 above. The results were published in J. Phys. G in 2021 [Bor21]

2.1.13 2022 NuDat3

NuDat is a web application that allows users to search and plot nuclear structure and nuclear decay data interactively. NuDat was developed by the NNDC in the early 2000s. It provides an interface between web users and several databases containing nuclear structure, nuclear decay, and some neutron-induced nuclear reaction information. It is by far the most used application of the NNDC web services, with over four million retrievals in FY21.

Despite its high usage and popularity among many user communities, NuDat was still making use of 15-year-old web technology. In January 2021, the NNDC began a project to modernize NuDat, led by BNL intern Donnie Mason. The project continued through the summer, with the internship converting to the DOE-funded Science Undergraduate Laboratory Internship (SULI) program. A beta version of NuDat3 was released at the end of FY21 and Donnie Mason was hired as a Technology Analyst at the NNDC.

New web technology gives NuDat3 a host of new features, as shown in Figure 2.8. New features in the interactive chart of nuclides include: (i) smooth pan and zoom using intuitive gestures, (ii) a movable current nucleus display with a search field and a zoom to slider, (iii) added ability to filter by ground and isomeric state properties, (iv) synchronized 1-D plots adjacent to the current chart view, and (v) options to export data, such as CSV, PNG, or a shareable link.



Ground and isomeric state information for $^{151}_{66}$Dy

E(level) (MeV)	Jπ	Mass Excess (keV)	$T_{1/2}$	Decay Modes	Q_α (keV)
0.0	7/2(-)	-68752 3	17.9 m 3	ε = 94.40% α = 5.60%	4180 3

The following are available

- List of levels
- Level scheme
- J vs. E* plot
- J vs. E(γ) plot
- E(γ)/J plot
- Band parameters
- Decay radiation information

Figure 2.8: Screenshot of NuDat3 showing the interactive chart of nuclides (top left), current nucleus display (bottom left), and two plots synchronized to the main chart of nuclides (top & bottom right).

2.2 Collaborative Accomplishments

This section describes recent USNDP accomplishments in collaboration with other federal and non-federal programs.

2.2.1 The Nuclear Data Working Group (NDWG) and the Nuclear Data Interagency Working Group (NDIAWG)

Following the NDNCA meeting in 2015 Dr. Catherine Romano, working in collaboration with DOE-NP leadership, led an effort to form a new Nuclear Data Working Group (NDWG) whose goal is to facilitate communication, collaboration, coordination, and prioritization of nuclear data efforts across multiple program offices, the national laboratories, universities, and industry. The group is composed of nuclear data and applications experts nominated to represent program or national laboratory mission interests. The NDWG currently represents 18 program offices and 10 national laboratories.

The NDWG identified and prioritized several of the most important cross-cutting nuclear data needs and presented a proposed solution, as well as general recommendations for funding nuclear data, to 25 federal program representatives at the Nuclear Data Exchange Meeting (NDEM) on April 15, 2016, in Washington, DC. The NDEM provided an opportunity for critical conversations between the nuclear data community and program managers to provide guidance in resolving nuclear data needs.

Figure 2.9: Collaborative goals of the WANDA workshops.

After the NDEM, a group of interested federal program managers created the Nuclear Data Interagency Working Group (NDIAWG) chaired by DOE NP to coordinate nuclear data funding between participating program offices. The NDIAWG is open to all interested federal program managers across DOE, NNSA, and other funding agencies. The NDIAWG communicates regularly on nuclear data needs and planned projects and releases an annual NDIAWG funding opportunity announcement (FOA), managed by DOE NP for all programs [3]. Table 1 lists the projects that have been funded through the NDIAWG FOA since 2018 representing a total of over $50 million in nuclear data improvements. Complimentary projects have also been funded through other mechanisms by agencies such as the DOD and DHS.

The annual NDIAWG FOA is guided by annual WANDA workshops organized by the NDWG. The NDWG determines cross-cutting mission-driven nuclear data needs and selects topics for the WANDA roadmapping sessions. In addition to the annual workshop, topical workshops such as the Nuclear Data for Reactor Antineutrino Measurements, the Nuclear Data Uncertainty Quantification Working Meeting, and the Nuclear Data Workshop for Classified Applications provide recommendations for nuclear data-related improvements impacting specific applications. These workshops are intended to achieve the following objectives:

1. To facilitate communication and collaboration among programs and organizations dependent on nuclear data;
2. To collect subject matter expert input, including nuclear data prioritization and recommended solutions;
3. To increase mutual awareness and understanding of different stakeholder segments of the nuclear data community, including experimentalists, evaluators, end users, and program managers;
4. To ensure recommended nuclear data improvements are mission driven and will provide impact.

The intellectual forum created by the NDWG, the WANDA meetings and the NDIAWG FOAs are shown schematically in Figure 2.9.

The NDWG has created a webpage hosted on the NNDC website[6]. The website contains links to the annual workshops and to resources on nuclear data.

Table 1: Funded NDIAWG projects.

FY start	Title	Lead	PI
FY18	Novel Approach for Improving Antineutrino Spectra Predictions for Nonproliferation Applications	ANL	Kondev, Filip
FY18	Improving the Nuclear Data on Fission Product Decays at CARIBU	ANL	Savard, Guy
FY19	Independent Fission Product Yields from 0.5 to 20 MeV	LANL	Winkelbauer, Jack
FY19	Energy Dependent Fission Product Yields	LLNL	Tonchev, Anton
FY19	Measurements of Independent Fission Product Yields	LANL	Duke, Dana
FY19	Beta-strength function, reactor decay heat, and anti-neutrino properties from total absorption spectroscopy of fission fragments	ORNL	Rykaczewski, Krzysztof
FY19	Integral Measurements of Independent and Cumulative Fission Product Yields Supporting Nuclear Forensics and Other Applications	LANL	Bredeweg, Todd
FY19	Evaluation of Energy Dependent Fission Product Yields	LANL	Kawano, Toshihiko
FY19	Improving the double-differential 238U(n,n’g) cross section using neutron-gamma coincidences	LBNL	Bernstein, Lee
FY20	Scoping Study of the Impact of (alpha,n) Reactions and Yields of Nonproliferation Applications	ORNL	Romano, Catherine
FY20	Assessment of Nuclear Data Needs for Neutron Active Interrogation	ORNL	McConchie, Seth
FY20	Fission product yield measurements using 252Cf spontaneous fission and neutron-induced fission on actinide targets at CARIBU	ANL	Savard, Guy
FY20	Modernization and Optimization of the Evaluated Nuclear Structure Data File	BNL	McCutchan, Elizabeth
FY20	238U(p,xn) and 235U(d,xn) 235-237Np Nuclear Reaction Cross Sections Relevant to the Production of 236gNp	LBNL	Bernstein, Lee
FY21	Neutron Scattering Cross Sections: (n,n'), (n,n'g), and (n,g) Measurements	USNA	Vanhoy, Jeff
FY19	State-of-the-art Gamma-ray Spectroscopy to Enhance the ENSDF	BNL	McCutchan, Elizabeth
FY22	Gamma Rays Induced by Neutrons	BNL	Brown, Dave
FY22	White-source neutron-gamma coincidence measurements of gamma production cross sections at LANSCE	LANL	Kelly, Keegan
FY22	Evaluation of Gamma-ray Production	LANL	Kawano, Toshihiko

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[6] https://www.nndc.bnl.gov/ndwg/

FY22	ß-energy spectral shapes in fission products affecting reactor decay heat and anti-neutrino flux	ORNL	Charlie Rasco
FY22	Two and Three-body Photodisintegration of the Triton at Energies Below 30 MeV	Duke Univ	Calvin Howell
FY22	Designing Nuclear-data Measurements that Resolve Discrepancies in Existing Data	LANL	Denise Neudecker
FY22	Modern Structure-based Nuclear Data Evaluations for Basic Science, Nuclear Safety & Security	LANL	Mark Paris
FY22	Solving the ^{56}Mn puzzle	Univ. of Mass-Lowell	Marian Jandel

2.2.2 Medical Applications

Both nuclear structure and decay data are important for the production and use of diagnostic and therapeutic radionuclides. USNDP personnel have been engaged in wide variety of nuclear data research on this topic.

2.2.2.1 Tri-laboratory Effort in Nuclear Data

Many important radionuclides needed for the diagnosis and treatment of disease are most effectively produced using high-energy (100-200+ MeV) proton beams and thick production targets. The DOE Isotope Program uses the Los Alamos Isotope Production Facility (LANL-IPF) and the Brookhaven Linear Isotope Production (BNL-BLIP) accelerators. Designing targets that are optimized for the production of a specific radionuclide while minimizing the concurrent production of chemically-identical contaminant isotopes requires the ability to properly model reactions with projectiles in this energy range.

Unfortunately, relatively little effort has gone into developing a robust modeling capacity for reactions in this energy range, where compound and pre-compound reaction mechanisms both play significant roles. Of the approximately 32,000 datasets in the EXFOR database, only 18 involve proton-induced reactions with energies greater than or equal to 100 MeV. Furthermore, the residual nuclei formed in these reactions are often very far from the valley of stability, resulting in more poorly-known discrete level structures and quasi-continuum properties, such as nuclear level densities (NLD) and radiative strength functions (RSF), which are needed to guide particle emission probabilities from excited composite nuclei.

The DOE Isotope program is aware of this deficiency and, in 2018, they started a program of targeted measurements at BNL-BLIP. LANL-IPF and the 88-Inch cyclotron at LBNL. This Tri-laboratory Effort in Nuclear Data (TREND) is a collaboration between staff at all three labs and was focused on the production of radiochemical generators for several promising Positron Emission Tomography (PET) emitters, namely ^{134}Ce, ^{68}Ge and ^{72}As and the development of the ^{93}Nb(p,4n) channel as a reaction monitor for high-energy (p,x) reactions.

Over nine months in 2021 the TREND collaboration published two papers that included [Fox21a, Fxo21b] not only measured values for the nuclides mentioned above, but also production cross sections for a total of 78 residual nuclides. The TREND collaboration includes USNDP staff at LBNL as well as staff from the IAEA NDS, ensuring that the data from these measurements were not only used to optimize production rates for these important medically-relevant isotopes, but also to guide improvements in reaction modeling. Some of these experimental results are shown in Figure 2.10.

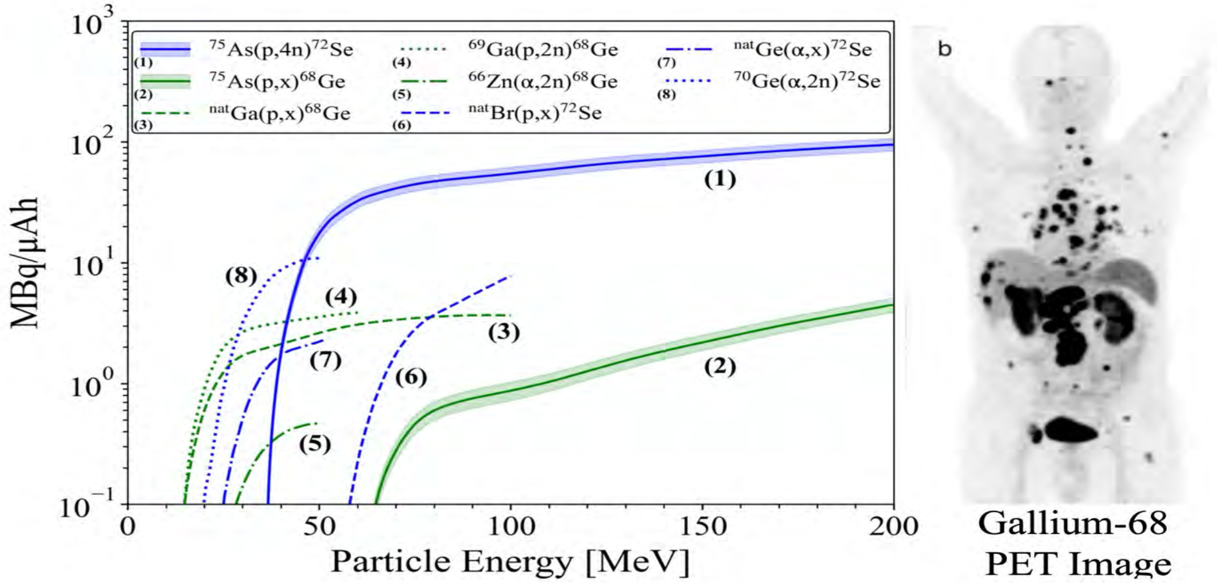

Figure 2.10: Production rate as a function of proton energy of parent radioisotopes ^{68}Ga and ^{72}Se used as radionuclide generators for PET nuclides ^{68}Ga and ^{72}As (left); a Ga PET image obtained with ^{68}Ga nuclides (right).

2.2.2.2 Correcting a long-standing error in decay data: the ^{137}Ce story

The DOE Isotope Program supported an R&D effort to produce ^{134}Ce as positron-emitting analog to the promising alpha-therapeutic radionuclide ^{225}Ac using the ^{nat}La(p,x) reaction. This effort resulted in two 2020 publications [Bec20, Mor20] between researchers at Los Alamos, the Berkeley Group and the research group at the University of Wisconsin.

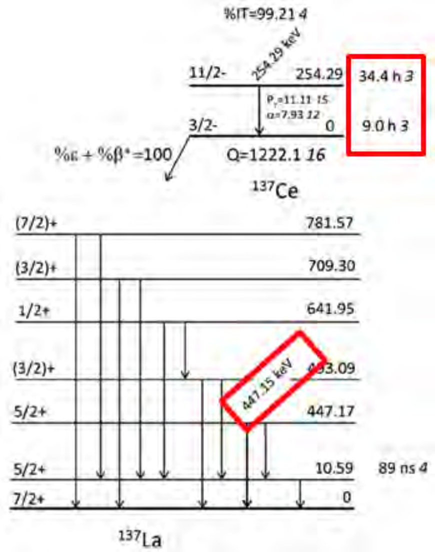

Fig 2.11: Partial level scheme (not to scale) showing 254- and 447-keV γ rays from ^{137m}Ce (34.4 h).

In addition to determining the production cross section for ^{134}Ce, the collaboration produced a large body of decay data for the longer-lived radionuclide ^{137}Ce via the ^{139}La(p, 3n)$^{137m,\gamma}$Ce reaction. At an IAEA-NSDD meeting, Caroline Nesaraja from ORNL had noted that in her evaluation for mass chain A=137, the 447 keV gamma-ray emission probability in ^{137}Ce had an anomaly in the literature. After further discussions with M.S. Basunia from Berkeley, a collaboration among the Berkeley, ORNL and Jülich groups was established to deduce the emission probability of the 447-keV γ ray from the EC+ β^+ decay of ^{137}Ce^g (9.0 h) relative to that of the 254-keV γ ray from the ^{137m}Ce (34.4 h) decay in transient equilibrium (see Figure 2.11). The time-dependent factor in the transient equilibrium was applied following the Bateman equation for a radioactive decay chain. The emission probability for the 447-keV γ ray deduced in this work is 1.21 ± 0.03 per hundred parent decays, which differed significantly from an earlier published value of 2.24 ± 0.10 per hundred decays. The source of this discrepancy was identified to be an incorrect use of the time-dependent factor.

This work [Bas20] highlighted the importance of explicit description of any time-dependent corrections made when reporting γ-ray intensities for nuclides in transient equilibrium and highlighted the value to the nuclear data community that can arise when an experienced evaluator is part of an application-oriented experimental effort.

2.2.2.3 Production and positron emission intensities for the medical radionuclide ^{86}Y

The positron-emitting radionuclide ^{86}Y ($t_{1/2}$= 14.7 h) has been gaining increasing importance due to its theranostic application, i.e. its diagnostic use prior to medication with the β⁻-emitting therapeutic radionuclide ^{90}Y ($t_{1/2}$ = 2.7 d).

However, significant discrepancies exist in the literature for the excitation function of the ^{86}Sr(p,n)$^{86\gamma+xm}$Y reaction which is the method of choice for its production. To address this issue a collaboration was formed between LBNL (USA), Shamsuzzoha Basunia from the Berkeley group and researchers from FZJ (Julich, Germany), BAEC (Bangladesh), Debrecen University (Hungary). The collaboration performed several cross-section measurements from threshold to

16.2 MeV at FZJ, Germany and from 14.3 to 24.5 MeV at LBNL. The experimental cross section data obtained agreed well with the results of a nuclear model calculation based on the code TALYS. The results are shown in Figure 2.12. The integral yield of ^{86}Y was calculated using the cross section data. Over the optimum production energy range E_p = 14 → 7 MeV the yield of ^{86}Y amounts to 291 MBq/μA for 1 h irradiation time. This value is appreciably lower than the previous literature values calculated from measured and evaluated excitation functions. It is, however, more compatible with the experimental yields of ^{86}Y obtained in clinical scale production runs. The levels of the isotopic impurities ^{87m}Y, ^{87g}Y and ^{88}Y were also estimated and found to be < 2 % in sum. The manuscript is published in [Udd20].

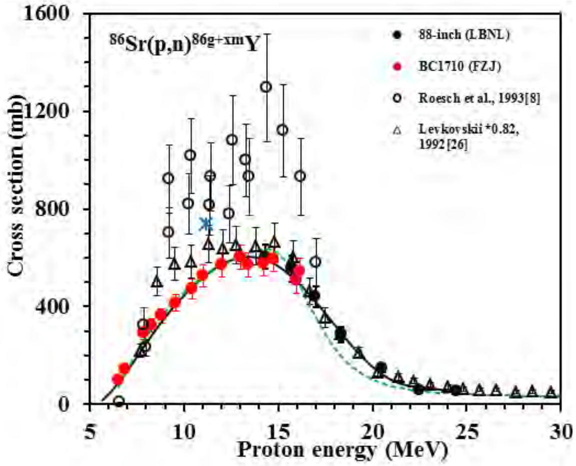

Figure 2.12: Excitation function of ^{86}Y production in the ^{86}Sr(p,n) reaction.

In addition to uncertainties in its production cross section, the use of ^{86}Y as a part of a theranostic pair with ^{90}Y demands a precise knowledge of the positron emission probability of the PET nuclide which was until recently rather uncertain for ^{86g}Y. To address this nuclear data need, the aforementioned collaboration use a high purity ^{86g}Y radionuclide source to perform a direct measurement of the positron emission intensity per 100 decays of the parent using high-resolution HPGe detector γ-ray spectroscopy and measuring the 511-keV annihilation radiation. The electron capture intensity was also determined as an additional check by measuring the K_α and K_β X-rays at 14.1 and 15.8 keV, respectively, using a low energy HPGe detector. Employing these measurements, normalized values of 27.2± 2.0% for β^+-emission and 72.8±2.0% for EC were obtained. These results are in excellent agreement with values recently reported in the literature based on a detailed decay scheme study. The result was published in 2022 [Udd22].

2.2.2.4 Recommended Nuclear Data Library for Medical Isotopes Production

USNDP member Filip Kondev (ANL), in collaboration with scientists from several European, South American, and Asian countries, participated in a project to improve the nuclear data needed in the production of medically-important radionuclides. The project was coordinated by the IAEA. A final set of recommended data files was prepared and are available at the IAEA Medical Isotopes Production Portal[7] Recommended data were also published in several review articles[8,9,10].

Many appropriate and potentially useful radionuclides have been identified for various life-saving diagnostic and therapeutic applications in nuclear medicine. Production routes and decay

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[7] https://www-nds.iaea.org/relnsd/vcharthtml/MEDVChart.html

[8] https://link.springer.com/article/10.1007/s10967-018-6142-4

[9] https://www.sciencedirect.com/science/article/abs/pii/S0090375219300031

[10] https://link.springer.com/article/10.1007/s10967-018-6142-4

properties of all such radionuclides need to be known with confidence. However, deficiencies do exist, especially for optimal production of specific radionuclides, minimization/elimination of impurities, and adequate quantification of the required nuclear data.

2.2.3 Collaborative Efforts for National Security and Nonproliferation

The National Nuclear Security Administration (NNSA) and select organizations within the Department of Defense are among the most longstanding collaborative partners of the USNDP. This section describes several recent collaborative efforts with these partner organizations.

2.2.3.1 Fission Yield Covariance Database

A Monte-Carlo method for the generation of correlation and covariance matrices for independent and cumulative yields for (*n*,f) on 10 elements has been developed and published in Atomic Data and Nuclear Data Tables [Mat21] and distributed on the web[11]. The method uses a constrained Monte Carlo resampling structure to vary evaluated fission yield libraries in a way that meets basic conservation principles. This results in the generation of correlation/covariance matrices with limited model bias and uncertainty; the matrices are primarily reflective of the evaluated fission yield uncertainties and correlations that arise from the evaluation process. This method has been applied to generate correlation and covariance matrices for all of the fissioning systems in the ENDF/B-VIII.0 and JEFF-3.3 evaluations, the first time such matrices have been generated for all of these systems. These covariance matrices have been published online for immediate public use for elements from Th through Fm. These correlation and covariance matrices can be used to improve uncertainty estimation in calculations of reactor antineutrino emission rates, decay heat problems, and nuclear forensics.

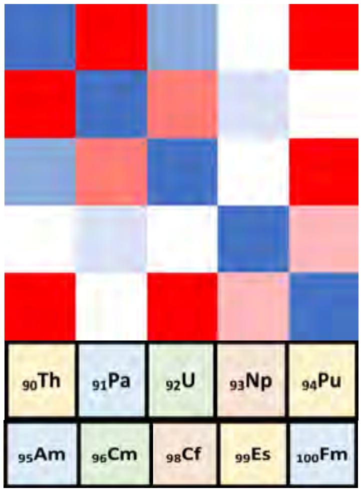

Figure 2.13 Fission product yield covariance database nuclides available at the Berkeley website

2.2.3.2 Gamma-X-ray coincident database

Current fieldable spectroscopy techniques for nuclear forensic applications often use single detector systems heavily impacted by interference from intense background radiation fields. These effects result in low-confidence measurements that can lead to misinterpretation of the collected spectrum. To help improve interpretation of the fission products and short-lived radionuclides produced in a composite sample, a coincidence-gamma database has been developed in support of a robust portable gamma/X-ray coincidence detector system concurrently under development at the Pacific Northwest National Laboratory (PNNL) for in-field deployment using support from both the Defense Threat Reduction Agency (DTRA) and the USNDP. This database is the first of its kind, containing coincident gamma/gamma and

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[11] https://nucleardata.berkeley.edu/FYCoM/index.html

gamma/X-ray intensities on an absolute scale and has the potential to greatly enhance isotopic identification for in-field applications.

In this first version of the database (soon to undergo beta testing at PNNL), more than 3200 decay data sets (α, β⁻, EC/β⁺) have been sourced from the ENSDF archive and successfully translated into a JavaScript Object Notation (JSON) format. All quantities from the primary and continuation records of the original ENSDF file have been serialized into key-value pairs and arrays in a JSON data structure using an intuitive syntax and representative nomenclature. The corresponding data have then been used to create further coincidence gamma/gamma and gamma/X-ray JSON data sets including all energy, intensity, and associated uncertainty information on an absolute scale. In addition, total calculated X-ray and singles gamma-ray decay spectra are stored in the coincidence JSON files along with normalized gamma, electron, and total transition intensities that are needed in the propagation of the coincidence-intensity calculations. The language-independent JSON format allows users to access and manipulate both the derived coincident data, as well as all original ENSDF-translated data, in a straightforward manner requiring little overhead. As an example, the effect of coincidence gating on the total-projection spectrum is demonstrated for the fission-product radionuclide ^{140}Ba (daughter nucleus ^{140}La) are shown in Figure 2.14.

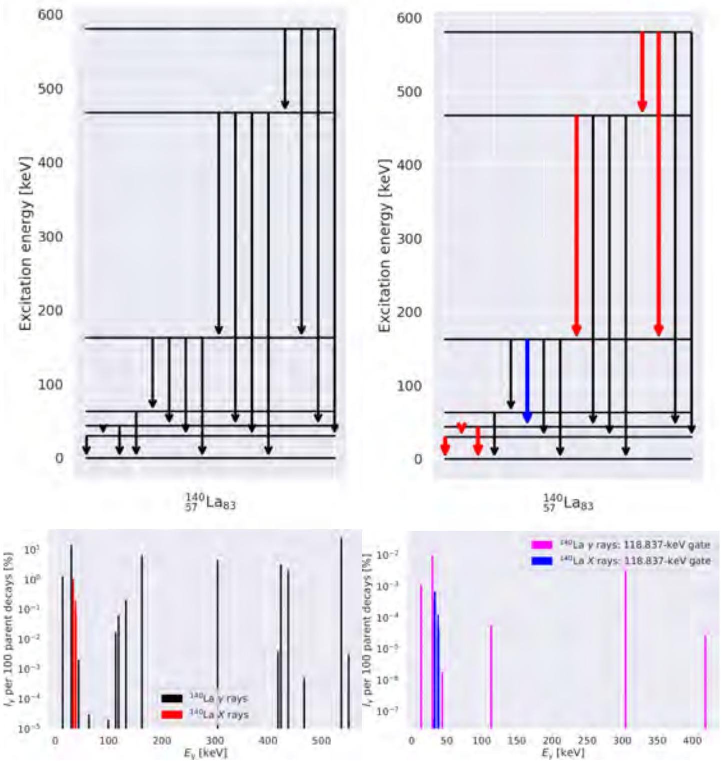

Figure 2.14: The left-hand side shows the decay scheme for ^{140}La and the corresponding total-projection spectrum of gammas and X-rays. The right-hand side shows the gamma rays in coincidence (indicated by the red arrows on the decay scheme) with the 118.8-keV gamma ray (blue arrow) in ^{140}La. The corresponding gated-projection of gammas and X-rays, weaker in intensity and fewer in number, is shown below. All data in this figure were generated from the deserialization of the JSON data structures described in the text.

2.2.3.3 Improved fission modeling (FREYA)

Prior to about 2007, fission was typically modeled deterministically in codes such as MCNP with all neutrons sampled from an average energy spectrum and no regard for conservation rules. In 2009, the FREYA code was developed by Jorgen Randrup (LBNL) and Ramona Vogt (LLNL/UC Davis) [Ran09]. It was intended to be a fast generator of fission events, conserving all quantities (mass, charge, energy, and linear and angular momentum) at each step of the process. The particular initial focus of FREYA was on correlated observables such as neutron-

neutron angular correlations [Vog11,Vog14,Ver18b]. The effort has expanded to cover other observables as well [Vog13,Ran14,Vog17].

Recently, FREYA has been used to study generation of angular momentum in fission [Ran21a,Mar21,Ran21b,Ran22] and the effects of changes in fission yields due to long-lived low spin isomeric states [Ran21a]. The authors have also been involved in two IAEA CRPs [Cap16] and worked with students on a number of topics, see e.g. [Mul14]. Jackson van Dyke, a UC Berkeley undergraduate, made a fit to the FREYA parameters for all the spontaneously fissioning isotopes in FREYA [Van19]. The authors have also made papers with several students and postdocs in the University of Michigan Nuclear Engineering Department, with studies covering photofission of ^{235}U [Cla17], neutron-neutron [Sch19] and neutron-gamma correlations in ^{252}Cf(sf) [Mar18,Mar19,Mar21,Mar22] and photon production as a function of excitation energy in ^{239}Pu(*n*,f) [Gih22]. University of Oslo student Dorthea Gjestvang worked with the authors on her master's thesis on ^{240}Pu(d,*p*f) studies of photon emission [Gje21]. FREYA was also used by the FIRE collaboration to study fission recycling in the r-process and its effect on nuclear abundances [Vas18] and late MeV-scale photon emission as a fission signature of neutron star mergers [Wan20].

FREYA has been published in Computer Physics Communications [Ver15,Ver18a] and is free to download. It was incorporated into MCNP6 through an NA-22 funded project [Tal18]. Indeed, much of the FREYA development has been sponsored by NA-22. The work mentioned here is just a sampling. FREYA has been used both in the US, e.g. [Sny21], and abroad, see e.g. [Wan16,Qi18].

2.2.4 Collaborative Efforts with Nuclear Energy

The next generation of nuclear energy systems involves materials and neutron spectra that are markedly different from the existing fleet of reactors. DOE Nuclear Energy recognizes this fact and has engaged with USNDP researchers to perform measurements and modeling of (*n,x*) reactions on specific nuclides. Two of these ventures are described below.

2.2.4.1 ^{35}Cl(n,p) for Molten Chloride Fast Reactors

Molten chloride salt reactors offer an inherently safe source of carbon-neutral energy that would aid in addressing anthropogenic climate change. The use of chloride salts results in a fast spectrum of neutrons which will allow fuel mixtures not suitable for use in light water reactors. In particular, the ability to use transuranics from spent fuel make this an attractive method for reactor design. Several companies are designing reactors using this technology including Terrapower and Elysium (US), Moltex Energy (Canada) and CEA/Orano (France). Reactor design is heavily dependent on nuclear data for neutron reactions.

The most recent ENDF evaluation of the ^{35}Cl(*n,p*) cross section treats resonances with energies above 1 MeV as unresolved, resulting in large cross sections for this reaction which would act as a "neutron poison" limiting the ability of the reactor to achieve criticality, necessitating the use of enriched ^{37}Cl in the reactor, adding cost and complexity to the reactor design. However, as of 2018, there were no measurements of the ^{35}Cl(*n,p*) cross section in the 0.1 to ≈5 MeV energy region of greatest importance for the reactor. To address this issue two complementary measurements were performed in 2019 at UC-Berkeley [Bat19] and 2020 at LANL [Kuv20].

Results from the Berkeley High Flux Neutron Generator (HFNG)

The ^{35}Cl(n,p) and ^{35}Cl(n,α) cross sections were measured at incident neutron energies between 2.42 - 2.74 MeV using the Berkeley High Flux Neutron Generator[12]. The cross sections for ^{35}Cl(n,p) were more than a factor of three to five less than all of the values in the neutron absorption data libraries (see Figure 2.15), while the ^{35}Cl(n,α) cross sections are in reasonable agreement with the data libraries. The measured energy-differential cross section is consistent with a single resonance with a width of 293(46) keV. This result suggested that, despite the high incident neutron energy, any attempt to model (n,x) cross sections in the vicinity of the $N = Z = 20$ shell gap requires a resolved resonance approach.

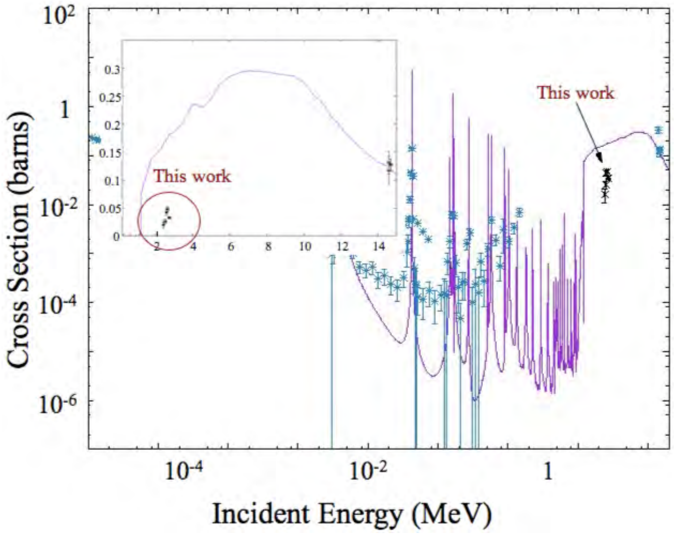

Figure 2.15: Comparison of cross section values of ^{35}Cl(n,p)^{35}S from [Bat2019] to the ENDF/B-VIII.0 evaluation. The inset shows the energy region of interest in a linear scale.

Results from WNR facility at Los Alamos Neutron Science Center

The ^{35}Cl(n,p) and ^{35}Cl(n,α) reaction cross sections were studied from 600 keV to 6 MeV using spallation neutrons from the WNR facility at the Los Alamos Neutron Science Center. Nonstatistical fluctuations in the ^{35}Cl(n, p) cross section were observed up to around 3 MeV and the magnitude of the cross section was systematically lower than all available data evaluations at energies above 1 MeV. The experimental data and resulting calculations show that ENDF/B-VIII.0 underestimates the (n, p) cross section below 1.25 MeV and overestimates it above 1.25 MeV, (Figure 2.16, from [Kuv20]). We note however, that the results were not in agreement with [Bat19] and did not cover the required energy range with the accuracy needed to optimize reactor design.

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[12] http://hfng.nuc.berkeley.edu

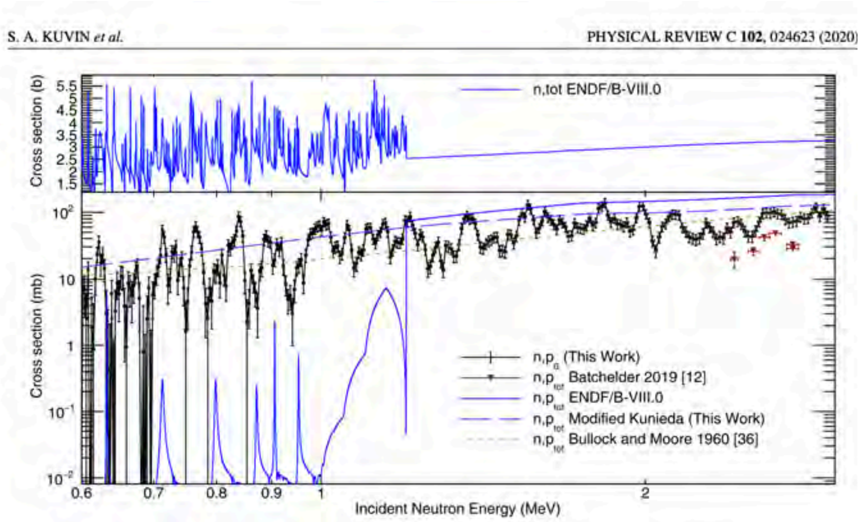

Figure 2.16: Results from the LANL work on ^{35}Cl(n,p)^{35}S [Kuv2020] (Fig. 13 in that ref). The top panel shows the ^{35}Cl(n,total) spectrum from ENDF/B- VIII.0.

Following these measurements, DOE Nuclear Energy and the Gateway to Accelerated Input for Nuclear Initiative provided funding for new cross section measurements to be performed at LBNL in 2021 and Los Alamos in 2023. The Berkeley experiment included measurements of not only the ^{35}Cl(n,p) cross section but also the ^{35}Cl(n,n') and ^{35}Cl(n,γ) cross sections needed for a complete evaluation of the reaction. The LANL effort also included support for complementary reaction evaluation work needed to produce a new cross section evaluation. Results from these efforts are expected in the next 2 years.

2.2.5 Workforce Development Accomplishments

The wide range of applications that rely on accurate, reliable nuclear data calls for an equally diverse and inclusive workforce. To this end, the USNDP has worked to integrate these goals into the program. This includes organizing nuclear data-related summer schools and participating in IAEA sponsored learning activities for the broader international community. The USNDP has also hosted numerous student trainees over the years including at its various centers and also has five centers located at universities (UC Berkeley, Michigan State, Duke and Texas A&M). These activities will be discussed in greater detail in the second portion of the subcommittee report scheduled to be completed on 1/30/23.

In this first status report we are calling out two recent student training opportunities hosted by the USNDP in partnership with other organizations and provide four recent Ph.D. recipients whose dissertation research was centered on nuclear data evaluation.

2.2.5.1 2022 Stellar Modeling for Nuclear Astrophysics Summer School

This conference taught stellar modeling using Modules for Experiments in Stellar Astrophysics (MESA) for nuclear astrophysicists, such as structure theorists and nuclear experimentalists, in order to apply new reaction rates and measure the effects on various features, such as abundances and astronomical observables. The school included brief lectures and extensive hands-on activities, with students learning to run models on their own. The school was held over 4 days in early June at Louisiana State University with local faculty as well as lecturers from the Max Planck institute and Los Alamos National Laboratory. The lead sponsor was Brookhaven National Laboratory and NNDC Research Associate Amber Lauer-Coles. The school was well attended and even exceeded parity in gender participation!

2.2.5.2 2022 NSSC Nuclear Data Summer School (August 1-12, UC-Davis)

The NSSC held a Nuclear Data Summer School August 1-12, 2022, at UC Davis in Davis, California. The program offered students a comprehensive overview of nuclear data as a subfield of nuclear science. Students learned how experimental and evaluated nuclear data is generated, how its corresponding uncertainties are estimated, and how nuclear data affects scientific applications. In addition to the lecture series, this summer school featured a lab practical where students performed a nuclear cross section measurement at the UC Davis Crocker Cyclotron. This lab practical gave students hands-on experience working with nuclear data and reaction modeling data and is intended to produce a set of cross section measurements suitable for publication.

Lecturers from the nuclear data community gave lectures on their various areas of expertise. Students had the opportunity to meet leading scientists and researchers in nuclear data as well as discuss the research and career opportunities that each institution and research group has to offer.

Topics covered included:

- nuclear data for isotope production;
- nuclear data evaluation;
- thermal scattering law and nTOF measurements;
- R-matrix theory and capture/inelastic gamma-ray data;
- cross section modeling, the optical model, and EMPIRE/TALYS;
- fission nuclear data and modeling;
- evaluation validation and integral benchmarks;
- artificial intelligence and machine learning methods

2.2.5.3 Recent Ph.D. Graduates

Nuclear Data Evaluation has traditionally not been considered an appropriate topic for a Physics or Chemistry PhD. However, this is not the case in nuclear engineering which is intrinsically more focused on applications than the physical sciences. In the past 4 years the Nuclear Engineering Department at UC Berkeley has graduated several students whose theses predominately centered on nuclear data evaluation. While these degrees were conferred by Berkeley, they were supported in their research by staff from the NNDC and Los Alamos. These students, their research topics and current employment are shown below.

Amanda Marie Lewis
Spring 2020*
Uncertainty Analysis Procedures for Neutron-Induced Cross Section Measurements and Evaluations
Current Position:
Staff at US Naval Nuclear Labs

Eric Francis Matthews
Spring 2021
Advancements in the Nuclear Data of Fission Yields
Current Position:
Researcher at UC-Berkeley

Morgan B. Fox
Spring 2021
Nuclear Data Evaluation of High-Energy Proton-Induced Reactions for Isotope Production
Current Position:
Terrestrial Energy Staff

Pedro Vincente-Valdez
Spring 2021
Machine Learning Augmented Nuclear Data Evaluations
Current Position:
Senior AI Software Engineer at Mythic

3 International Collaborations

The wide-ranging importance of the applications that depend on nuclear data is recognized throughout the industrialized world. Most international nuclear data efforts take place as a part of international collaborations covered under the Organization of Economic Cooperation and Development's Nuclear Energy Agency (OECD-NEA) and the International Atomic Energy Agency IAEA.

The NEA addresses the nuclear technology interests of its 33 member states, and in the area of nuclear reaction data, the Working Party on Evaluation Coordination (WPEC) is the main forum for collaborative effort between the nuclear data library projects from the NEA countries, namely ENDF/B (United States), JENDL (Japan), Joint European Fission Fusion (JEFF) (NEA), TENDL (Europe), and BROND (Russia), as well as the non-OECD file project CENDL (China).

A powerful instrument of WPEC to drive progress in nuclear data is the so-called Subgroup, or SG: Members of WPEC identify a common area in nuclear data that requires improvement and, if enough support from the various data library projects is present, a Subgroup is formed. Subgroups typically operate on a 3–5-year time frame. A recent successful example of a WPEC Subgroup, with specific relevance to the United States, includes the large-scale horizontal CIELO effort (SG40) on worldwide nuclear data evaluation for the most important fission energy-related materials. The CIELO initiative has led to new ENDF/B-VIII.0 evaluations for ^{235,238}U, ^{56}Fe, and ^{16}O, among others. Other successful Subgroups include one centered on developing a new Generalized Nuclear Database Structure (GNDS) format (SG38)[13], one focused on covariance adjustment for improvement of nuclear data files (SG39)[14] and one on the development of a new format for experimental nuclear reaction data that would facilitate the use of machine-learning algorithms for nuclear data evaluation (SG50)[15].

WPEC also hosts long-term expert groups. Current groups are working on the development of the GNDS format mentioned above, which will provide a data library interface between nuclear physics and applications more modern than the ENDF-6 format, and the High-Priority Request List, which assembles the most important nuclear data requests from applications in a unified format to stimulate experimentalists and evaluators to provide these data. A full list of past and current WPEC Subgroups is available on the web[16].

A key player in nuclear data evaluation is the IAEA, which covers the interests of its 170 member states. The main task of the IAEA NDS is to provide fundamental nuclear databases for basic and applied use, with data originating from experiments and theoretical simulations covering both nuclear structure and nuclear reaction data. An important collaboration coordinated by the IAEA is the Nuclear Reaction Data Center Network, which is responsible for keeping the EXFOR database of experimental nuclear reaction data up to date. The NNDC is responsible for the US input to EXFOR.

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[13] https://www.oecd-nea.org/science/wpec/sg38
[14] https://www.oecd-nea.org/science/wpec/sg39
[15] https://www.oecd-nea.org/download/wpec/sg50
[16] https://www.oecd-nea.org/ science/wpec/

In addition, the IAEA organizes Coordinated Research Projects (CRPs) and technical meetings as instruments to align international nuclear data efforts toward the production of validated databases ready for applied use. Examples of recent and current CRPs include a 2018 venture centered on nuclear data for primary radiation damage, which has been completed; an ongoing effort to improve nuclear model parameters for fission reaction calculations by modern nuclear model codes such as EMPIRE [Her07], CCONE [Iwa16], COH3 [Kaw10], and TALYS [Kon12]; and an effort to create the first-ever evaluated database of radiative strength functions [Gor19]. In 2019, a CRP on fission yields started and aims to produce updated fission yield libraries for the major actinides to respond to requests from reactor technology, safeguards, and nonproliferation.

Nuclear data evaluations of neutron-induced reactions for fission applications are covered by the International Nuclear Data Evaluation Network (INDEN), an IAEA initiative that continues the CIELO efforts of the NEA for differential nuclear data developments, and evaluations, for the most important materials relevant for fission technology. Other long-term projects are cross sections for beam current monitor reactions used in medical isotope production cross section measurements, neutron standards, the Fusion Evaluated Nuclear Data Library (FENDL), and most notably, the Nuclear Structure and Decay Data (NSDD) network.

3.1 Nuclear Structure and Decay Data: international collaboration

Nuclear structure and decay data are important data for a wide range of applications, from the basic nuclear sciences to other fields such as medicine, reactor design and operation, geophysics, environmental sciences, radiation safety and materials sciences. The data in ENSDF are evaluated and maintained by an international group of experts who form the international network of NSDD evaluators. The network has been under the auspices of the IAEA since 1974. It includes 16 data centers and over 20 internationally-recognized experts from more than 10 countries who compile and evaluate nuclear structure and decay data for all known isotopes on an agreed basis. A complete list of the NSDD Centers is available on the web[17]. The role of the IAEA is to coordinate the network, organize biennial technical meetings and expert training workshops for the evaluators, provide technical support where needed, and disseminate the results of the ENSDF evaluations.

Seven data centers funded by the USNDP form the most important component of the NSDD network: NNDC-BNL hosts the ENSDF database and manages both the evaluation pipeline and the publications in Nuclear Data Sheets. MSU is involved in development of ENSDF Analysis and Checking Codes. TUNL is responsible for evaluation and dissemination of light element evaluations ($2 < A < 19$). All USNDP data centers make important contributions to the evaluation of mass chains incorporated into ENSDF.

In addition to NSDD evaluation activities, USNDP evaluators collaborate with the IAEA on various international projects aiming at improving nuclear structure and decay data for specific energy and non-energy applications. Some of these projects are:

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[17] http://www-nds.iaea.org/nsdd/datacenters.html

3.1.1 ICTP Workshops

The organization of joint ICTP-IAEA training workshops on nuclear structure and decay data by the IAEA have been essential to the introduction of new evaluators to the network for ENSDF evaluation over the years. Apart from introducing the evaluation procedures and methodologies, as well as useful online tools, to young nuclear scientists from all over the world, the workshops allow participants to become actively engaged in compilation and evaluation work which eventually will be included in the XUNDL and ENSDF databases, respectively, and published in Nuclear Data Sheets. USNDP evaluators are involved in co-directing the workshops and/or lecturing and supervising compilations and evaluations. Four mass-chain evaluations have been published in Nuclear Data Sheets from the 2012, 2014, 2016 and 2018 workshops.

3.1.2 Project to improve ENSDF processing codes

The IAEA is coordinating a data development project to address the need for maintenance, revision, proper documentation and re-writing of codes in modern programming languages so that they can be used by future generations of programmers and evaluators. Three meetings were held at the IAEA in 2014, 2015 and 2018, respectively (INDC(NDS)-0665, 0696, 0774). USNDP code developers and evaluators participated in this project and contributed to the improvement and development of ENSDF codes in collaboration with other non-US experts (Australian National University, CEA-France, IAEA).

3.1.3 Decay Data for Monitoring Applications

USNDP decay data evaluators contribute to the updating and improvement of decay data of long-lived radionuclides required in monitoring applications by organizations such as Comprehensive Test Ban Treaty Organization (CTBTO) and the IAEA Radiation Safety Laboratories. The coordinated project engages nuclear data experts from Australia, Romania, UK, and the IAEA (INDC(NDS)-0828).

3.1.4 Decay Data for Decay Heat and Anti-neutrino spectra calculations

Accurate estimates of the decay heat produced by reactor fission products after shutdown of the reactor operation are required in safety assessments of all types of reactor and fuel-handling plant, the storage of spent fuel, the transport of fuel-storage flasks, and the intermediate-term management of any resulting radioactive waste.

The most important fission products contributing to decay heat are re-assessed with respect to their decay data to ascertain the impact of the Pandemonium effect and the need for further Total Absorption or Discrete Gamma-ray Spectroscopy measurements. The impact of all the available TAGS data on decay heat calculations as well as reactor anti-neutrino spectra calculations are investigated within an IAEA-lead collaboration. Several USNDP experts collaborate with experts from France, Japan, Spain, India, and the IAEA in this project (INDC(NDS)-0551, 0577, 0676).

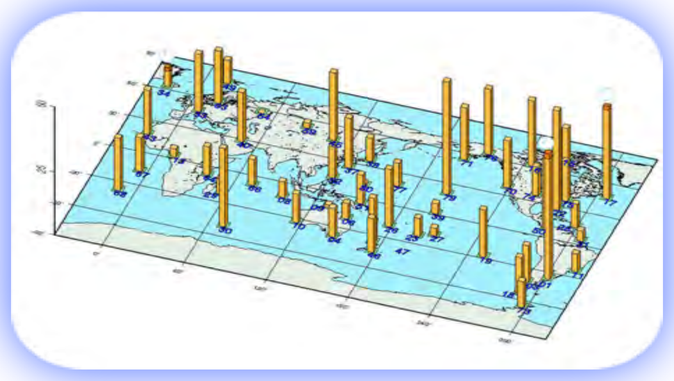
3.1.5 Beta-delayed neutron emission data

A Reference Database[18] for beta-delayed neutron emission data has been developed by an international collaboration led by the IAEA. USNDP experts collaborated with experts from Canada, China, France, Japan, Spain, UK, and Russia to produce recommended beta-delayed neutron data for individual precursors, as well as aggregate total delayed neutron yields, spectra, and group constants for reactor applications. The results are in discussed in section 2.1 above and in the publication by *Dimitriou et al.,* [Dim21].

3.1.6 New Decay Data Library for Monitoring Applications

USNDP members Jun Chen (MSU), Filip Kondev (ANL) and Balraj Singh (McMaster U), in collaboration with scientists from Australian National University (Australia), University of Surrey (UK), IPNE-HH (Romania) and IAEA-NDS (Austria) are contributing to the development of a new decay data library for monitoring applications. The project, coordinated by the IAEA, aims to improve and update the decay data for 27 selected long-lived fission products considered to be of high priority for worldwide radionuclide monitoring efforts. A final set of recommended data files is currently being prepared. It will be published and made available to laboratories and international bodies such as the CTBTO involved in the monitoring of such radionuclides.

Radionuclide monitoring involves measurements of the concentrations of radioactive particles and noble gases in air, soil, and liquid samples. After collection and appropriate treatment of the samples, γ and β emissions are measured by means of Ge detectors and β counters, respectively. Quantification of such spectra relies heavily on up-to-date evaluations of the nuclear structure and decay data of all potential candidate radionuclides. R&D work and Monte-Carlo simulations for identification and quantification of radionuclides also depend on a sound knowledge of the intensities of the γ and β^-, EC/β^+ emissions, along with the equivalent atomic radiation.



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[18] https://www-nds.iaea.org/beta-delayed-neutron/database.html

3.1.7 Future perspectives

The evaluation and dissemination of nuclear structure and decay data is an international effort coordinated by the IAEA. For many years, the NSDD network has been witnessing a shortfall in effort attributed to lack of adequate funding and the retirement of several experienced evaluators.

On the other hand, the advent of modern radioactive beam facilities combined with advances in detector technologies are leading to a rapid growth in new measured data while the demand for up-to-date and reliable nuclear data is increasing due to developments in basic and applied sciences.

To meet the growing demands, a concerted effort is required to develop new approaches to nuclear data evaluation exploiting modern computing tools and enhance international cooperation while maintaining the existing expertise and know-how.

4 Nuclear Data Needs

In this section of the report nuclear data needs are presented for six topical area with the writing leads listed in parentheses:

4.1 Basic Science (Michael Smith and Michael Carpenter);
4.2 Nuclear Energy (Ayman Hawari and Friederike Bostelmann);
4.3 Medical Applications (Syed Qaim, Michael Carpenter, Caroline Nesaraja, Calvin Howell, Cristian Vermeulen and Lee Bernstein);
4.4 National Security (Mark Chadwick and Jennifer Jo Ressler);
4.5 Nonproliferation (Catherine Romano);
4.6 Space Applications (Lee Bernstein, Jennifer Jo Ressler and many others from WANDAs 2019-2022).

4.1 Basic Science

The majority of the staff in the US Nuclear Data Program come from a background in low energy nuclear structure physics. It is not surprising therefore that this community has worked tirelessly to ensure that nuclear data needs for low energy nuclear science be met. In the first part of this section a high-level summary of nuclear data needs for nuclear structure are presented. In the second part, input from USNDP member Michael Smith on nuclear data needs for nuclear astrophysics is presented.

4.1.1 Nuclear Structure

Low energy nuclear science facilities generate a large quantity of nuclear data each year. The experiments performed at accelerator facilities are typically reviewed by a program advisory committee (PAC) and, based on the scientific justification, are allocated beam time. One of the dominant criteria for judging the scientific merit of a proposal is whether it aligns with the Long Range Plan for Nuclear Science (see the cover of the 2015 report) which is re-assessed approximately every 7 years. Consequently, there is a well-established mechanism which determines which nuclear data are important for basic nuclear science and how these data are collected.

In order to quantify the needs of the basic science community with regards to Nuclear Data, a 1.5-day workshop entitled "*Nuclear Data Needs and Capabilities for Basic Science"* (NDNCBS) was organized on August 10-11, 2016 at the University of Notre Dame, in conjunction with the annual Low Energy Community Meeting [Kon16]. A white paper was generated based on the presentations and a list of six items, summarizing the needs of the community going forward as it related to Nuclear Data and the USNDP, was produced. This list centered around the interaction of the research community with the evaluated databases. A list of actual nuclear data needs was not elucidated since the community already has a well-funded process that allows the nuclear data to be collected through experiments.

The workshop participants expressed overwhelming and unequivocal support for the existence, maintenance, and future development of the nuclear structure database (ENSDF). A set of ***specific recommendations*** were made in the NDNCS report and are updated below to reflect the changes that have occurred in the intervening 6 years, including the opening of the Facility for Rare Isotope Beams (FRIB) as the new US flagship facility for low energy nuclear physics.

1. ***The evaluated data should be reliable, comprehensive and up-to-date. To achieve this goal there should be continuous funding support for the existing data evaluators. An expansion of the pool of skilled nuclear structure data evaluators is imperative for succession planning.***

   Experimenters rely on the ENSDF and ENDF databases to assist in their experimental programs, both in planning experiments and in data analysis. For the databases to be useful, one assumes that the underlying databases are a) reliable and credible – data must be correctly evaluated; b) comprehensive – should include all measured quantities and their uncertainties; c) up-to-date – results from all measurements should be promptly incorporated; and d) accessible – easy and rapidly available in user-required formats.

   The current US facilities utilized for basic science research include ATLAS, FRIB, and the ARUNA laboratories. These facilities will continue to generate new data that need to be compiled and evaluated. While most of these data are generated from experiments motivated by basic science, overlap with applications should also be noted. Consequently, it is important to evaluate and compile all of these data into the relevant database *e.g.* ENDF or ESNDF. It is notable that a number of ENSDF mass chains have not been re-evaluated in excess of 10 years and there is a sense from the community that evaluations are falling further and further behind.

2. ***Capabilities for the compilation and evaluation of new and more complex data types should be developed.***

   In the FRIB era, many new types of data, including data with increased complexity, will be generated, which will require upgrades of current database formats and policies. For example, γ-ray strength function data and results from calorimetric γ-ray spectroscopy studies are currently not uniformly incorporated in ENSDF. Nevertheless, they provide important nuclear structure information about the properties of excited states. A new Generalized Nuclear Data format (GNDS) has already been devised and implemented and one for ENSDF is currently being developed. It is expected that these new formats will address these needs.

3. ***Connections to nuclear astrophysics research need to be strengthened and expanded.***

   The interdisciplinary field of nuclear astrophysics has extensive data needs in both reaction and structure physics. It also requires specialized data processing steps in order to enable these data to be used as critical input for simulations of cosmic systems. Current efforts in this area are subcritical. To maximize the scientific return on recent facility investments for measurements in this area, USNDP activities should be expanded to include efforts in evaluations, databases, and tools specifically targeted for nuclear astrophysics. A more detailed explanation of these needs is given in the next subsection.

4. ***Connections to theoretical databases should be established.***

   Progress in all areas of nuclear physics requires the critical comparison of theoretical predictions to experimental data. Theoretical models have, however, greatly expanded their predictive power in scope and complexity and the number of groups producing such sophisticated data sets has also expanded. The USNDP should explore the establishment of databases and tools necessary to facilitate the comparison of large theoretical nuclear data sets with evaluated nuclear data.

5. ***Accessibility to the databases should be improved.***

   The generation of comprehensive and up-to-date databases by itself is not sufficient to fully exploit the potential of scientific discoveries. Appropriate interfaces that allow the users to easily interrogate the evaluated data are required. In close collaboration with the nuclear physics research community, USNDP should develop innovative software tools for display, extraction and manipulation of the evaluated data. In addition, establishing a version-controlled publication of ENSDF would allow unambiguous citations of reproducible quantities. Much progress has been made in this area and methods for both interrogation and accessibility issues have been addressed by the USNDP.

6. ***Compilation of new data should be ensured.***

   The data needs expressed at the workshop make it apparent that the demand on the USNDP is considerable. The basic nuclear science community should also take on a greater responsibility in the compilation of data they produce, which would allow the data scientists to concentrate their efforts on the evaluation process. Thus, it is imperative that the experimenters publish all data in sufficient detail and in a readable format so they can be easily incorporated into the databases. Data-related pre-review of journal manuscripts is encouraged and should be pursued. Finally, there is a large quantity of historical data which has not been evaluated because it is not available in a directly readable format. In many cases, these data are relevant to current research activities, and it would be beneficial to recover them. This would be much more cost effective than to repeat the experiments. Digitizing the old results is the only option for some data because the experimental capabilities for taking these data no longer exist. Again, steps have been taken to engage experimentalists in the process, but more engagement is certainly needed.

4.1.2 Nuclear Astrophysics

4.1.2.1 Executive Summary

The field of nuclear astrophysics addresses many exciting puzzles in the cosmos and is an essential, growing component of the low energy nuclear physics research program in the US and abroad. Nuclear astrophysics studies require a specialized set of nuclear data, especially low-energy cross sections. The principal focus of the US Nuclear Data Program's efforts have involved support for structure and neutron-induced reaction evaluation that often don't entirely match the needs of the nuclear astrophysics community. These needs include timely evaluation of new data sets, including thermonuclear reaction rates and structure data relevant to modeling neutron capture on nuclei far from stability. Targeted investments are needed to make nuclear astrophysics data efforts viable and sustainable for the long-term future. Such investments will enable researchers to fully explore the scientific impact of new measurements and thereby expand our understanding of the universe.

4.1.2.2 Background

Importance of Nuclear Astrophysics

Nuclear astrophysics addresses some fascinating unsolved puzzles in the cosmos, including the origin of the elements heavier than Fe [NRC03]; the formation of light elements in the early universe and their constraint on the total amount of baryonic matter [Wal91, Smi93]; the cosmic origins of specific nuclides such as the rare ^{180}Ta [Lae05], $^{92-94}$Mo and $^{96-98}$Ru [Bli18] and the very abundant ^{19}F [Sie18]; the mechanism of thermonuclear supernova explosions [Pol19]; the nucleosynthesis in neutron star mergers as driven by neutron captures on *n*-rich unstable nuclei [Wan21]; the heaviest elements created in nova explosions [Lia20, Bod12]; the possible ejection of p-nuclides from X-ray bursts [Pet19]; the formation of ^{7}Li three minutes after the Big Bang [Cyb08]; the formation of heavy elements in core-collapse supernovae [Yam22]; and the evolution of stars as influenced by the ^{12}C(α,γ) reaction rate [Pep22a]. The popularity of the field of nuclear astrophysics is growing due to new astrophysical observations (neutron star mergers [Wan21a]), new observatories (the James Webb Telescope [Nat17]), and new accelerator facilities like FRIB [Wei19]. For these (and many other) reasons, nuclear astrophysics remains a major component of low energy nuclear physics research, as reflected in the 2015 NSAC Long Range Plan [NSA15a].

Importance of Nuclear Data for Nuclear Astrophysics

Nuclear data is essential for carrying out studies of the above-mentioned puzzles. There are numerous reasons for this: nuclear interactions drive the evolution of stars and their role in synthesis of elements; nuclear data is essential to plan new measurements of cross sections and level properties critical for nuclear astrophysics; and nuclear data provides valuable benchmarks for reaction models that provide thousands of unmeasured cross sections.

Additionally, *processed* nuclear data in the form of thermonuclear reaction rates (see [Rol88] are required input for astrophysical simulations. These critical simulations are used to determine the sensitivity of billion-dollar satellites to detect exploding stars, to identify high priority measurements at radioactive beam facilities, to determine the astrophysical impact of recent measurements, and to assess the uncertainties of astrophysical model predictions which thereby enable quantitative comparisons with observations.

Specialized Nuclear Data Needs

The nuclear data needs for nuclear astrophysics studies are quite specialized (see, [Smi03, Smi08, Smi11]), spanning both nuclear reaction and nuclear structure data. The broad-based needs are exemplified by thermonuclear reaction rates, which are a convolution of a reaction cross section and the Maxwell-Boltzmann temperature-dependent energy distribution in a star. A reaction cross section can be measured directly and converted to a rate, or a rate can be determined indirectly by measuring the structure properties of relevant nuclear levels. Some of the required structure properties include resonance energies, partial widths, total widths, proton- and neutron-separation energies, single-particle level energies, spectroscopic factors, nuclear masses, optical model parameters, beta-delayed neutron decay probabilities, beta-decay lifetimes, alpha-nucleus potentials, level densities, and more.

As another indication of the specialization needed, particle-induced cross sections at low center of mass energies (less than ~1 MeV) are of particular interest, as are the properties of single-particle levels that are within ~ 1 MeV of a particle threshold. Since these data types are not critical needs in most other nuclear physics applications, they require specialized efforts to produce. Furthermore, it is important to present the relevant nuclear data, like cross sections and level information, in a way that is user-friendly for the astrophysical model

In the subsections below, the contributions to nuclear data for nuclear astrophysics by the USNDP, the US nuclear astrophysics research community, and the international community will be detailed. The top priority nuclear data needs will be listed, and the status of existing efforts will be discussed.

4.1.2.3 USNDP Contributions

The mission of the USNDP is to "provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering." The National Nuclear Data Center heads up the USNDP, with the other data centers located at ANL, LANL, LBNL, LLNL, McMaster University, MSU, ORNL, TAMU, TUNL, and UC Berkeley. Collectively, these USNDP centers serve the low-energy nuclear physics community and a broad range of applied users. For nuclear structure research, for example, the DOE Office of Nuclear Physics funds, and USNDP coordinates, efforts for bibliographies (NSR), compilations (XUNDL), evaluations of mass chains and individual nuclides, databases (ENSDF), dissemination (NuDat), software development, methodology development, national and international coordination, and more. In FY21, 40% of the scientific permanent FTEs in the USNDP were involved in ENSDF-related work.

Since nuclear astrophysics is also a critical component of the low-energy nuclear physics program in the US, the USNDP should strive to meet the nuclear data needs of the nuclear astrophysics community. However, the USNDP has very little effort directed at the specialized needs of nuclear astrophysics – only 1% of the scientific permanent FTEs in FY21 – and therefore many of these data needs are unmet.

There are, however, several USNDP efforts that are beneficial to nuclear astrophysics. For example, ENSDF contains evaluations of the properties of many low-lying, single-particle resonances that are critical for thermonuclear reactions; many USNDP centers contribute to ENSDF evaluations. Another critical effort is the Atomic Mass Evaluation (AME) effort [Hua02, Wan21]. The nuclear masses generated in the AME are critical for determining the energy release in thermonuclear reactions and calculating cross sections of unmeasured reactions. While the AME is an internationally led effort, ANL makes a significant contribution from the USNDP.

The USNDP reaction database ENDF [Bro18] contains most of the neutron-induced cross sections needed to study the slow neutron capture process (*s*-process) [Kae11], except for some reactions on branch-point isotopes [Bis15] that are a few mass units from stability. Studies at the NNDC [Pri10, Pri20] and the CALCMACS webpage[19] have determined the Maxwellian-averaged cross sections needed for s-process studies from cross sections in ENDF and those from other databases (JEFF[20], JENDL[21], ROSFOND[22], CENDL[23]). It should be noted, however, that these cross sections are adjusted to agree with benchmarks from nuclear criticality safety and nuclear energy applications and are therefore optimized at energies well beyond those appropriate for astrophysics studies. Streamlined reaction assessments that are focused on lower energies often generate significantly different cross sections, some that subsequently produce different element synthesis and energy generation in astrophysical simulations [Zha22]. Also, ENDF is focused on neutron-induced reactions on stable nuclei, making its utility limited to only certain astrophysical scenarios such as AGB stars [Bus99].

There have also been developments in nuclear theory that have been coordinated in part by the USNDP. These include the development of statistical reaction models at LANL Kaw10, Kaw16] and NNDC [Her07], as well as other reaction theory efforts at LLNL [Tho09].

There is one USNDP effort directed at nuclear astrophysics: the Computational Infrastructure for Nuclear Astrophysics[24] [Smi05, Nes05a, Nes05b, Smi06]. This is an online cloud-computing data pipeline created at ORNL that provides a simple graphical interface that enables users to: upload, manipulate, and save reaction cross sections; convert these into thermonuclear reaction rates; modify, parameterize, and save rates into rate libraries; combine libraries for use in custom nucleosynthesis simulations; execute post-processing nucleosynthesis calculations with the XNET

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[19] https://www.nndc.bnl.gov/astro/calcmacs.jsp

[20] http://www.nea.fr.html/

[21] http://wwwndc.jaea.go.jp/index.html

[22] http://www.ippe.obninsk.ru/podr/abbn/libr/rosfond.php

[23] http://www.ciae.ac.cn

[24] https://nucastrodata.org/infrastructure/

code[25]; quickly change nuclear physics input and determine astrophysical impacts, including automated sensitivity studies; and save, visualize, analyze, and share simulation results.

Finally, the Fission In R-process Elements (FIRE) effort[26] was a nuclear theory topical collaboration [Cot18] that was closely aligned with some ongoing USNDP work. The focus of this work, a collaboration of LLNL, LANL, NNDC, North Carolina State, and Notre Dame, was to integrate the most advanced models of spontaneous, neutron-induced, and β-delayed fission into rapid neutron capture (*r*-process) nucleosynthesis codes and examine the subsequent astrophysical impacts.

4.1.2.4 US Research Efforts

The majority of nuclear astrophysics data efforts in the US are small projects within the nuclear astrophysics research community. A prime example is the JINA REACLIB thermonuclear reaction rate library[27] [Cyb10] managed at MSU. This library contains over 160,000 parameterized rates and inverses that are widely used for astrophysics simulations. While a few hundred of these rates are based on streamlined assessments performed by the nuclear astrophysics community, the overwhelming majority of the rates in REACLIB are based on the 2008 version of the NON-SMOKER Hauser-Feshbach reaction code[28] [Rau00].

Another effort is the STARLIB reaction rate library[29] [Lon10], which has advanced the methodology of reaction rate determinations via Monte Carlo propagations of nuclear level uncertainties through the calculation of 63 reaction rates to provide their uncertainties. STARLIB, created at North Carolina Chapel Hill, provides tabulated rates on a temperature grid and adds rates from other sources (REACLIB, decays from ENSDF, and theoretical rates from statistical models) to produce a "full" library useful for astrophysical simulations.

Bibliographic data is also critical for progress in research. One valuable bibliographic service is the JINA Virtual Journal of Nuclear Astrophysics[30], which scans 42 journals for articles in nuclear astrophysics. A second is the NASA Astrophysical Data System ADS[31] that contains references from hundreds of journals in astrophysics and related fields including nuclear astrophysics.

Additionally, numerous projects to produce astrophysical simulation codes – an important "end-user application" of nuclear astrophysics data – have efforts to delineate (and in some cases update) a "default" set of thermonuclear reaction rates. The CINA system, described above, runs the XNET code with default REACLIB parameterized rates and a GUI to build customized rate libraries. The NUGRID post-processing nucleosynthesis code[32] [Den14] takes pointwise reaction rates from

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[25] https://github.com/starkiller-astro/XNet
[26] https://www.osti.gov/servlets/purl/1668514; https://www.osti.gov/biblio/1776653-fission-process-elements
[27] https://reaclib.jinaweb.org
[28] https://nucastro.org/nonsmoker.html
[29] https://starlib.github.io/Rate-Library/
[30] https://journals.jinaweb.org/jinavj/
[31] https://ui.adsabs.harvard.edu/
[32] https://nugrid.github.io/content/codes_collab.html

numerous sources including REACLIB, has an associated Jupyter-based platform and python scripts and resources, and accepts hydrodynamics profiles from MESA stellar evolution code[33] [Pax11]. The Portable Routines for Integrated nucleoSynthesis Modeling (PRISM) nucleosynthesis code [Spr20, Spr21] is a modern code from LANL used for a novel "nucleosynthesis tracing" technique; PRISM uses theoretical reaction rates of r-process nuclei calculated with the statistical Hauser-Feshbach code CoH [Kaw16]. The SkyNet modular nuclear reaction network library [68] is a new code that features significant attention to neutrino-induced nucleosynthesis. This LANL code uses reactions from REACLIB and from other sources as defaults. Finally, the Webnucleo/Libnucnet nuclear reaction network[34] [Mey12], a modular system for nucleosynthesis calculations from Clemson, is available in Jupyter notebooks and as downloadable source code. This system, especially useful for student projects, accepts user-specified pointwise reaction rates as default inputs.

4.1.2.5 International Efforts

There are numerous international efforts that have provided valuable data resources for nuclear astrophysics research. The most active of these are associated with the reaction code TALYS[35] [Gor08]. This code performs advanced global nuclear modeling with uncertainties and outputs data for applications. It contains multiple reaction components including pre-equilibrium reaction effects, multi-particle emission, width fluctuations, coupled channels, nuclear deformation, fission products, and a wide variety of level density models. TALYS has been used to generate TENDL, the TALYS Evaluated Nuclear Data Library[36] [Gor08, Kon19], which combines reaction evaluations with TALYS calculations to obtain complete coverage of the chart of the nuclides making it useful for some astrophysics studies. However, TENDL is optimized at higher energies and provides cross sections in ~ 1 MeV bins for many reactions, of insufficient fidelity at the low energies needed for astrophysics research. Recently, the TENDL-Astrophysics database[37] was released, which contains neutron capture reactions on 8892 isotopes with uncertainties generated from 288 models that combine different choices of input parameters – gamma strength functions, level densities, optical models, collective enhancements, width fluctuations, and mass models. The incorporation of uncertainties and the complete coverage of neutron-induced reactions on stable and neutron-rich isotopes make this library useful for investigations of s-process and r-process nucleosynthesis.

Another theoretical effort is the NON-SMOKER Hauser-Feshbach reaction model code which has inputs optimized for astrophysical applications [Cyb10, Rau20]. It has been used to calculate rates for (n, γ), (n, p), (n, α), (p, γ), (p, α), (α, γ), and their inverse reactions for $10 \leq Z \leq 83$ (Ne to Bi) and a mass range reaching the neutron and proton driplines. This code, from the Univ. of Basel, provided most of the rates for REACLIB. Nucleosynthesis simulations were used to benchmark these rates and demonstrate their advantages over other statistical model rate collections [Hof99].

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[33] https://docs.mesastar.org/en/release-r22.05.1/

[34] https://sourceforge.net/p/libnucnet/home/Home/

[35] https://www-nds.iaea.org/talys

[36] https://tendl.web.psi.ch/tendl_2021/tendl2021.html

[37] https://tendl.web.psi.ch/tendl_2021/tar_files/astro/astro.html

The Karlsruhe Astrophysical Database of Nucleosynthesis in Stars (KADONIS)[38] [Dil06] is a collection of experimental neutron-induced cross sections on stable nuclei from the Institute for Nuclear Physics at the Karlsruhe Research Center. KADONIS contains a 2005 update to the previous Bao and Kaeppeler collection [Bao00] of experimental (n, γ) cross sections relevant for s-process nucleosynthesis. This database was subsequently extended to contain neutron capture rates on 32 p-process nuclei [8Szu150].

Another effort is the Brussels nuclear reaction rate library (BRUSLIB)[39] [Xux13, Gor04, Aik05] from the Univ. of Brussels. This contains experimentally based rates from the 1999 NACRE reaction rate library [Ang99] and the 2013 follow up library NACRE II [Xux13], as well as theoretical rates determined from TALYS. BRUSLIB is accompanied by the Nuclear Network Generator NETGEN[40] [Aik05], a tool to generate nuclear reaction rates on a user-specified temperature grid for subsequent use in nucleosynthesis calculations.

Finally, the Reference Input Parameter Library (RIPL)[41] [Cap09] is a valuable collection of nuclear information needed for nuclear reaction calculations as well as for nuclear data evaluations. It includes nine sub libraries – masses, nuclear levels, resonance spacing, optical models, level densities, giant dipole resonances, fission barriers, and codes. RIPL has been widely used by the nuclear data community but has had only limited use in nuclear astrophysics research.

4.1.2.6 Nuclear Astrophysics Data Needs and Current Status

The highest priority nuclear data needs for nuclear astrophysics are assessments of low energy cross section measurements of critical reactions [Ang99, Xux13], and assessments of properties of critical (near threshold, low angular momentum transfer) resonances [Ili01, Nes07]. Global nuclear structure and reaction calculations needed to fill in measurement gaps are required to generate datasets with complete coverage of the nuclear chart [Kon19]. Software tools and resources are required to: access and process the data into thermonuclear reaction rates [Bar97]; incorporate these rates into databases; and disseminate the libraries to the community [Cyb10]. Without these processing steps, the nuclear data will not be broadly used for astrophysics research.

The next highest priority nuclear data needs include: benchmarking datasets with astrophysical simulations [Hof99, Zha22]; carrying out sensitivity studies [Zhu21, Smi11] to identify the most critical reactions and nuclides to help focus research efforts; improving uncertainty quantification efforts [94]; advancing evaluation and processing methodologies [Spr21, Lon10, Smi11, Ili16] to improve capabilities, insights, and productivity, and to aid in workforce development; developing software tools as needed for all of the above; assessing some higher energy cross sections of spallation reactions needed to study cosmic ray nucleosynthesis [Kus18] and other exotic phenomena [97, 98]; and collecting and indexing bibliographic listings of nuclear astrophysics papers in experiment, theory, and simulation.

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[38] https://exp-astro.de/kadonis1.0/

[39] http://www.astro.ulb.ac.be/bruslib

[40] http://www.astro/ulb.ac.be/Netgen/form.html

[41] https://www-nds.iaea.org/RIPL-3

It is important to note that the efforts described here are insufficient to meet all nuclear astrophysics data needs. First and foremost, there is no effort directed at regularly evaluating new astrophysics-related measurements, either within the USNDP or in the research community. Second, the processing required to subsequently generate reaction rates into libraries is far too infrequent. In general, these efforts in the research community lack the required personnel and longevity. REACLIB went 8 years without a major update to add new rates, and NON-SMOKER cross sections were last converted to REACLIB format in 2009. Furthermore, those rates used nuclear masses from the 2003 Atomic Mass Evaluation [Wap03, Aud03], which have since undergone numerous updates (most recently AME2020 [24,25]). The NACRE [85] effort ended in 1999, RIPL-3 [88] ended in 2009, NACRE II [Xux13] ended in 2013, KADONIS was completed in 2005 (with some updates in 2013), and BRUSLIB and NETGEN were last updated in 2015. Finally, STARLIB has only added a few rates since 2015 and has announced no plans for a further update.

While no single effort could provide all the needed data in all formats requested by end-users, the efforts to date have lacked standardization and coordination. Another issue has been a reliance on outdated methodologies and a tendency to work independently of the data community. As a result, the nuclear data resources for nuclear astrophysics are far below the level of those for other areas of basic scientific researcher such as nuclear structure. Much current research in nuclear astrophysics therefore utilizes simulations with outdated nuclear inputs, and the scientific impacts of new measurements cannot be fully explored. Targeted investments are needed to improve this situation and enable forefront measurements to be used to expand our understanding of the universe. Such investments would also enable the field to expand and evolve to address new observations and challenges and be sustainable long into the future.

4.1.2.7 Summary

The field of nuclear astrophysics addresses many exciting puzzles in the cosmos and is an essential, growing component of the low energy nuclear physics research program in the US and abroad. Nuclear astrophysics studies require a specialized set of nuclear data, especially low-energy cross sections. The primary focus of the USNDP on discrete structure and reaction evaluation on stable nuclei doesn't match many of the specific requirements of nuclear astrophysics including the timely evaluation of new measurements, processing thermonuclear reaction rates and updating the information needed for understanding neutron capture on unstable nuclei. Targeted investments would enable researchers to fully explore the scientific impact of new measurements and thereby expand our understanding of the universe.

4.2 Nuclear Energy

Nuclear energy currently plays a major role in electricity generation in the United States and worldwide. In the US, nuclear energy produces nearly 20% of the needed electricity and contributes 55% of the carbon-free energy portfolio. These numbers need to rise significantly if clean energy objectives are to be met.

The current US nuclear reactor fleet consists of light water reactors (LWRs) that are based on thermal fission, where neutrons produced in fission in the uranium dioxide fuel, with an average energy of nearly 2 MeV, are moderated and thermalized in light water (i.e., water with almost exclusive ^{1}H content) to drive the fission chain reaction. These thermal reactors are expected to continue to be major contributors to electricity generation in the future.

US government R&D funding for nuclear energy is currently being revived with the objective of rebuilding US leadership in nuclear technology. This support targets not only the improvement of LWRs but also support for reactor concepts beyond current designs. These so-called advanced reactor technologies (also called Generation-IV) cover a wide range of different designs with different materials and geometries. This includes smaller versions of LWRs to reactors that, for example, use different fuels (e.g., High Assay Low Enrichment Uranium, Pu etc.), coolants such as gas, salt (e.g., FLiBe), or liquid metal (e.g., Na or K), and other moderator materials (e.g., graphite or ZrH) if any.

Given the limited operating experience with non-LWRs, the accurate simulation of reactor physics and the quantification of associated uncertainties are critical for ensuring that advanced reactor concepts operate within the appropriate safety margins. For nuclear energy applications, the correct simulation of reactivity involves a good understanding of k_{eff}, control rod worth (e.g., the change in reactivity that caused by control rod motion), xenon reactivity, and temperature-dependent reactivity feedback. It also includes kinetic parameters (e.g., effective delayed neutron fraction and neutron generation time) at a certain point in time to inform the prediction of transient behavior, and it includes fission yield and decay data to correctly predict the nuclide inventory over the time of operation. Nuclear data are one—if not the most important—source of input uncertainties in these reactor physics calculations.

Some of the most relevant nuclear data for reactivity and burnup calculations include:

- Cross section, thermal scattering, and angular scattering distribution data;
- Recoverable energy from fission and capture reactions;
- Independent and/or cumulative fission product yields;
- Decay constants;
- Branching fractions;
- Effective delayed neutron fraction;
- Fission spectra.

4.2.1 Key nominal and uncertainty nuclear data

Tables 2 and 3 provide an overview of key nominal (e.g., recommended) and attendant uncertainty data for various reactor concepts compiled for NUREG/CR-7289 [Bos21]. The data was collected based on extensive literature searches and by performing sensitivity and uncertainty analyses of various non-LWR systems using publicly available specifications. While the mentioned study was performed for non-LWRs, the key published nominal and uncertainty data for traditional LWRs are included in Tables 2 and 3 under “All concepts”.

The literature research was performed as follows:

1. Publicly available literature and identified descriptions of representative geometrical and material definitions relevant to reactor physics analysis of the selected advanced reactor technologies were explored;
2. Modern evaluated nuclear data libraries were interrogated to identify important updates in nominal values and uncertainties of relevant nuclear data;
3. Results from previous studies performed at various research institutions with respect to the impact of nuclear data on the key figures of merit associated with advanced reactor safety were reviewed;
4. Based on this survey and previous studies, identified key nuclides and nuclear data impacting reactivity during operation, considering both fresh and irradiated fuel, and assessed their impacts on the selected advanced reactor technologies.

The impact of nominal nuclear data and uncertainties in nuclear data was assessed for selected benchmarks as available. Nominal, sensitivity, and uncertainty analyses were performed for selected quantities of interest (QOIs) using multiple ENDF/B nuclear data libraries: ENDF/B-VII.0, ENDF/B-VII.1, and ENDF/B-VIII.0.

The sensitivity and uncertainty analyses were performed as follows:

1. New computational models for the benchmarks were developed.
2. Neutron transport calculations were performed, and agreement confirmed with existing benchmark results or other published results.
3. Selected QOIs were assessed for each of the considered benchmarks, based on availability of measurements and key figures of merit associated with reactor safety, and the estimated modeling and computational effort.
4. Relevant nuclear data was identified for the selected QOI through calculations performed with different nuclear data library releases and through nuclear data sensitivity analyses (ranking of top sensitivities).
5. The uncertainties on the QOI's due to nuclear data uncertainties were quantified and the top contributing nuclear data to the observed uncertainties were identified.

The main QOIs selected for performing in-depth uncertainty analysis for the considered advanced reactor technologies included the following: (1) core reactivity, (2) control rod (CR) worth, (3) temperature and expansion coefficients, and (4) power distribution, including axial or radial peak power. The QOI's level of importance to reactor safety differed between various advanced reactor concepts. No judgment of the performance of one ENDF/B library release over another is made since no or little validation data is available. The tables merely provide an overview of identified important nuclide reactions.

The following list summarizes the key observations related to various reactor concepts that stood out from either the literature survey or the analyses. Significant updates between ENDF/B libraries indicate that further studies, especially for non-LWRs and comparisons with measurements, are necessary to understand which data results in values closer to the corresponding experimental measurements. Furthermore, additional measurements and evaluations should be added to improve confidence in the data. Observations related to large uncertainties indicate the need for further measurements to reduce these uncertainties. The findings regarding thermal scattering data only refer to library releases up to ENDF/B-VIII.0. There are several activities to add thermal scattering data which will become available in the next ENDF/B releases (see below).

- All concepts:
    - Large differences between different ENDF/B library releases for relevant nominal and uncertainty data: neutron multiplicity, fission, capture, scattering for ^{235}U, ^{238}U, major Pu isotopes
- LWR:
    - There was a significant update in the ^{1}H elastic scattering cross section and its uncertainty between ENDF/B-VII.1 and VIII.0.
- Fluoride-salt-cooled high-temperature reactor (FHR):
    - No thermal scattering data uncertainties on graphite (see below)
    - No thermal scattering data for salts (see below)
    - Carbon (n,γ): significant update from ENDF/B-VII.0 to VII.1
    - Large ^{7}Li (n,γ) uncertainty
    - ^{6}Li (n,t): significant cross section update from ENDF/B-VII.0 to VII.1
- Heat Pipe Reactor (HPR) and Sodium-cooled Fast Reactor (SFR):
    - No angular scattering uncertainties
    - **Large ^{235}U (n,γ) uncertainty for HEU fuel**
    - Large ^{238}U inelastic scattering uncertainty for U/Transuranic (TRU) fuel
    - Large impact of scattering reactions of coolant and structural materials
- High Temperature Gas Reactor (HTGR):
    - Carbon (n,γ): significant update from ENDF/B-VII.0 to VII.1
    - No thermal scattering data uncertainties graphite (see below)
- Graphite-moderated Molten Salt Reactor (MSR):
    - No cross section data for ^{135m}Xe in the ENDF/B libraries
    - No thermal scattering data for salts (see below)
    - No thermal scattering data uncertainties graphite (see below)
    - **Large ^{7}Li (n,γ) uncertainty**
    - ^{6}Li (n,t): significant cross section update from ENDF/B-VII.0 to VII.1
- Fast spectrum MSR:
    - ^{35}Cl (n,p): significant cross section update from ENDF/B-VII.0 to VII.1
    - Large impact of ^{24}Mg elastic scattering uncertainty

Table 2. Overview of key *nominal* nuclear data for selected advanced reactor concepts

Reactor type	Key nuclear data	Missing/discrepant/additional data, important data changes
Thermal spectrum pebble-bed HTGR*	**Fuel:** ^{235}U , ^{235}U fission, ^{235}U (n,g), ^{238}U (n,g), ^{16}O elastic **Moderator:** ^{12}C (n,g), ^{10}B (n,g), ^{10}B (n,α) graphite thermal scattering	^{12}C (n,g) (ENDF/B-VII.0 vs. VII.1), 0%, 10% and 30% graphite porosities in ENDF/B-VIII.0, new SiC thermal scattering data in ENDF/B-VIII.0
Thermal spectrum FHR	**Fuel:** , fission, and (n,g) of ^{235}U, ^{239}Pu, and ^{241}Pu (n,g) of ^{238}U (n,g), ^{238}U and ^{240}Pu **Coolant:** ^{7}Li,^{19}F,^{9}Be(n,g), ^{7}Li(n,el), ^{6}Li (n,t), ^{19}F elastic, ^{9}Be(n,2n),(n,el) **Moderator:** ^{12}C (n,g), graphite thermal scattering	^{12}C (n,g) and ^{6}Li (n,t) (ENDF/B-VII.0 vs. VII.1), 0, 10% and 30% graphite porosities in ENDF/B-VIII.0 New SiC thermal scattering data in ENDF/B-VIII.0 ^{19}F inelastic discrepancies (ENDF/B-VIII.0 vs. JENDL 4.0), no thermal scattering data for salt (e.g., LiF, BeF_2)
Thermal spectrum, graphite-moderated MSR*	**Fuel/coolant:** ^{235}U , ^{235}U fission, ^{235}U (n,g), ^{238}U , ^{238}U fission, ^{238}U (n,g), ^{238}U elastic, ^{19}F elastic, ^{19}F (n,g), ^{7}Li (n,g), ^{6}Li (n,g), ^{6}Li (n,t) **Moderator:** ^{12}C (n,g), graphite thermal scattering **Structure:** ^{58}Ni elastic, ^{58}Ni inelastic, ^{58}Ni (n,p)	^{12}C (n,g) and ^{6}Li (n,t) (ENDF/B-VII.0 vs. VII.1), 0%, 10% and 30% graphite porosities in ENDF/B-VIII.0, new SiC thermal scattering data in ENDF/B-VIII.0, no data for ^{135m}Xe, ^{19}F inelastic discrepancies (ENDF/B-VIII.0 vs. JENDL-4.0), no thermal scattering data for salt (e.g., LiF, BeF_2)
Fast spectrum, molten chloride MSR	**Fuel and coolant salt:** and fission of ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{238}U (n,g), ^{238}U inel., ^{239}Pu (n,g), ^{37}Cl inelastic, ^{37}Cl elastic, ^{23}Na inelastic, ^{23}Na elastic, ^{35}Cl (n,p), ^{35}Cl (n,g)	Missing ^{135m}Xe, ^{35}Cl (n,p) (ENDF/B-VII.0 vs. VII.1)
Fast spectrum, oxide and metal fueled HPR*	**Fuel:** ^{235}U , ^{235}U fission, ^{235}U (n,g), ^{238}U , ^{238}U fission, ^{238}U (n,2n), ^{16}O elastic, elastic and inelastic scattering, as well as (n,g) of ^{238}U, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{96}Zr **Coolant:** ^{23}Na elastic, ^{23}Na inelastic, ^{39}K capture, ^{39}K (n,p), ^{39}K elastic **Structure/Reflector:** ^{56}Fe (n,g), ^{56}Fe elastic, ^{56}Fe inelastic, ^{27}Al elastic, ^{9}Be elastic, ^{16}O elastic, ^{10}B (n,g), ^{10}B (n,α), BeO thermal scattering	
Fast spectrum, metal and oxide fueled SFR	**Fuel:** and fission of ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{245}Cm; ^{238}U (n,g), ^{238}U inelastic, ^{239}Pu (n,g), ^{241}Am (n,g), ^{243}Am (n,g), ^{16}O elastic **Coolant:** ^{23}Na elastic, ^{23}Na inelastic **Structure/Reflector**: ^{52}Cr elastic; elastic and inelastic scattering, as well as (n,g) of ^{56}Fe, ^{52}Cr, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{96}Zr	
All concepts	Fission yields, decay constants, branching ratios, energy release per fission, fission spectra, fission products (e.g., Xe, Sm, Gd), fission and capture of actinides that build up during depletion	

*Based on the availability of data, the findings reported here for this reactor type are focused on systems with fresh fuel. Additional relevant reactions are expected for systems including irradiated fuel.

Table 3. **Overview of key nuclear data *uncertainties* for selected advanced reactor concepts**

Reactor type	Key nuclear data	Missing/discrepant/additional data, important data changes
Thermal spectrum, pebble-bed HTGR*	**Fuel:** ^{235}U , ^{235}U χ, ^{235}U fission, ^{235}U (n,g), ^{238}U (n,g), ^{28}Si (n,g), ^{28}Si elastic **Moderator:** ^{12}C/graphite: (n,g), elastic, inelastic, ^{10}B (n,α)	No thermal scattering data uncertainties for graphite
Thermal spectrum, FHR	**Fuel:** , fission, $^{\text{and}}$ (n,g) of ^{235}U, ^{239}Pu, and ^{241}Pu, (n,g) of ^{238}U and ^{240}Pu **Coolant:** ^{7}Li (n,g), ^{7}Li elastic, ^{6}Li (n,t) ^{19}F (n,g), ^{19}F elastic, ^{9}Be elastic **Moderator:** ^{12}C/graphite (n,g) and elastic	No thermal scattering data uncertainties for graphite components
Thermal spectrum, graphite-moderated MSR*	**Fuel/coolant:** ^{235}U , ^{235}U fission, ^{235}U (n,g), ^{238}U , ^{238}U fission, ^{238}U (n,g), ^{238}U elastic, ^{19}F elastic, ^{19}F (n,g), ^{7}Li (n,g), ^{6}Li (n,g), ^{6}Li (n,t) **Moderator:** ^{12}C/graphite (n,g) and elastic **Structure:** Structure: ^{58}Ni elastic, ^{58}Ni inelastic, ^{58}Ni (n,g), ^{58}Ni (n,p)	No thermal scattering data uncertainties for graphite or salt components
Fast spectrum, molten chloride MSR	**Fuel and coolant salt:** and fission of ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{238}U (n,g), ^{238}U inel., ^{239}Pu (n,g), ^{37}Cl inelastic, ^{37}Cl elastic, ^{23}Na inelastic, ^{23}Na elastic, ^{35}Cl (n,p), ^{35}Cl (n,g) **Reflector:** ^{24}Mg elastic	Angular scattering distribution uncertainties: limited availability and usability; ^{238}U inelastic scattering uncertainty ENDF/B-VII.1 vs. VIII.0
Fast spectrum, oxide and metal fueled HPR*	**Fuel:** ^{235}U , ^{235}U fission, ^{235}U (n,g), ^{238}U , ^{238}U fission, ^{238}U (n,2n), ^{16}O elastic; elastic and inelastic scattering, as well as (n,g) of ^{238}U, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{96}Zr **Coolant:** ^{23}Na elastic, ^{23}Na inelastic, ^{39}K capture, ^{39}K (n,p), ^{39}K elastic **Structure:** ^{56}Fe (n,g), ^{56}Fe elastic, ^{56}Fe inelastic, ^{27}Al elastic, ^{9}Be elastic, ^{16}O elastic, ^{10}B (n,g), ^{10}B (n,α)	Angular scattering distribution uncertainties: limited availability and usability No thermal scattering data uncertainties for BeO; ^{235}U (n,γ) uncertainty ENDF/B-VII.1 vs. VIII.0
Fast spectrum, metal and oxide fueled SFR	**Fuel:** and fission of ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{245}Cm; ^{238}U (n,g), ^{238}U inelastic, ^{239}Pu (n,g), ^{241}Am (n,g), ^{243}Am (n,g), ^{16}O elastic **Coolant:** ^{23}Na elastic, ^{23}Na inelastic **Structure/Reflector:** ^{52}Cr elastic; elastic and inelastic scattering as well as (n,g) of ^{56}Fe, ^{52}Cr, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{96}Zr	Angular scattering distribution uncertainties: limited availability and usability ^{238}U inelastic scattering uncertainty between ENDF/B releases
All concepts	Fission yields, decay constants, branching ratios, energy release per fission, fission spectra, fission products (e.g., Xe, Sm, Gd), fission and capture of actinides that build up during depletion	Missing correlations between , fission and χ; ^{235}U/^{239}Pu and fission uncertainty ENDF/B-VII.1 vs. VIII.0 Missing uncertainty for ^{242}Am, ^{244}Am, ^{244m}Am, ^{243}Pu, ^{237}U, ^{239}U, ^{240}U, ^{241}U

*Based on the availability of data, the findings reported here for this reactor type are focused on systems with fresh fuel. Additional relevant reactions are expected for systems including irradiated fuel.

4.2.2 Covariance Data

While ENDF/B provides a great many uncertainty data, other nuclear data libraries contain uncertainty data not yet included in ENDF/B. For example, the SCALE covariance library not only contains ENDF/B data, but also data on fission spectrum uncertainties from JEFF. Furthermore, the SCALE libraries contain low-fidelity uncertainty data generated through the Low-Fidelity Covariance Project, which used simple procedures to estimate data uncertainties in the absence of high-fidelity covariance data [Wie20]. The available nuclear data libraries are still missing a significant number of uncertainties on various materials and reactions. For example, covariance data on inelastic scattering, $(n,2n)$, and other neutron interactions are missing for relevant nuclides such as ^{197}Au.

The covariance matrices in the ENDF/B libraries sometimes do not show their intrinsic attributes. For example, they may be not positive semi-definite (sometimes caused by limited precision when stored in a particular format), they can show non-physically large correlations, or they present correlations that seem incorrect because the data in certain energy ranges are independent. Depending on the application need (e.g., required matrix inversion), it may be necessary to modify the matrices to be able to perform the uncertainty calculations. Even if all relevant uncertainty data were available, the following three requirements must be met before the data can be used in sensitivity and uncertainty analyses:

1. The tools for nuclear data processing must be able to handle the data.
2. The data must be stored in a format suitable for subsequent use in uncertainty/sensitivity analysis tools.
3. The uncertainty/sensitivity analysis tools must be able to read and use the data.

Not all available nuclear data processing codes can process all data provided in the evaluated nuclear data files. Furthermore, the output format of processing codes might not allow storage of the data (e.g., consider the addition of a second dimension to the data). Modifications of the output format usually require modifications of the analysis tools that use the data.

The utility of current nuclear data is impacted by the available computational capabilities that use these data. The perturbation theory–based approach to uncertainty calculations relies on calculating sensitivity coefficients for an output quantity with respect to the input data uncertainty. However, such sensitivity coefficients are not yet implemented for all available nuclear data in commonly-used sensitivity analysis tools. In sampling-based approaches, two dimensional data (e.g., fission spectra) cannot necessarily be sampled. Furthermore, many tools can only consider data in multigroup representations, but not in continuous-energy representations. For example, the AMPX code system used to process nuclear data for SCALE cannot currently store angular scattering uncertainties. Furthermore, it is not yet possible to consider the incident neutron energy dependence of the fission spectrum; uncertainties are currently included only for mean incident energies [Wia16].

During the challenging process of developing ENDF/B libraries, nuclear data mean values are adjusted based on data from criticality experiments in the ICSBEP Handbook. As a result of this adjustment, the mean values can accurately predict the multiplication factors for such experiments. The covariance data development does not include or reflect this type of adjustment which can sometimes lead to inconsistencies in the predicted uncertainties on integral quantities such as the multiplication factor. The variation of calculated vs. experimental (C/E) multiplication factors for large sets of ICSBEP experiments was shown to be significantly smaller than that predicted using ENDF/B covariance data [Wil17]. However, methods are available to account for available information on the experiments in the generation of adjusted covariance data, enabling a more consistent calculation of C/E. The nuclear data community is currently engaged in discussing an optimal approach to address the adjustment of the covariance data to better represent uncertainties on integral quantities [CSE18, CSE19].

4.2.3 Decay Data Consistency

In addition to the ENDF/B libraries, the NNDC maintains ENDSF. The ENDSF repository contains evaluated nuclear structure and decay data in a standard format. There is a complicated interplay between the two repositories, as some of the data in ENDSF can also be represented in the ENDF format. For example, the decay pathways through both discrete and continuous excitation levels appear in ENDSF, but are also used in the ENDF File 8, section 457. Unfortunately, these data are not updated in ENDF/B nearly as frequently as the ENDSF repository so outdated (or erroneously translated) data can live through many ENDF/B cycles before being identified and corrected. Due to the current limitations of the codes that translate the ENDSF data into the ENDF format, the data translated into ENDF are often much less informative than the original ENDSF data, missing emission spectra information or level distributions with associated decay energies. The data that is impacted by potential discrepancies between the repositories includes delayed neutron and gamma data which is important for several applications, such as for reactor transient analysis, spent fuel decay heat analysis, and active interrogation analysis. This is one example to demonstrate the need of assuring consistency between different data resources.

4.2.4 Thermal scattering data

The underlying physical phenomenon that defines the operation and safety of thermal reactors is the neutron thermalization process. In this process, neutrons born in fission, and after moderating to thermal energies, achieve a state of pseudo-equilibrium by exchanging energy with the atoms and molecules of the moderating medium (e.g., light water, graphite, etc.). This phenomenon is quantitatively described using double differential cross sections in energy and angle. In a given moderating medium/material, the cross section is directly proportional to a quantity known as the thermal scattering law (TSL), i.e., $S(\alpha,\beta)$, which is a material property (i.e., independent of the interacting particle) that represents a probability distribution function of the available momentum and energy exchange states in the material. As it may be expected, the TSL is also temperature dependent [Haw14].

TSL data sets for various materials are captured in a number of databases such as ENDF/B-VIII.0 [Bro18]. The $S(\alpha,\beta)$ libraries [OEC20] are produced for each temperature of interest. Typically, users of TSL data are responsible for converting such libraries to cross section data that are used in the design and/or operational assessment of nuclear reactors.

4.2.4.1 Production of TSL Data

The generation of TSL data has historically been computationally based. Codes such as NJOY, or more recent variants of it, and FLASSH were developed to perform this task [Mac16, Fle22]. These codes also have the ability to process the TSL data into cross section libraries using various group or continuous structures for the incoming neutron energy. However, these codes require input information describing the available excitation (e.g., vibrational, rotational, etc.) of the medium, contained in a quantity known as the density of states (DOS). Over the past 20 years, DOS data for a number of materials became readily accessible due to the development of atomistic/molecular simulation techniques such as molecular dynamics and density functional theory. In addition, computational tools have become significantly more powerful. Consequently, the ENDF/B-VIII.0 database, which was released in 2018, presented the largest contribution to TSL data since the 1960s.

However, the evaluation of TSL data has evolved to include, in addition to the computational steps described above, validation and benchmark steps that are necessary before the data are accepted into the ENDF/B database. As a result, the evaluators are often utilizing relevant benchmarks in the International Criticality Safety Benchmark Evaluation Program (ICSBEP) [ICS20] and the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE) databases [IRP20]. Alternatively, specific benchmark experiments that isolate the phenomena of neutron moderation and thermalization have been designed and implemented to support the process of TSL benchmarking [Fle22]. In terms of data validation, it is typical to seek and utilize measurements of quantities such as total and differential neutron cross sections and, if available, the scattering law for selected conditions. The validation process was also extended to utilizing measured properties of the material of interest including microstructure information and possibly the DOS at given temperatures.

4.2.4.2 Current Status and Needs

As mentioned above, the latest TSL evaluations appear in the ENDF/B-VIII.0 database, released in 2018, and reflect the evaluation process described previously. Tables 4 and 5 summarize the TSL data content in ENDF/B-VIII.0 and data submitted to ENDF/B-VIII.1. As shown in the tables, new first-of-a-kind evaluations were included that support the description of neutron thermalization in materials of relevance to energy production and to critical systems in general. This includes data for graphite and molten salt FLiBe that have been produced to directly support the needs of advanced reactor concepts currently under development. Furthermore, for materials such as beryllium and ideal graphite, the ENDF/B-VIII.1 library is expected to include advanced physics modeling that relaxes the incoherent approximation typically used in TSL evaluations.

Nonetheless, the significant contributions described above may still fall short of the needs of nuclear reactor designers. The following activities need to be carried out:

1. Expand the TSL portfolio to include more materials that support advanced nuclear reactor concepts;

2. Perform customized evaluations that address particular designs at varying steady state and transient operational conditions;
3. Supplement all TSL data with the corresponding covariance data
4. Perform validation and benchmark experiments that directly support TSL evaluations;
5. Develop modern techniques that continue to enhance the fidelity of the evaluations to address the requirements of advanced multi-physics simulations.

4.2.4.3 Conclusions for thermal scattering data

The current ENDF/B-VIII.0 and the upcoming ENDF/B-VIII.1 databases contain new TSL libraries for energy and criticality applications. These include new evaluations for nuclear graphite, molten salt FLiBe, metal hydrides, and reevaluated libraries for light and heavy water. The ENDF/B-VIII.1 database is also anticipated to include libraries with high fidelity physics content that illustrate the relaxation of the incoherent approximation, which has been the typical assumption that is utilized in TSL evaluations.

4.2.5 Time-dependent analyses

Time-dependent behavior involves data on fission yields, decay constants, branching ratios, recoverable energy for capture and fission, and effective delayed neutron fractions (β_{eff}) for transient analysis. The current ENDF/B format does not allow correlations for fission product yields or decay data. However, correlations for fission product yields can be determined via constraints such as a limited number of fission products per fission event. Such correlation matrices were generated for use in the SCALE code [Wie20, Pig15]. Additionally, updates were implemented in SCALE for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu to ensure consistency between the measured cumulative fission yields and the independent fission yields taken from ENDF/B-VII.1. Considering that fission yield uncertainties and the details of their constraints can have a noticeable impact on fission product evolution in depletion calculations, as has been shown for LWR systems [Aur17].

A survey of the relevant literature did not reveal any consideration or availability of branching ratio uncertainties in any computational tool or data library. If they were available and accounted for, then additional correlations would be introduced for the independent fission yields since they are always required to sum up to 2 as demonstrated in the recent work by the Berkeley group [Mat21]. No uncertainty data in the recoverable fission and capture energies were found. In fact, the energy release per fission is often hard coded in many of the computational tools. If such uncertainties were available and considered, then they could affect the power distribution calculation.

The propagation of cross section uncertainties on β_{eff} reveals significant uncertainties (up to 15% for depleted fuel) [Rad19]. Different studies found β_{eff} uncertainties of up to 4% for thermal and fast systems [Aur16, Kod13]. The ^{238}U scattering reactions were identified as major contributors to the uncertainty on fast systems while the delayed neutron multiplicity for ^{235}U and ^{239}Pu are important for thermal systems

Due to the buildup of Pu during depletion in a LWR, the value of β_{eff} decreases over time. Consequently, its uncertainty grows more relevant for safety analyses. Advanced reactor systems such as SFRs fueled by a mixture of U and Pu have a smaller β_{eff} than LWR systems. The impact of nuclear data uncertainties on β_{eff} in these systems is expected to be significant.

Some correlations in β_{eff} are expected between correlated data such as fission cross sections, neutron multiplicity, and fission spectra. However, no correlations are included in ENDF/B. In fact, the current ENDF/B format cannot even store correlations between these reactions. In a recent ORNL study, the existing covariance library was augmented with such correlations [Sob18] which demonstrated that these additional correlations are relevant and have a visible impact on uncertainty analyses. Since all the above-mentioned data are used in the calculation of β_{eff}, a significant impact on the β_{eff} uncertainty is expected when such correlations are included.

Table 4 (left): Evaluations in ENDF/B-VIII.0 that are relevant to energy and criticality applications.
Table 5 (right): Evaluations submitted to ENDF/B-VIII.1 that are relevant to energy and criticality applications

Material	ENDF Library Name	Evaluation Basis
Beryllium metal	tsl-Be-metal.endf	DFT/LD
Beryllium oxide (Be)	tsl-BeinBeO.endf	DFT/LD
Beryllium oxide (O)	tsl-OinBeO.endf	DFT/LD
Light water (H)	tsl-HinH2O.endf	MD
Light water ice (H)	tsl-HinIceIh.endf	DFT/LD
Light water ice (O)	tsl-OinIceIh.endf	DFT/LD
Heavy water (D)	tsl-DinD2O.endf	MD
Heavy water (O)	tsl-OinD2O.endf	MD
Polymethyl Methacrylate	tsl-HinC5O2H8.endf	MD
Polyethylene	tsl-HinCH2.endf	MD
Crystalline graphite	tsl-graphite.endf	MD
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD
Silicon dioxide (α phase)	tsl-SiO2-alpha.endf	DFT/LD
Silicon dioxide (β phase)	tsl-SiO2-beta.endf	DFT/LD
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD
Uranium dioxide (O)	tsl-OinUO2.endf	DFT/LD
Uranium dioxide (U)	tsl-UinUO2.endf	DFT/LD
Uranium nitride (N)	tsl-NinUN.endf	DFT/LD
Uranium nitride (U)	tsl-UinUN.endf	DFT/LD

Material	ENDF Library Name	Evaluation Basis
Beryllium metal+Sd	tsl-Be-metal+Sd.endf	DFT/LD
FLiBe (Be)	tsl-BeinFLiBe.leapr	MD
FLiBe (F)	tsl-FinFLiBe.leapr	MD
FLiBe (Li)	tsl-LiinFLiBe.leapr	MD
Crystalline graphite+Sd	tsl-graphite+Sd.endf	DFT/LD
Reactor graphite (20% porosity)	tsl_20pGraphite.endf	MD
Calcium hydride (H)	tsl-H1inCaH2.endf	DFT/LD
Calcium hydride (Ca)	tsl-CainCaH2.endf	DFT/LD
Uranium carbide (C)	tsl-CinUC.endf	DFT/LD
Uranium carbide (U)	tsl-UinUC.lendf	DFT/LD
Hydrogen fluoride	tsl-HinHF.endf	MD
Paraffinic oil (H)	tsl-HinParaffinicOil.endf	MD
Beryllium carbide (Be)	tsl-BeinBe2C.endf	DFT/LD
Beryllium carbide (C)	tsl-CinBe2C.endf	DFT/LD
Uranium hydride (H)	tsl-HinUH3.endf	DFT/LD
Lithium hydride (H)	tsl-Hin7LiH-mixed.endf	DFT/LD
Lithium deuteride (D)	tsl-Din7LiD-mixed.endf	DFT/LD
Lithium deuteride (Li)	tsl-7Liin7LiD-mixed.endf	DFT/LD
Light water (H)	tsl-HinH2O.endf	MD

4.3 Medical Applications

Nuclear tools and techniques, together with surgery and chemotherapy, provide targeted diagnostic and treatment options in the battle against cancer. The most commonly used nuclear medical tools include single-photon emission computed tomography (SPECT) and Positron Emission Tomography (PET), which rely on a steady supply of radionuclides. The promise of nuclear medical treatments dates back to Marie Curie's development of mobile x-ray machines used during World War I to treat wounded soldiers on the battlefield to Emilio Segre and Glenn Seaborg's recognition that ^{99}Mo ($t_{½}$=66 h) could be used to generate the 141 keV photon-emitter ^{99m}Tc ($t_{½}$ =6 h) to guide surgical procedures [Hof00].

An incomplete list of radioisotopes important for nuclear medicine include: ^{195m}Pt, ^{177}Lu, ^{131}I, ^{124}I, ^{123}I, ^{111}In, ^{99}Mo, ^{99m}Tc, ^{90}Y, ^{89}Zr, ^{86}Y, ^{68}Ga, ^{67}Cu, ^{64}Cu, ^{61}Cu, ^{51}Cr, ^{47}Sc, ^{44}Sc, ^{43}Sc, ^{18}F and ^{11}C [Qai17, Ste19, Jan19].

More recently, *Theranostic pairs* of imaging isotopes combined with chemically-similar high-dose radionuclides provides particularly promising pathway for the precision treatment of disease with limited collateral damage to healthy tissues and organs. A particularly promising class of theranostic treatments involves the use of targeted alpha therapies (TAT) that take advantage of the limited range (and therefore high dose) of alpha-emitting nuclides. Examples of viable theranostic radioisotope pairs (i.e., radioisotopes with similar chemical bounding efficiency with carrier pharmaceuticals) are listed in table 6.

Table 6: Examples of theranostic radioisotopes from [Qai18]

Imaging (PET/SPECT)	Therapy
^{123}I, ^{124}I	^{131}I
^{86}Y [Rös17]	^{90}Y
^{61}Cu, ^{64}Cu [Qai18,Qai19]	^{67}Cu
^{111}In, ^{68}Ga	^{90}Y, ^{177}Lu
^{43}Sc, ^{44}Sc [Sin15, Meu15, Rös11]	^{47}Sc [Dom17]

However, all of these treatments rely on a robust, contamination-free, high specific-activity (i.e., Ci/g) supply of radionuclides produced either at the treatment location using hospital-based cyclotron or regionally using reactors, high-energy particle accelerators or multi-MeV photon sources. Furthermore, high-quality decay data, including absolute positron yields and alpha yields for PET imaging and TAT, are also needed to ensure that patient dose is optimized for imaging or treatment purposes.

This portion of the report includes subsections that cover all of these needs, including:

4.3.1 Decay Data (M. Carpenter, C. Nesaraja and S.M. Qaim);
4.3.2 High energy accelerator production and stopping power (C. Vermeulen & L. Bernstein with input from A. Koning);
4.3.3 Low energy charged-particle isotope production (S.M. Qaim);
4.3.4 Gamma-ray production (C. Howell);
4.3.5 Integral Validation (S.M. Qaim and others)
4.3.6 Ion Beam Therapy (L. Bernstein with input from C. Keppel and Ceferino Obcemea from the WANDA 2022 Stopping Power Session).

4.3.1 Decay Data

A recent review had been performed [Nic22] to assess the status of available decay information of radionuclides that are in use or proposed for medical diagnostics and therapeutics, and to identify possible deficiencies in the currently available nuclear data. This assessment was made by consulting various nuclear databases including evaluated and unevaluated data such as ENSDF, XUNDL, NUBASE2020 and AME2020. In a previous review by S.M. Qaim [Qai17], the status and existing discrepancies of decay data associated with standard and nonstandard or novel radionuclides as well as the need for further nuclear data for producing radionuclides using newer technologies were also discussed [Ber15].

While much is known with regards to the decay properties of many isotopes utilized and proposed for diagnostics and therapeutic purposes, there is still work to be done for the determination of more accurate information. In the case of developing novel radionuclides, there still exist a significant amount of decay data needs. The isotopes used for SPECT, PET, and therapeutics are summarized below from recent work and needed studies.

Diagnostic γ emitters and single-photon spectroscopy (SPECT). The isotopes utilized for these diagnostic investigations typically have short half-lives (< 3 days), emit γ rays in the energy range of 100 -200 keV, and have relatively simple and well-known level schemes. The isotope ^{99m}Tc is the most utilized for these types of studies but ^{67}Ga, ^{81m}Kr, ^{111}In and ^{123}I and ^{201}Tl have also been employed. Other isotopes that have been proposed as diagnostic tools for SPECT include ^{133}Xe, ^{178m}Ta ^{196}Au, ^{199}Tl and ^{202}Tl. In some cases, the isotope of interest is produced as a parent-daughter generator e.g., ^{81}Rb/^{81m}Kr and ^{99}Mo/^{99m}Tc. The isotopes ^{147}Gd and ^{155}Tb have also been proposed as candidate nuclides for SPECT even though their decay schemes are more complicated than the others. In some cases, these isotopes can have a dual purpose and be utilized in microdosimetry studies which require a more thorough quantification of emitted radioactivity including X-ray, internal conversion and Auger electron emission. While much is known about the γ-decay properties of these isotopes, most of the listed isotopes require additional decay data studies to better determine the decay emission for all levels whether this be by γ-ray or electron emission. For nuclides with complex decay schemes, Total Absorption Gamma Spectrometry (TAGS/TAS) [Rub05, Kar16, Alg21] would be beneficial to ensure the γ-ray spectrum of these isotopes is correctly measured, considering the consequences of the "pandemonium effect" [Har77]. Hence, by measuring gammas depopulating high nuclear energy levels with TAGS, a more accurate determination of the individual EC/β+ branching will be possible. Some specific examples related to achieving more comprehensive and accurate decay data for the diagnostic γ emitters and SPECT are improved internal conversion measurements for ^{99m}Tc, improved measurements of Auger-electrons for ^{67}Ga, ^{111}In, ^{123}I and ^{193m,195m}Pt; improved K X-rays for ^{201}Tl; and improved decay schemes for ^{147}Gd and ^{155}Tb using TAGS/TAS studies.

A particularly significant data gap involves detailed low-energy yields and spectra for the development of high-dose Auger therapeutics. This was pointed out by Roger Howell at the WANDA 2019 meeting [Ber19a] and echoed in a recent review article on the topic [Val22].

β^+ emitters for PET. There are a large number of isotopes which can be deployed in PET. PET relies on back-to-back emission of 511-keV γ radiation from positron annihilation. The most commonly used isotopes are ^{11}C, ^{13}N, ^{15}O, and ^{18}F. The decays of these light isotopes are well characterized, and no additional studies appear to be required. There are also a few isotopes of medium mass nuclei including ^{55}Co, ^{61}Cu, ^{64}Cu, ^{68}Ga, ^{75}Br, ^{82}Rb and ^{86}Y that are utilized and, in some cases, coupled with another radioactive isotope of the same *Z* to be used as a theranostic pair *e.g.,* ^{64}Cu with ^{67}Cu [Qai17]. At first glance it appears that most of these isotopes are also well characterized, with recent work either confirming previously measured isotope half-lives or extending knowledge of the decay structure of the daughter. For example, two decay measurements of ^{82}Rb [Nin16] and ^{86}Y [Gul20] have been performed with the Gammasphere detector array at ANL with the later changing the ^{86}Y β^+ yield by 14% to 27.9(12)%.

This is a critical result since a good knowledge of the *β^+ yield, not the total EC/β^+ rate*, is needed to fully exploit PET as a *quantitative* nuclear imaging diagnostic. Qaim [Qai17] mentioned that the emission probabilities of positrons from novel radionuclides are not precisely defined in the existing data files. The values are generally deduced from decay schemes and not measured directly. This is a drawback. Positron Emission Tomography (PET) is the only diagnostic technique which delivers quantitative results. Therefore it demands an exact knowledge of the intensity of the emitted positron. A recent experimental study on ^{86g}Y [Udd22] has attracted great attention of nuclear physicians/medical physicists with regard to quantitative dosimetry in the theranostic use of the ^{86g}Y/^{90}Y pair of radionuclides [Qai18]. A general recommendation is therefore to measure the intensity of the positron directly, wherever possible. A systematic review of PET radionuclides using this method could be used to guide a targeted measurement program for other PET nuclides, such as ^{61}Cu.

Non-standard β+ emitters are potentially promising radionuclides that have either been proposed or are in pre-clinical trials. This includes ^{30}P, ^{34m}Cl, ^{38}K, ^{44}Sc, ^{45}Ti, ^{51,52,52m}Mn, ^{52}Fe, ^{57}Ni, ^{62}Cu, ^{66}Ga, ^{73}Se, ^{76}Br, ^{77}Kr, ^{82m}Rb, ^{83}Sr, ^{89}Zr, ^{90}Nb, ^{94m}Tc, ^{110m}In, ^{120,121,124}I, ^{132}La and ^{152}Tb as well as parent-daughter generators ^{52}Fe/^{52m}Mn, ^{72}Se/^{72}As, ^{118}Te/^{118}Sb, ^{122}Xe/^{122}I, ^{128}Ba/^{128}Cs and ^{140}Nd/^{140}Pr. While the half-lives of these isotopes appear to be well-established, more detailed studies of nearly all these isotopes are required to better characterize the decay branches and requires measurements similar to those done for ^{82}Rb and ^{86}Y using Gammasphere and/or the absolute β+X-ray method from *Uddin* (see above) in conjunction with TAGS/TAS studies. Although several have well defined decay schemes, there exist nuclides with complex decay schemes that are either incomplete, questionable or have unplaced and/or inconsistent gammas, as highlighted in Ref. [NIC22]. They include ^{38}K, ^{45}Ti, ^{52}Fe, ^{73}Se, ^{76}Br, ^{82m}Rb, ^{83}Sr, ^{90}Nb, ^{94m}Tc, ^{110m}In, ^{120,121,122}I, ^{128}Cs, ^{132}La and ^{152}Tb.

Pallative and therapeutic radionuclides. One of the many applications of therapeutic radionuclides is palliative care, which is intended to relieve pain in bone metastasis, prostate, and breast cancer [ALS:20]. A broad range of isotopes have been considered for palliative treatment and/or other forms of radiotherapy such as brachytherapy. These isotopes, listed in Ref. [NIC22], include ^{32,33}P, ^{89}Sr, ^{109}Pd, ^{125,131}I, ^{137}Cs, ^{153}Sm, ^{161}Tb, ^{165}Dy, ^{169}Yb, ^{175}Yb, ^{177}Lu, ^{192}Ir, ^{198}Au, ^{225}Ac (and α-decay daughters ^{221}Fr, ^{217}At, ^{213}Bi), and ^{227}Th (and α-decay daughter ^{223}Ra) as well as parent-daughter generators ^{90}Sr/^{90}Y, ^{103}Pd/^{103m}Rh and ^{188}W/^{188}Re. Characterizing the decays of these nuclides is ongoing and recent progress in defining ^{177}Lu decay and improved characterization of the ^{227}Th and subsequent daughter decays has been undertaken. Since these isotopes are being used for therapy, it is important to quantify their decay radiations, to the extent possible, possible, including levels fed in the daughter nucleus and emission of α–, β–, γ– and electron emissions. In some cases, the aforementioned Pandemonium effect occurs when many unresolved states are populated in the decay, resulting in a continuous spectrum of γ rays which are not characterized by the deduced level scheme. This unresolved emission can account for a substantial amount of γ-ray energy emitted in the decay, > 20%, and is typically characterized utilizing TAS. Nuclides targeted in Ref. [Nic22] for further investigation include ^{103,103m}Rh, ^{125}I, ^{161}Tb, ^{169}Er, ^{225}Ac and ^{227}Th.

Potential therapeutic radionuclides. These isotopes were identified in Ref. [Nic22] and include ^{47}Sc, ^{67}Cu, ^{114m}In, ^{117m}Sn, ^{131}Cs, ^{135}La, ^{149}Tb, ^{166}Ho, ^{186}Re, ^{193m},^{195m}Pt, ^{228}Th (and decay daughters ^{224}Ra, ^{212}Pb, ^{212}Bi) and ^{230}U (and α-decay daughter ^{226}Th) along with parent daughter generators: ^{195m}Hg/^{195m}Au, ^{197m}Hg/^{197}Hg and ^{211}Rn/^{211}At. Recent work includes a study of ^{67}Cu which resulted in significant changes to the β^- branches, with implications for radiation dose [Che15], and more accurate half-lives of ^{117m}Sn, ^{135}La, ^{166}Ho, ^{195,195m}Hg. Regarding future work, more precise information is required on ^{67}Cu (full evaluation of the decay scheme); ^{114m}In, ^{117m}Sn, ^{193m}Pt, ^{195m}Au (reassessment of IC electron emission probabilities and re-evaluation of decay schemes;^{131}Cs, ^{135}La, ^{197,197m}Hg (re-evaluation of decay data); and ^{228}Th and ^{230}U decay chains (more extensive α and γ singles spectroscopy as well as γ–γ coincidence measurements).

4.3.2 High Energy Accelerator Production

Many of the most promising radionuclides for use in the treatment and diagnosis of cancer are most effectively produced using radiochemical generators with multi-day half-lives made using high-energy ($E > 100$ MeV) protons rather than more commonly available low-energy beams due to the dramatically longer effective range. An example of this was shown in figure 2.10 comparing the production rates for two radiochemical generators for two emerging PET isotopes; ^{72}Se and ^{68}Ga [Fox21b]. While the peak production cross sections for lower energy beam/target combinations may be larger, the greater range of the proton, together with the longer half-life of the ^{72}Se generator, clearly makes it the preferred regional production pathway. However, the energetic proton-induced reaction approach carries the risk that a long-lived contaminant radionuclide could be co-produced, rendering the isotope unsuitable for clinical use. Any high-energy isotope production plan requires predictive modeling based on measured data and a robust reaction modeling capability, e.g., nuclear reaction modeling, to ensuring that the radionuclide will be appropriate for human use.

Unfortunately, high-energy reaction modeling has a number of features that distinguish it from $E_n < 20$ MeV neutron-induced reactions that make up the vast majority of ENDF data, including significant pre-equilibrium particle emission and the formation of residual nuclei far from stability, poorly known nuclear level densities and radiative strength functions. Furthermore, there are relatively few comprehensive reaction data sets available to guide modeling of these production routes. This deficit has been acknowledged by the Isotope Program at the US DOE which has funded a nuclear measurements campaign for targeted proton-induced reactions with

$E_p < 200$ MeV which produced two peer-reviewed publications in 2021 [Fox21a, Fox21b]. This effort is described in the Accomplishments section (2) of this report.

The advent of commercial availability of higher energy cyclotrons, capable of delivering protons, deuterons and alpha particles for the bulk production of radioisotopes, increases the need for comprehensive evaluated cross sections for relevant production routes at these energies including both the radionuclide of interest together with any co-produced radio- and stable impurities. Figure 4.1 below shows the cross sections for isotopes produced during bombardment of ^{139}La for the production of ^{134}Ce, illustrating the very fine balance needed to optimally produce the isotope of interest while avoiding co-produced impurities. ^{134}Ce has been identified as a valuable imaging analog for both ^{225}Ac as well as ^{227}Th [Bai21].

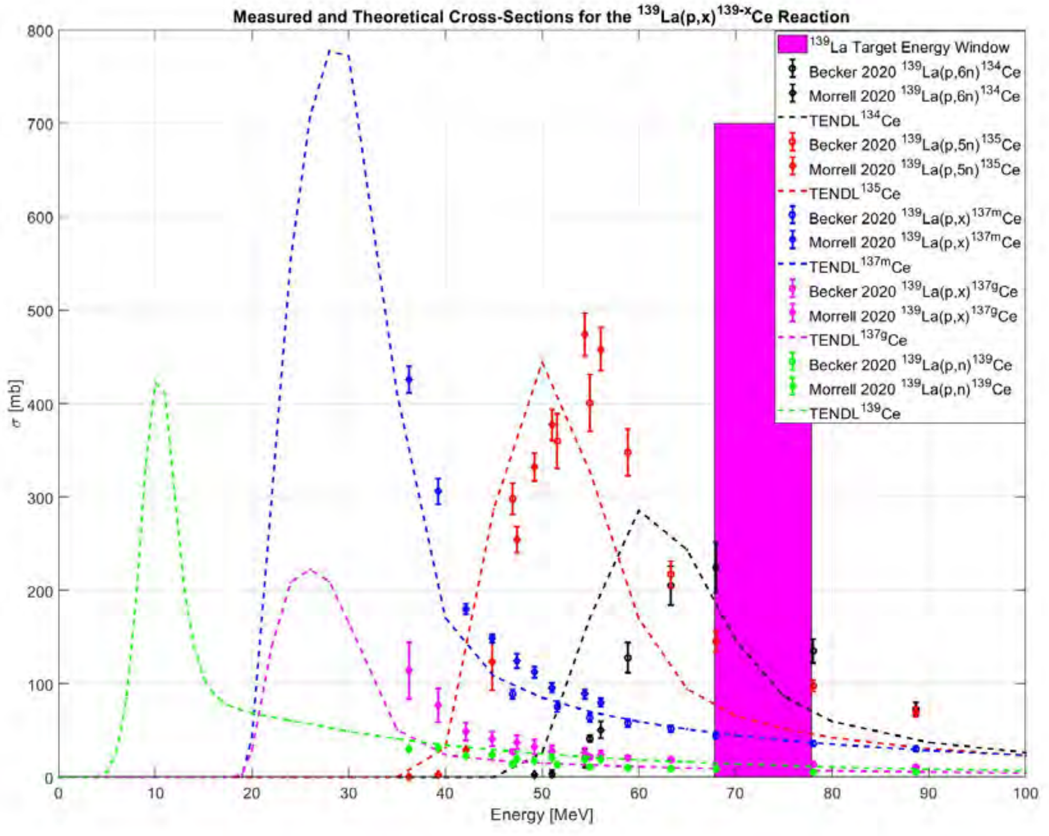

Figure 4.1: Cross sections for protons on ^{139}La from TENDL along with measurements from Becker [Bec20] and Morrell [Mor20].

Precise knowledge of the stopping power of the particles delivered at these higher energies are couple to cross section measurements because the targets will typically be irradiated in a stacked configuration to make optimal use of the full energy range of the machine.

While nuclear data have been measured at higher energies for many years, these data sets are not as comprehensive as the measurement campaigns at lower energies where many machines have been available for measurements. Higher energy measurements have been performed exclusively at a handful of national laboratories around the world. Those facilities will continue to dominate research in high energy isotope production because commercial machines will almost exclusively be occupied with bulk production.

One of the isotopes of great interest for TAT is ^{225}Ac and, by extension, other alpha emitters. Currently, production routes from natural Thorium targets are being investigated at proton energies above 70 MeV. Higher energy commercial machines are not inconceivable within this context, emphasizing the need for better data at higher energies and alternate particles, such as alphas and deuterons, are already available albeit with fewer data.

To ensure that systematic measurements of both the cross sections as well as the stopping powers are performed, **collated into a searchable, evaluated database** and provided to the production community at large, funding is required to support the research groups at our national laboratories to produce the data in a comprehensive and systematic way.

Another cross-cutting need is precipitated by the necessity of using high Z targets for the production of alpha-emitting isotopes and as is already being seen in Th irradiation for ^{225}Ac. There is little data on fission fragment formation and, consequently, poor representation in reaction modeling codes.

Finally, with the tremendous interest in TAT, the question of the alpha particle energy and consequent recoil becomes incredibly important because this determines the stability of the isotope in a targeting molecule and can significantly influence the efficacy, as well as the side effects, in a therapy regime [Koz18].

4.3.3 Low Energy Accelerator Production

An updated review published in 2021 [Qai21] describes the various needs. In view of the increasing number of small cyclotrons all over the world, combined with the use of a solution target to produce small amounts of novel positron emitters for local use, the demand on the quality of data near the threshold of the reaction is increasing. It is suggested that a low-energy LINAC be used rather than a cyclotron with an initial projectile energy of about 20 MeV. Furthermore, the calculation of stopping power at low energies becomes critical. Accurate studies have been recently performed in the low-energy range for the ^{64}Ni(p,n)^{64}Cu and ^{86}Sr(p,n)^{86g}Y reactions [Udd16, Udd20]. Such studies are needed for many other radioisotopes as well.

With the increasing significance of theranostic approach in medicine, termed as **personalized medicine**, the need for a suitable therapeutic partner of a novel positron emitter is increasing. The best example is ^{86g}Y/^{90}Y where ^{90}Y is obtained from the reactor-produced ^{90}Sr/^{90}Y generator system. Other promising systems are ^{44}Sc/^{47}Sc and ^{64}Cu/^{67}Cu. Whereas ^{44}Sc and ^{64}Cu are easily produced at small cyclotrons, the longer lived ^{47}Sc and ^{67}Cu therapeutic radionuclides are difficult to produce. A few promising reactions are induced by 70 to 100 MeV protons and/or with bremsstrahlung radiation up to 50 MeV. Thus there is considerable need of data measurements using intermediate energy accelerators and powerful LINACs.

In radionuclide targeted therapy, the use of suitable chemical compounds of trivalent metal radionuclides like ^{47}Sc, ^{90}Y, ^{177}Lu and ^{225}Ac, is attracting great attention. The reactor-produced ^{90}Y and ^{177}lu are commercially available but great efforts are underway to produce ^{225}Ac using accelerators. This α-emitting radionuclide appears to be superior to all over β^- emitting radionuclides used in internal therapy. In view of the large number of potentially useful routes for its production, further extensive nuclear data efforts are needed. It may be added that for quantification of dose from ^{177}Lu or ^{225}Ac, a PET measurement using the chemically analogous positron-emitting radionuclide ^{68}Ga is necessary. The latter is commercially available via the ^{68}Ge/^{68}Ga generator system. In recent years, however, it is also produced directly via the ^{68}Zn(p,n)^{68}Ga reaction locally at small medical cyclotrons using a solution target. The nuclear data for this reaction have been well measured and evaluated [Qai19].

In addition to the necessity of new measurements with protons in the low and intermediate energy regions discussed above, the possible use of the α-particle beam in the production of some special radionuclides may also be mentioned [Qai16]. Some low-lying high-spin isomeric states of a few radionuclides decay via internal conversion or isomeric transition, and thereby emit a large number of Auger electrons which are of great potential in Auger therapy. Those isomeric states are easily populated in α-irradiations than in proton irradiations. Two examples are ^{117m}Sn and ^{193m}Pt. The availability of the α-particle beam at a cyclotron should therefore be an added advantage.

Finally, a small word of caution appears to be appropriate. Most of the non-standard positron emitters are produced at small cyclotrons using highly-enriched target materials. In Europe the major supplier of the enriched materials has been Russia. In view of the new developing political landscape, it is strongly suggested that USA pay more attention to the enrichment and supply of important target substances.

4.3.4 Gamma-ray Production

Most radioisotopes are produced in either nuclear reactors via (n,γ) reactions or by reactions induced with light-ion beams. However, radionuclides produced in nuclear reactors typically have low specific activity and are not optimum for use in nuclear medicine applications. The DOE/NSF Nuclear Science Advisory Committee recently named production of radioisotopes with electron LINACs as one of the most compelling and largest-impact opportunities for the production of high-specific-activity radioisotopes for medical applications [NSA15b].

Simulations (using transport codes like GEANT4) are a cost effective approach for designing systems for radioisotope production via photon-induced reactions. The reliability of such simulations depends on access to libraries with accurate photonuclear reaction data at photon energies across the GDR (Giant Dipole Resonance) region (e.g., from 10 to 40 MeV) where most of the photo-absorption strength resides. Most simulations use reaction cross sections from the well-established evaluated data libraries (TENDL, JENDL, ENDF, JEFF, CENDL, BROND, etc.), which are based on extrapolations of theoretical fits to data. The problem with many of the calculated photo-nuclear reaction cross sections relevant to medical isotope production in these libraries is that the fits are based on very scarce experimental data.

These libraries can provide general guidance on photo-production of radionuclides, but they are unreliable for many reactions that need precise, quantitative predictions. Nearly all photo-nuclear reactions relevant to medical isotope production have yet to be experimentally verified [Kon14, Shi11a, Shi11b, Iwa11, Chi11, Cha11, Cha06, OEC09, OEC06, OEC05, OEC00, Gex11, Chi91, Blo94]. Cross section measurements are needed to improve the accuracy and fill gaps in photo-nuclear databases for reactions relevant for production of radioisotopes important for medical treatment and diagnostics, including reactions such as (γ,*n*), (γ,*p*), (γ,2*n*), (γ,3*n*), and (γ,*pn*). The most straightforward way to measure photo-nuclear reaction cross sections is to use quasi-monoenergetic gamma-ray beams produced by Laser Compton Scattering sources. A collaboration of groups from ANL and TUNL have begun such measurements using the quasi-monoenergetic photon beam at the High Intensity Gamma-ray Source.

4.3.5 Integral Validation of Production Data

Production data of many radionuclides have been evaluated through Coordinated Research Projects (CRPs) of the IAEA. Some of the evaluated data appear to be very reliable but a few others do not have the same authenticity. A general weakness of all evaluated data is that almost no validation work has been done. Although in a few isolated cases the integral yield has been determined experimentally and compared with the yield calculated from the excitation function (ARI 56, 685, 2002; ARI 65, 247, 2007), the result is not very conclusive. There is a great necessity to plan benchmark type experiments at low currents to avoid radiation damage effects. On the other hand validations at high beam currents are necessary to make the data useful for robust type irradiations in large production runs at powerful accelerators. Guidance should be sought from experts in integral measurements at reactors.

A related concern is that often unvalidated or inaccurate data is used in some of the high-energy modeling codes used for isotope production, such as MCNP and FLUKA. These codes are used to define the proper irradiation conditions at cyclotrons. This practice is not reliable. Big IAEA evaluated data files are now available which are more authentic than the model calculated results, and the user is therefore urged to use those data as inputs. Furthermore, a large number of new groups simply use TALYS or some other code to calculate the data, without having a real insight in the theory or the production intricacies. Those data should be treated with caution.

4.3.6 Ion Beam Therapy

At the WANDA 20222 meeting Dr. Cynthia Keppel provided an overview of ion beam therapy, describing how data from Positron Emission and Computer Tomography (PET/CT) are used to guide treatment plans. She pointed out that, in many cases, calculated rather than measured stopping powers are used. Lastly, she pointed out that, in the case of carbon beam therapy, the production of secondary particles, including both ions and neutrons, are responsible for a significant portion of the dose [Mat10]. The importance of secondary neutrons to beam therapy highlights the interrelationship between topical areas that is a recurring theme in the WANDA meetings. The dose attributable to secondary ions from high-energy ion beams such as carbon can cause significant unwanted dose beyond the Bragg curve. This effect was pointed out in the recent work of *Ruvitoso* and *LaTessa* [Rov17] and is demonstrated in figure 4.2 reproduced from the paper by *Kempe* [Kem07].

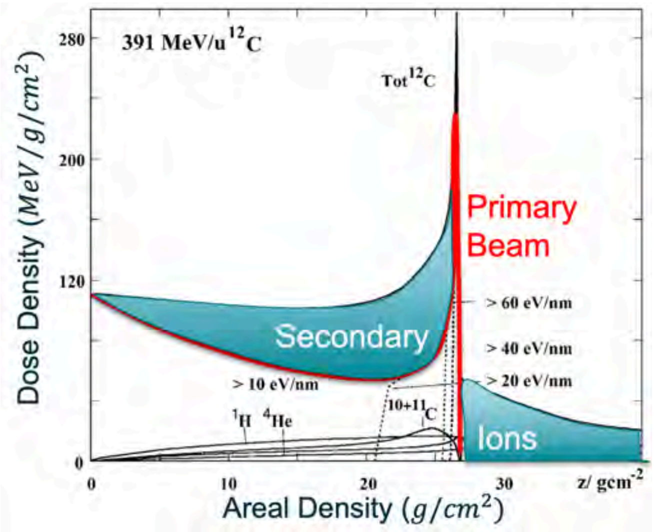

Figure 4.2: Depth dose distribution of a 391 MeV/u ^{12}C beam showing the primary and secondary contributions to the dose, with separation into different LET components. Reused from (Kem07).

Also at WANDA 2022, Dr. Ceferino Obcemea presented a high-level overview of how stopping powers and dose are modeled in multi-component tissues through Bragg Additivity. He pointed out that, at low energies (in the vicinity of the Bragg Peak), additivity may no longer be valid due to changes in the charge state of the beam and the collective excitations and electron wake effects causing stopping powers to deviate significantly from those in water [Rot17]. Furthermore, he noted there is little knowledge of the stopping powers of different cellular structures, including DNA, and that recent results suggesting that DNA was an electrical conductor has profound implications for beam-based cancer treatments [Bar15]. It is worth noting that, while Dr. Obcemea's talk was centered on beam therapy, the issues at low energies he pointed out were equally relevant to energy deposition from targeted alpha-therapeutic radiopharmaceuticals such as ^{225}Ac and ^{211}At. Lastly, he suggested that, at high-fluence, a 60-80% enhancement in stopping powers would take place due to collective excitations [Obc16]. This vicinage, or local area effect [Ari91] can be described via the Lindhard formulation and would be particularly important for modeling dose from laser plasma accelerator ion sources.

It is worth noting that the primary custodian of stopping power data is the IAEA, which hosts a website including electronic stopping for H, He, Li to Ar, and K to U ions. The data can be found at https://nds.iaea.org/stopping/.

4.4 National Security

US national security efforts encompass sustained support and certification of our nuclear stockpile as well as nuclear threat assessment and detection capabilities. These applications rely on analyses from complex, multi-physics simulations where accurate nuclear data are needed. For stockpile stewardship applications, high accuracy is necessary for predictive capabilities. Nuclear data are also used in the interpretation of diagnostic measurements from experiments, both historical and modern. Last, and certainly not least, nuclear data play an important role in the design and implementation of new experimental facilities and capabilities.

A variety of multi-agency sponsors support this work, particularly program offices within the NNSA. The NNSA work is coordinated with DOE/Science investments in related areas, most notably in the enduring support of the ENDF (Evaluated Nuclear Data File) databases. ENDF represents a collaboration of US national laboratories and universities, with some international participation (notably the IAEA) and is coordinated by the Cross Section Evaluation Working Group (CSEWG). ENDF incorporates continued improvements in our best understanding of the nuclear reactions, based on experiment, theory, and simulation. The current U.S. version is ENDF/B-VIII.0, and new releases are made on a roughly 5-year time frame. Our U.S. ENDF capabilities are continually intercompared with European and Asian counterparts through collaborative groups under the IAEA and the OECD/NEA.

In the present document, only a high-level overview is given on the priority areas for future national security nuclear data work. We note that nuclear data improvement extends beyond data needs and includes the infrastructure for developing and using these data. Data needs may be met by improved evaluations or theoretical capabilities or new measurements of theoretical inputs or correlated data.

4.4.1 ENDF databases and the NNDC

Nuclear data are shared across application spaces through an evaluated database. In the US, the ENDF is compiled through a multi-national collaboration and vetted with a range of experts. This is a priority, since the ENDF databases are the interface by which simulation codes access high-fidelity nuclear data. Although ENDF is mature in the sense that versions of that database have existed for decades, much continued attention is needed to maintain quality, and ensure continued trust by our user communities. The ENDF database is extraordinarily complex, including detailed information on reaction cross sections and products, including energy and angular distributions of emitted (secondary) particles. Uncertainties and correlations are also included and warrant increased attention. New methods for using these uncertainties are being developed for applications, helping to quantitatively identify nuclear data needs. Other priorities needed for continued product quality include (a) education and mentoring, to transfer “expert judgment” of our senior researchers to the next generation; (b) development of staff who have expertise in the range of capabilities needed to successfully create a nuclear data evaluation – understanding experiments, nuclear reaction and structure theory, statistical uncertainty-quantification (UQ) analyses, integral nuclear criticality, and new opportunities such as AI/ML;

(c) computational capabilities to rapidly process, test and validate the data; (d) new computational formats to robustly deliver data capabilities to our codes.

4.4.2 Nuclear data advances needed for nuclear security

The priorities are established by nuclear data researchers in nuclear security who work with their colleagues to determine where key application uncertainties can be most valuably reduced. This has led to the categories listed below. Further details can be found in the referenced documents:

1. Precision fission data, including reaction cross sections and products such as prompt fission neutron spectra, neutron multiplicities, and fission gamma-rays. Collaborative work between Los Alamos and Livermore has led to high-accuracy data through complex experiments and continued work is needed to build on this success.
2. Fission product yields. An ongoing multi-agency collaboration is advancing our capabilities here with a goal to update the current capability (the three decade old “England and Rider’’ [Eng93]) widely used in many applications.
3. Neutron inelastic and elastic scattering. A number of studies, both for national security and nuclear energy applications, have pointed to the need to better determine these data for a broad range of isotopes, including environmental isotopes, structural materials, and actinides. Experimental methods are being developed that could transform our understanding here, including the “semi-differential” method pioneered by RPI.
4. Neutron capture measurements, for both stable and unstable nuclides. Advances are needed especially in the hundreds of keV region for applications, taking advantage of new detector instrument and neutron source capabilities.
5. Light nucleus thermonuclear cross sections, including both increases in accuracy and more detailed computational representations (e.g. allowing for charged-particle transport in high-fidelity simulations).
6. Diagnostic cross sections, both for radiochemical and prompt diagnostics. An increased understanding of key cross sections can allow us to “mine” historical test data so as to better validate and constrain our simulation models. Since the easier measurements have already been done, what remains is to exploit new methods to accurately determine the more challenging cases, notably those involving shorter-lived species.
7. Nuclear criticality & criticality safety. As well as the aforementioned fission-related data for actinides, improved data needs continued to be identified and addressed for a variety of materials.

4.4.3 Training

Various DOE programs help develop pipelines of scientists into this research field. These include the Stewardship Science Academic Alliance Program (SSAAP) and Predictive Science Academic Alliance Program (PSAAP)-funded universities and centers of excellence (NA10), and the NA-22 nuclear security consortia. Additional opportunities, through internships (e.g. SULI) and summer programs are also critical toward educating the next generation and developing the future workforce.

4.4.4 Facilities and detectors/instruments

Nuclear cross section measurements are made at various facilities across the USA. For nuclear security applications, key facilities include the Los Alamos Neutron Science Center (LANSCE), the ATLAS and CARIBU facilities at Argonne National Laboratory, the 88-inch Cyclotron at Lawrence Berkeley National Laboratory, Livermore's National Ignition Facility (NIF), and the Nevada NCERC facility for nuclear criticality experiments. New opportunities are on the horizon with the Facility for Rare Isotope Beams (FRIB) in Michigan, particularly for decay studies and reactions on unstable isotopes. Many other facilities also provide needed data, including universities through DOE alliances (e.g. TUNL, RPI, Texas A&M, Notre Dame). Measurements are also exchanged with foreign facilities in Europe and Asia.

4.4.5 Simulation Codes

A key element for the application of nuclear data is the connection to neutronics transport codes. Data evaluations compiled into libraries must be further processed for use in transport applications. Processing and transport code support and development is also necessary. Although it is beyond the scope of this document to discuss the processing and simulation codes used in national security, one example is the MCNP transport code, which is widely used in unclassified neutron transport and criticality safety applications. The ENDF data are validated and improved through comparisons of calculated and measured nuclear criticality, and in this way, the MCNP code plays an important role in the development of the ENDF databases. It is not only an important US code, but it is widely used across the world, especially by IAEA and OECD partners as a gold-standard for transport applications.

4.4.6 Further information

The NNSA Stockpile Stewardship Management Plans (SSMP)[42] for the past 7 years are available online. They provide an overview of the program. Additional resources include the reports by Mosby and Tolar [Mos21], Gibson [Gib22], Lee [Lee21], Keksis [Kek21] and the NDNCA [Ber15], NDREW [Rom18] and WANDA workshop reports [Ber19a, Rom20a, Kol21].

4.5 Nonproliferation

This section describes how the nuclear data impact the missions within nuclear nonproliferation. This includes a description of specific topics that comprise nonproliferation as well as a section organized along specific nuclear data topics.

4.5.1 Nuclear Forensics

In nuclear forensics samples of collected material are investigated to infer the source of that nuclear material, information about the process in which the material was produced, or other relevant quantities such as enrichment levels. Nuclear data is key in understanding reaction networks, fission yields and radioactive decay, and has therefore been an active area of research

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[42] https://www.energy.gov/nnsa/articles/stockpile-stewardship-and-management-plan-ssmp

for the nuclear forensics community for many years. The NNSA Defense Programs (DP), Defense Threat Reduction Agency (DTRA) and the Air Force Technical Applications Center (AFTAC) missions have overlapping mission and nuclear data needs, and coordination of efforts is important in order to prevent duplication of effort.

Required data include improved actinide cross sections, independent and cumulative fission yields, short lived fission product decay data, long lived fission product capture data, other isotope capture cross sections and neutron induced secondary particle information.

4.5.2 Safeguards

The objective for International Safeguards is “the timely detection of diversion of significant quantities of nuclear material from peaceful nuclear activities to the manufacture of nuclear weapons or of other nuclear explosive devices or for purposes unknown, and deterrence of such diversion by the risk of early detection” [INF72]. To carry out these measurements, the community employs a range of passive and active non-destructive assay (NDA) techniques that measure γ-rays, neutrons and X-rays. Many of these methods rely on accurate nuclear data to interpret measurement results. Because large quantities of materials are processed, and a significant quantity can be collected by diverting small quantities over time, physical inventory measurements require very low uncertainties.

With the production of advanced reactors using molten salts, new nuclear data needs have emerged. For example, these reactors use fuels with higher enrichments (near 20%) and will experience buildup of minor actinides and have a higher neutron energy flux spectrum. In addition, the passive neutron source term from spontaneous fission and (α,n) reactions will be stronger and more important.

Some measurement systems are calibrated to standards and repetitive measurements are conducted where outliers are the primary concern. In these cases, nuclear data has minimal importance once the calibration is made.

Safeguards needs are broad due to the variety of NDA measurements of multiple processes in the nuclear fuel cycle that overlap with all other mission objectives. Some of these needs have been collected from users in a previous study and are presented in [Bah14, Hux14].
Some of the priority nuclear data requirements for safeguards are:

- Spontaneous fission yields (fissions/sec/gram)
- Spontaneous neutron multiplicity factorial moments and distributions, ν_{sn}, $P_s(\nu)$
    - Uncertainty is typically 1% (far higher than what is required for safeguards assay of PuO_2 products and MOX
- Fission neutron induced neutron multiplicity moments and distributions, ν_{in}, $P_i(\nu)$
- Fission neutron energy distributions, $\chi(E)$
- (α,n) cross sections and neutron emission spectrum
- He-ion stopping cross sections
- Photoelectric cross sections for Pu and U in the 60 to 300 keV region to support XRF and K-edge measurements

    - Shape & absolute magnitude of K-edge actinide cross sections
- Gamma-ray and X-ray mass attenuation coefficients to significantly improve performance of gamma-ray and X-ray analysis methods
- Gamma decay half-lives and branching ratios
- Neutron induced gamma emission

4.5.3 Near-field Detection

Apart from safeguards, there are multiple applications using radiation detection with dependencies on nuclear data, including wide-area searches, nuclear counterterrorism, treaty verification, and arms control scenarios.

4.5.4 Emergency Response

In Emergency Response (ER) situations the responders rely on multiple detection techniques and calculations to locate and characterize an object of interest. Of the characteristics measured are both passive and active neutron and gamma intensities and energies. Measurement of neutron multiplicity and correlated neutron-gamma emissions are powerful techniques developed for characterization. In addition, the characterization and calibration of detectors is often achieved through benchmark measurements compared to modeling and simulation, which requires nuclear data.

Needs for emergency response include [McN05]:
- Gamma intensities and energies
- Neutron multiplicities and energies
- Correlated neutron and gamma information
- Neutron induced secondary particle emission

4.5.5 Fissionable Materials Production Detection

Fissionable materials production and detection requires the knowledge of fission products and other isotopes produced during the burnup of reactor fuel and the processing of materials. Specific fission product ratios may be useful for materials production detection. Isotopic ratios of actinides can allow inference of the source of material and process of interest. The fission products and actinides found in LWR fuels important for reactor operations are benchmarked within international collaborations and the data is stored in the Spent Fuel Composition Database (SFCOMPO). However, much of the nuclear data requires improvement to accurately model the variety of reactors and processes of interest from first principles Improving nuclear data for systems that could be used for fissionable material production would support the detection of such facilities. Detailed information on uncertainties in reactor fuel isotopics of interest can be found in [Fra14].

Nuclear data needs for Fissionable materials production detection include:
- Independent and cumulative fission product yields
- Fission product gamma emission energies and intensities

- Actinide cross sections up to 1 MeV for thermal reactors
- Capture cross sections up to 1 MeV for thermal reactors

4.5.6 Nuclear Data Topical Areas

Nuclear data can be organized into categories that in many cases are relevant to more than one mission area in Nonproliferation R&D.

4.5.6.1 Fission Product Yields

Scientific interest is focused on the part of the fission process that occurs after scission, the point of separation between the two fragments. The newly formed fission fragments emit prompt neutrons and gamma rays within ~10^{-14} s, with some prompt gammas coming later, within ~1 ms, due to the presence of isomers. The fission fragment yields as a function of mass and charge, *Y(A,Z)*, *after* prompt neutron emissions, are called independent fission yields (IFYs). Eventually, the neutron-rich fragments undergo beta-decay, when a neutron transforms into a proton, an electron, and an antineutrino. Following beta-decay, more neutrons and gamma rays can be emitted. Those are called beta-delayed emissions. The final fission product yields, after prompt and delayed emission has ended, are referred to as cumulative fission yields (CFYs). A consistent, coherent description of this decay chain has yet to be developed for nuclear data evaluation purposes, although all the necessary pieces of physics theories, experimental data, and model codes are available to do so. However, many important, unanswered questions remain regarding the details of this decay chain. Also, the correlations expected in a coherent description of the complete process present significant challenges and opportunities.

Specific requirements to improve fission product data include:

- Reevaluation of independent and cumulative fission yields [Pig15]
- Targeted experiments to resolve areas of high uncertainty such as:
  - Short lived independent yield data
  - Population of metastable states
  - Fission yield variations as a function of neutron energy including in the keV energy region
- Fission gamma and beta energy spectra
- Neutron multiplicity and energy spectrum as a function of incident neutron energy, including in the *keV* energy region.
- Fission product decay data
- Delayed gamma and neutron spectra

<u>State of the Data</u>: Several studies of fission yield decay data important to forensics missions have been accomplished using codes such as ORSEN. Extensive work has been completed on reactor depletion models using ORIGEN to identify fission products with high uncertainties. Information from users indicates that ratios of many fission yields need to be better understood. While differential fission yield measurements as a function of incident neutron energy have been conducted in the US and internationally, differential yields are difficult to measure in the fast region. The fission yields can change substantially in the resonance region when compared to thermal neutron induced fission and these changes should be understood in order to interpret fission product ratios and uncertainties in nubar (the average neutron multiplicity in a fission event).

Integral measurements encompass higher energies but are limited to measurements of gamma decays from fission fragments or mass spectrometry. Work is currently underway to measure very short-lived fission products by measuring gamma emission < 1 second after irradiation [FLU20]. In addition, surrogate measurements of neutron multiplicity have been measured, but with unknown uncertainty. Several projects to measure beta decay in support of antineutrino calculations contribute to the required decay data for cumulative yields.

A new fission yield evaluation was initiated in 2019 and is ongoing. Office of Science is currently funding several studies on beta decays of fission fragments to support antineutrino calculations. Other offices are funding fission yield experiments. These data should be incorporated into the fission yield decay evaluations.

4.5.6.2 (α,n) reactions and neutron emission

Passive neutron source terms can be generated in (α,n) reactions to determine material properties. In addition, the SOURCES4C code calculates the (α,n) neutron source term used in neutron transport and depletion. The ^{19}F(α,n) and O(a,n) source terms are the most frequently measured during NDA in emergency response and safeguards. These (α,n) reactions are also important for neutronics codes. In addition, PuBe, AmBe and other neutron sources are used as calibration standards for some active interrogation systems.

State of the data: Currently, the (α,n) library maintained by the NNDC contains few new evaluations. Many of the cross sections have not been measured for decades. The cross sections that are available are low resolution, missing energy ranges or disparate data sets. The neutron emission spectrum is not well known and should be measured for the most common reactions. In addition, the gamma spectrum and intensity is also a useful signature that should be verified. It is unknown how alpha stopping power influences reaction rates or neutron emission spectra. Specific needs for (α,n) data include:

- New measurements of high priority isotopes: ^{19}F, ^{17,18}O, ^{13}C, ^{7}Li, ^{9}Be, ^{10,11}B, and ^{27}Al.
    - Measurements of both neutron and gamma emission energies are needed for a proper evaluation and to support NDA measurements
- New evaluations of all measured isotopes
- Modernization of the charged particle database to support new data and covariances

These issues are discussed in greater detail in a report from *Romano* [Rom20b].

4.5.6.3 Actinide Cross Sections and Decay Data

The capture, fission, $(n,2n)$ and (n,xn) reactions and decay of actinides creates a network of minor and short-lived actinides important in forensics and reactor calculations, an example of which is shown in figure 4.4 below. Many of the minor actinides of interest have short half-lives and are thus difficult to measure, leading to large cross section uncertainties. However, these cross sections are important for understanding the production of measurable quantities when actinides are exposed to a large neutron flux. Small uncertainties can compound quickly, leading to large uncertainties in accumulation and decay rates. These uncertainties in the cross sections and decay chains in an actinide network can be reduced through a combination of differential and integral measurements supported by theoretical models. The approach includes bounding the problem with the isotopes where energy-differential cross sections can be well measured and filling gaps with integral measurements, capture/fission ratios and theory.

State of the Data: There has been much recent work on minor actinides, specifically, isotopes of Pu and U. An example of a reaction network of interest is given in Figure 4.3. Other actinides such as Am, Np, Cm have received less attention and require improved data. In particular, there are little to no direct measurements of short-lived actinides. Integral measurements are the only way to validate other methods, such as surrogate measurements combined with theory. Theoretical work includes the recently completed FIRE project as well as theoretical models to support surrogate measurements.

- The IAEA CIELO project has created new evaluations of ^{235}U, ^{238}U, and ^{239}Pu. In the next cycle, ^{240}Pu and ^{242}Pu will be examined.
- Recently, TUNL measurements have included ^{238}U *(n,2n)* and *(n,γ)* (0.1–15 MeV), and
- Chi-Nu at LANL has measured scattering on ^{235}U and ^{239}Pu.
- LLNL has completed evaluations of (*n, γ*), (*n,n'*), (*n,2n*), *(n,3n),* and *(n,f)* reactions on ^{236,237,238}Pu, as well as Am isotopes, but these are not available in ENDF format and have undefined uncertainties.

Specific needs for actinide cross sections include:

- Half-lives and branching ratios
- Improved theoretical models
- Differential (beam) and integral (in-reactor) measurements of available actinides
- Indirect measurements to fill in gaps
- Precise measurements of reaction cross sections on long-lived isotopes to bound those on short-lived isotopes.

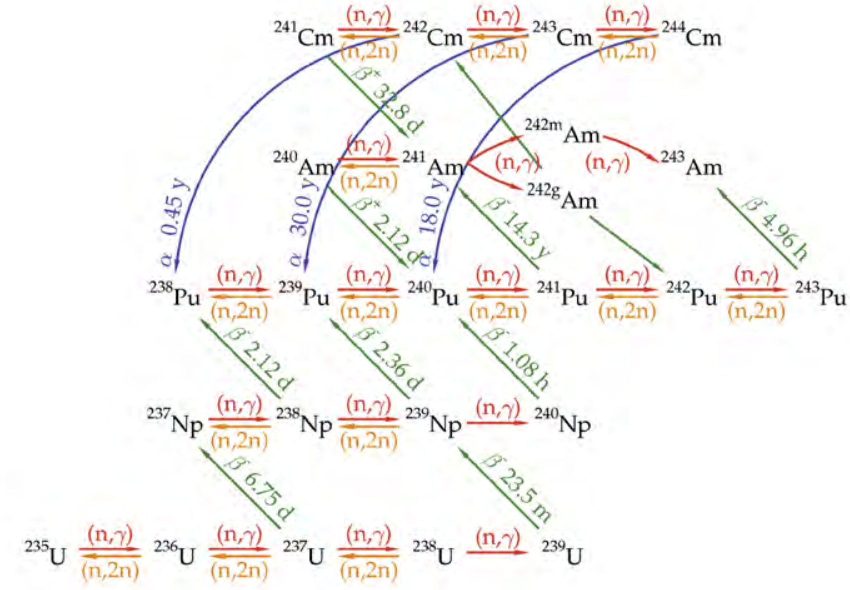

Figure 4.3: An example of an actinide reaction network.

4.5.6.4 Neutron induced gamma-ray production

Neutron-induced gamma-ray production includes those emitted in capture and inelastic scattering reactions. These interactions are particularly important for identification of materials during active neutron interrogation, including ratios of isotopes present in the material.

State of the data:
A recent scoping study [McC21] provided a set of recommendations, many of which were funded the past two years. One project will ensure that ENDF decay data, pulled from ENSDF data files, is complete and consistent with ENSDF. Several experiments were recently funded by multiple agencies to provide new neutron-induced gamma data as well as benchmarks for real-world Non-Destructive Analysis (NDA) experiments.

DNN R&D has previously funded a project to evaluate and incorporate new thermal neutron data from the Budapest reactor. Some files were improved before the project ended. In addition, UC Berkeley created the Atlas of Gamma-Ray Spectra from the Inelastic Scattering of Reactor Fast Neutrons from the Baghdad reactor in Iraq [Hur21][43].

Discrete gammas are not always modeled correctly for each interaction. Whether this is caused by the processing the data sets or by the physics included in the model is unclear. However, improvements can be made by developing a complete, physically-consistent γ-ray cascade event generator.

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[43] https://nucleardata.berkeley.edu/atlas/index.html

In addition to the newly funded projects described above, the following work is recommended:

- Extend GNDS to include level density information and allow states to be embedded in the continuum.
- Develop a computationally-practical gamma event generator for modeling excitation to the continuum for incorporation into radiation transport codes that model processes event-by-event.
- Correct existing cross section data in ENDF and fill in gaps for gamma emission data for energies from thermal to 14 MeV for priority elements: H, C, N, O, Al, Si, Fe, Cu, W Pb, U and Pu.

4.5.6.5 Capture and other Cross Sections on non-actinides

Capture cross sections on fission fragments are important for reactor and activation analysis. NCSP and the Navy Reactors program measures capture, scatter and total cross sections of many isotopes of interest and those with high uncertainties. Any work in this area should not conflict with prior and planned NCSP work. The NCSP 5-year plan, Appendix B [NCS22] lists the nuclear data work and priority needs.

State of the data: There are several materials found in reactors that have large uncertainties arising from capture cross sections and decay data.

- High energy (0.5 to 20 MeV) Co, Cu, Ta and Fe transmission and (n, γ) measurements are in progress at RPI
- $^{63,65}\mathrm{Cu}(n,\gamma)^{64,66}\mathrm{Cu}$ and $^{191,193}\mathrm{Ir}(n,2n)^{190,192}\mathrm{Ir}$ measurements are in progress at TUNL
- NCSP planned work listed in Appendix B

4.5.6.6 Gamma-induced reactions

Gamma-induced fission and activation reactions are useful for active interrogation in the 6 – 9 MeV range for search missions [Gon09, Ged17]. The fission cross section changes rapidly in this energy range, resulting in large uncertainties. Lack of characterization of a bremsstrahlung source may contribute to the uncertainty more than the cross section. In addition, gamma-induced reactions need to be included in fission models, including those of cross sections and fission yields.

State of the data: Department of Homeland Security (DHS)-funded benchmarks highlight large discrepancies between measured and calculated fission rates, requiring a reassessment of the data. The discrepancies may be due to improper characterization of the beam. In addition, there is little or no gamma/neutron emission data available from (γ,f) reactions. The delayed neutron emission data for $^{18}\mathrm{O}(\gamma,n)$ is off by an order of magnitude. One recent DHS-funded project will obtain gamma-induced fission cross sections and yields as a function of incident gamma energy.

Comprehensive compilations of photo-neutron cross section data can be found in the work by Dietrich and Berman and in IAEA-TEC-DOC 1178. More recent photofission work includes relative measurements of bremsstrahlung-induced photofission yields performed by A. S.

Soldatov for 19 nuclei from ^{232}Th to ^{249}Cf relative to ^{238}U. This work includes photofission yields for U and Pu isotopes of interest in nuclear safeguards and nonproliferation.
The following are nuclear data needs for photon interactions:

- The photofission cross section in the 6–9 MeV region of interest.
- Measurement of outgoing neutron and gammas including angular information for gamma-induced reactions.

4.5.6.7 Benchmark Development and Uncertainty Quantification/Sensitivity Studies

Benchmarks are well controlled experiments that can be used to examine model uncertainties and find sources of nuclear data deficiencies. Benchmarks are useful for bounding evaluations of differential data.

The NCSP conducts criticality experiments for multiple missions including defense programs and nuclear material processing facilities to determine material safety limits. These experiments tend to be expensive because they require large amounts of fissile materials. There are currently no standards for conducting benchmarks for NDA measurements for nuclear data, but useful and well controlled experimental data exist.

Data uncertainty, sensitivity, and covariance needs include:

- Further developing tools that can be used to quantify nuclear data uncertainties and sensitivities for certain systems of relevance
- UQ/S studies to inform nuclear data priorities for specific systems
- Creating comprehensive and consistent covariance data
- Defining nuclear data end-use uncertainties
- Creating a standard for the user community to determine relevant benchmarks for validating and testing nuclear data as well as identifying deficiencies

4.5.6.8 Code development:

Code development is needed to support the creation and testing of new data and for users to take advantage of those data. Each program should support the code development required to provide the nuclear data for their specific applications. For example, fission yield covariance data sets will be extremely large and new methods will be needed to process the data and capture the uncertainties of these data in neutron transport codes.
Data processing and transport code needs:

- Developing codes to handle new nuclear and covariance data as they become available to ensure proper use of the data, including processing and transport codes.

4.6 Space Applications

In this section we present a partial overview of nuclear data needs related to space and aerospace applications

4.6.1 Introduction

Unlike nuclear energy, national security, nonproliferation and isotope production, the nuclear data needs for space applications have only recently started to be examined by the nuclear data community. At WANDA 2020, a session on gamma-rays induced by neutrons included a talk by Mauricio Ayllon from NASA Goddard that specifically addressed nuclear data required for planetary spectroscopy applications, such as the Dragonfly mission to Titan. Many of these needs were also found to complement those of terrestrial-based oil-well logging, which also features active interrogation using DT neutron generators. However, the majority of the topics covered in this session were focused on addressing data needs related to active interrogation for nonproliferation, providing limited coverage of space-related needs. As a result, the NDWG decided to make nuclear applications relevant to space exploration a primary focus of WANDA 2022, with three session covering high-energy charged particle-induced reactions, neutron-induced reactions and stopping powers.

In this section we reproduce virtually the entire WANDA 2021 space applications section with the planetary spectroscopy needs augmented using the contributions from WANDA 2020 Also included are summaries of the high-energy charged particle and stopping power sessions from WANDA 2022.

4.6.2 Introduction to the WANDA 2021 Space Applications Report

As humanity works to extend its technological reach deeper and more resolutely into space, the sophistication of the missions and equipment being launched has also been accelerating. In turn, the engineering and scientific needs to support those missions have continued to grow and nuclear data is no exception. From anticipating effects due to the vast collection of cosmic rays that moves freely in the vacuum of space to humans sending sources of radiation into space to support their missions, utilizing nuclear data and models – generated mostly for terrestrial uses – for space applications is becoming more widespread. To that end, all the prominent users of nuclear data for space-related technology gathered for the first time to summarize their work as well as their current or future anticipated data needs. These topics included shielding from space radiation, planetary nuclear spectroscopy, space reactors, planetary defense, and detecting nuclear detonations in space.

As the impact of nuclear data to applications is recognized by a growing number of programs, it is important to examine the many cross-cutting nuclear data needs for the space mission. Enhancing outreach to relevant programs will enable more comprehensive discussions and collaboration among interagency partners. Those interested in nuclear data needs for space should seek to build awareness of these applications in the nuclear data community; document critical data gaps, especially those affecting multiple applications; and suggest steps for meeting those needs. The remainder of this section introduces each space-based research topic, the pertinent nuclear data, and what improvements would be most useful..

4.6.3 Space Radiation Protection

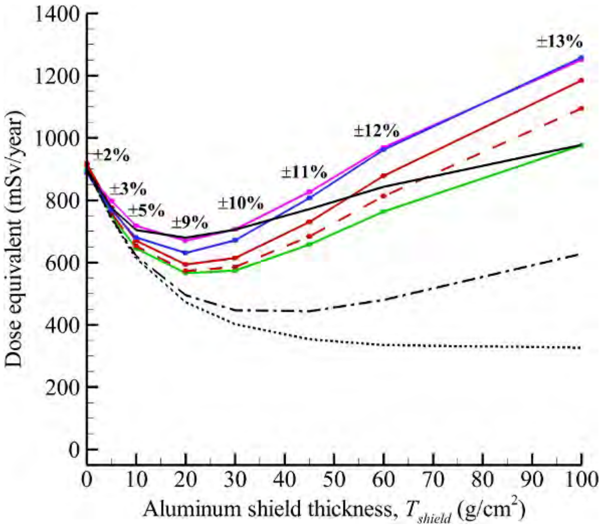

Figure 4.4: Predicted dose equivalent rates from neutrons and ions behind varying thicknesses of aluminum using several transport models.

The radiation environment in space poses unique risks to humans and electronics, necessitating an understanding of the interactions of galactic cosmic rays (GCR), solar energetic particles (SEP), and trapped Van Allen belt radiation. The range of particle energies, species and materials included in those interactions is vast, spanning energies ranging from keV per nucleon to up to several tens of TeV per nucleon; ion species that span the naturally occurring isotopes in the periodic table; and materials composed of elements that also span the periodic table [Guo15,Koh14,Ehr16]. The effort to understand those interactions includes measurements in space [Nor12,Wal13,Sla17,Nor20,Lin61,Ree73], measurements at particle accelerators [Adl72], and modeling [Fel98].

The free-space radiation environment is generally well understood [Guo15]. Except for cases where instruments and electronics are exposed to the free-space environment, the radiation environment for most operations in space will be composed of the particles and energies present after the primary radiation field has passed through varying thicknesses of materials that make up spacecraft and habitats. In shielded environments, the radiation environment is composed of primary, free space ions that have slowed down due to electromagnetic interactions (stopping power), and a secondary radiation field created by nuclear interactions of primary ions with shielding materials. The secondary radiation field is complex and also includes particles not present in free space, such as neutrons. The calculated yields of secondary light ions (p, ^2H, ^3H, ^3He, ^4He, and n) have been predicted to contribute 50% of the dose equivalent behind 5 g/cm^2 of Al and 80% of the dose equivalent behind 30 g/cm^2 of Al [Law98]. The calculated secondary light ion yields are also responsible for most of the differences seen between the various codes [Pre06] behind shielding thicknesses greater than 5-10 g/cm^2 and are the largest source of uncertainty in those calculations (see figure 4.4 above). As such, the secondary radiation field created by nuclear interactions within spacecraft, habitat, and other materials requires an accurate quantification of the electrons, protons, heavy charged particles, and neutrons that make up that field.

Radiation transport models, both Monte Carlo and deterministic, are the primary tools used for mission design and prediction of crew doses and electronic effects in space. Experimental nuclear data is needed for verification of code predictions, improvements in the physics models used in those codes, and reduction of the uncertainties in their predictions. A review of the double-differential and total reaction cross sections important to the understanding of GCR and SEP transport was conducted [ADl72, Fel02], and key gaps in the experimental data have been identified. For GCR transport, He- induced inclusive double differential light ion (p, ^{2}H, ^{3}H, ^{3}He, ^{4}He, n) cross sections at beam energies from 0.1 up to several GeV per nucleon and on targets of H, C, O, Al and Fe have been identified as a critical need, as well as total reaction cross sections for most GCR ion species and targets at beam energies above 1.5 GeV per nucleon. In some cases, such as Fe + O, no total reaction cross section data exists. Secondary particle production includes hadronic and electromagnetic particle showers which spread dose geometrically as well as impact the depth of particle penetration through some material thickness. The angular dependence of production cross sections is critical for understanding showers. These data needs for the planetary spectroscopy community are similar to needs of the isotope production and medical physics communities.

In addition to a better understanding of secondary (and higher order) particle production cross sections from GCR and SEP sources improvements are needed in stopping power data to better quantify not only dose to astronauts, but the related quantity, Linear Energy Transfer (LET) in electronics. The interactions of energetic particles from GCR cascades with materials in electronics causes heavy-ion recoils that can impart significant energy in the electronics near the location of the Bragg peak. These high-LET interactions can in turn lead to Single Event Effects (SEE) that can cause resets in electronics leading to failures of critical systems with potentially devastating consequences. These needs were discussed at greater length in the stopping powers session at WANDA 2022. A recent paper by Jason Osheroff discussed damage from heavy-ion recoil in GaN electronics [Osh21]. Figure 4.5 shows the LET and range from heavy-ion recoils in GaN from this publication.

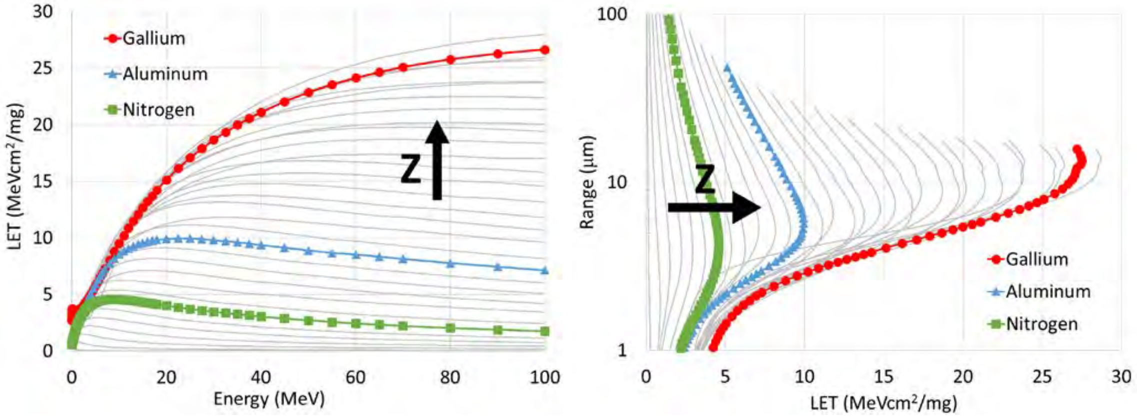

Figure 4.5: LET vs. Energy (left) and Range vs. LET (right) in GaN for ions with Z=1-32 resulting from interactions of GaN nuclides with GCR ions.

In general, there is wide interest in having better data on proton/neutron cross sections and the recoil characteristics in many materials, including, but not limited to wide-bandgap semiconductors such as SiC, GaN and Ga_2O_3, as other materials such as GaAs, SiGe, and HgCdTe, and elemental Cu, Ag, W, Ti, Ta, Sn and Pb. The question was raised if there is the potential for even higher LET particles from proton/neutron reactions on these materials.

In addition to heavy-ion recoils there is also evidence of damage from GCR-induced fission on high-Z materials in electronics, including gold contacts. Thomas Turflinger discussed this at

WANDA 2022 and noted that simple phenomenological models are being used for fragment mass and energy dependence [Vio86, Zha00].

4.6.4 Planetary Nuclear Spectroscopy

Planetary nuclear spectroscopy is an established sub-field of planetary science where measurements of gamma-ray and neutron emission from planetary surfaces are used to characterize the chemical composition of the surface. First proposed as a means of characterizing the hydrogen [Boy07] and major-element composition [Pep11] of the Moon, the technique has now been applied to a wide variety of planetary objects. To date, nuclear spectroscopy experiments have been carried out from orbit around the Moon [Eva12, Law13, Pep16, Pre12], Mars [Pre17, Vin73], Mercury [Pep15, Mit14, Elk20], and the asteroids 433 Eros [Law19], 4 Vesta [Pep22b], and 1 Ceres [Cas19]. Although less common, in situ experiments by landed spacecraft have also been carried out on Venus [Yam06], asteroid 433 Eros [Brü11], and Mars [Ago18]. Missions are currently planned for asteroids 16 Psyche [Wer18], the Mars moon Phobos [Pep21], and Saturn's moon Titan [Ree02].

Most planetary nuclear spectroscopy experiments rely on galactic cosmic rays to stimulate neutron and gamma-ray emission from planetary surfaces, as shown in Fig. 4.6. In this scenario, high-energy primary cosmic-ray particles (>30 MeV), primarily protons, initiate nuclear spallation reactions to depths of a few meters in the surface. Spallation neutrons can escape the surface and the energy-dependent shape of the neutron spectrum provides constraints on the bulk composition and hydrogen content of the surface. Moreover, the neutrons interact with subsurface materials and stimulate gamma-ray emission via inelastic scattering and neutron radiative capture reactions. The resulting gamma rays provide element-diagnostic measurements of the surface composition to depths of tens of centimeters. NASA's upcoming Dragonfly mission to Titan will use a D-T neutron generator to stimulate gamma-ray emission from the surface. However, the underlying nuclear reactions of interest are neutron inelastic scattering and radiative capture.

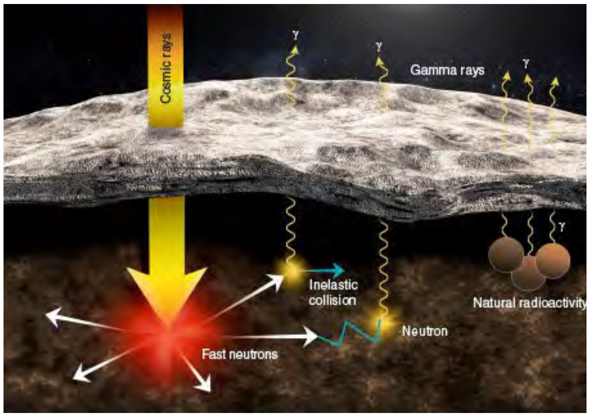

Figure 4.6: Schematic of cosmic ray interactions with planetary surfaces. Rendering by V. Chen [Cas19].

Although a number of benchmark experiments have been conducted [Bec15, Gib17], the wide variety of processes that are important for nuclear spectroscopy experiments means that data analysis efforts require intensive radiation transport simulations that rely on cross section libraries to provide the knowledge of the physics processes of interest. Relevant processes include:

1. Spallation cross sections for protons and alpha particles, on a wide variety of materials, from energies of a few tens of MeV to hundreds of GeV.
2. Neutron elastic scattering cross sections from energies of ≈50 MeV to thermal ≈0.2 eV).
3. Neutron inelastic scattering, $(n,n'\gamma)$, cross sections for major elements, from energies of 50 MeV down to threshold (typically 0.1 to 1 MeV), for elements with concentrations of 0.1 weight % (percentage by weight) or higher.
4. Neutron radiative capture, (n,γ), cross sections also for elements with concentrations of 0.1 weight % or higher

In the case of items 3 and 4, both primary, (*e.g.*, $n,n'\gamma$), and secondary cross sections for gamma-ray production are relevant as both contribute to the final measured gamma-ray environment. While exact detection limits vary based on the nature of the gamma-ray detectors, spacecraft orbit, and measurement time, typically gamma-ray spectroscopic investigations are sensitive to elements with > 0.1 weight % concentrations. For known planetary materials, this can include H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni. Currently, uncertainties on neutron interaction cross sections are the dominant source of systematic uncertainty. Planetary geochemists require measurements with less than 1% uncertainty while 5-25% uncertainties are currently the best that can be achieved.

The highest priority nuclear data need for planetary nuclear spectroscopy is $(n,n\,\gamma)$ for H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni, from threshold (≈ 0.1 to ≈ 1 MeV) to 50 MeV with less than 5% uncertainty. This overlaps with data needs from safeguards and stewardship applications, where neutrons are used for nondestructive characterization of nuclear waste materials and homeland security applications. The data must be provided to the community via cross section libraries, *e.g.*, ENDF and JENDL , that are compatible with the GEANT4 [Pos20] and MCNP6 [Dun21] transport codes, which are widely used by the planetary nuclear spectroscopy community. Comparisons of laboratory-measured gamma-ray production via neutron inelastic scattering to predictions based on ENDF/B- VI, ENDF/V-VII, and ENDFB/VIII reveal a significant degradation in the accuracy of the secondary gamma-ray energy distributions since the release of ENDF/B-VI [Tri17]. Cross sections for secondary gamma generation are also affected. *Ayllon* provided a particularly comprehensive assessment of the $(n,x\gamma)$ data needs for a number of these missions at the WANDA 2020 meeting. Those needs are summarized in table 7 below.

Table 7: Gamma-ray spectroscopy data needs from *Ayllon*

Target isotope	Reaction	Energy level (MeV)	Gamma energy (MeV)	Moon (M), Titan (T) Phobos (Ph), Psyche (Ps)	Data Library (ENDF)	Notes
0 -16	$(n,n'\alpha)$	4.439 (C-12)	4. 439	M, T, Ph	B6.8	MCNP6 overpredicts***
0 -16	$(n,\alpha\gamma)$	3.089 (C-13)	3.089	M, T, Ph	B6.8	MCNP6 underpredicts***
N-14	$(n,n'\gamma))$	2.313	2.313	T	B7.0	MCNP6 overpredicts•
C-12	$(n,n'\gamma)$	4.439	4.439	T	B6.8	Angular dependent cross section needs reevaluation*
Al-27	$(n,n'\gamma)$	2.734	1.72	M, T, Ps	B6.8	MCNP6 underpredicts***
Al-27	$(n,n'\gamma)$	2.212	2.212	M, T, Ps	B6.8	MCNP6 underpredicts***
Si-28	$(n,n'\gamma)$	6.276 → 1.779	4.497	**M**, T, Ph, Ps	B6.8	Important for correcting C***
Si-28	(n,x)		>6	**M,** T, Ph, Ps	B6	MCNP6 underpredict s**
Fe-56	$(n,n'\gamma)$	0.847	0.847	**M,** T, Ph, Ps	B6.8	MCNP6 overpredicts***
Fe-56	$(n,n'\gamma)$	2.085 -> 0.847	1 .238	**M**, T, Ph, Ps	B6.8	MCNP6 underpredicts***
Cl-35	(n,d)	2.127 (S-34)	2.127	T	B7.0	MCNP6 overpredicts*
Cl-35	$(n,n'\gamma)$	3.163	3.163	T	B7.0	MCNP6 underpredicts*
Na-23	$(n,n'\gamma)$	2.076 → 0.440	1.636	M, T, Ph	B7.0	Lar11:e relative error*
Na -23	(n,d)	1.275 !Ne-21)	1.275	M, T, Ph	B7.0	MCNP6 underpredicts*
Na-23	$(n,n'\gamma)$	0.440	0.440	M, T, Ph	B7.0	MCNP6 underpredicts*
Ni-58	$(n,n'\gamma)$	1.454	1.454	T, Ps	87,0	MCNP6 overpredicts*
Ca-40	$(n,n'\gamma)$	3.736	3.736	**M**, T, Ph, Ps	B7.0	MCNP6 overpredicts*
Ca-40	$(n,n'\gamma)$	3.904	3.904	**M**, T, Ph, Ps	B7.0	MCNP6 overpredicts*
Ca-40	(n,p)	0.800 →0.030	0.77	**M,** T, Ph, Ps	B7.0	MCNP6 overpredicts*
Mg-24	$(n,n'\gamma)$	4.238	4.238	M, T, Ph	B6	MCNP6 underpredicts, future ENDF releases wrong**
Mg-24	$(n,n'\gamma)$	1.369	1.369	M, T, Ph	B6	MCNP6 underpredicts, future ENDF releases wrong**
Mg-24	(n,d)	2.076 →440 (Na-23)	1.636	M, T, Ph	B6	MCNP6 underpredicts, future ENDF releases wrong **
Mn-55	$(n,n'\gamma)$	1.292 → 0.126	1.166	**M**	B6	Future ENDF releases wrong **
S-32	$(n,n'\gamma)$	2.23	2.23	T, Ps	?	
La-139	?	?	?	**M,** T, Ph,Ps	?	Detector material
Br-nat	?	?	?	M, T, Ph,Ps	?	Detector material
Ce-nat	?	?	?	M, T, Ph,Ps	?	Detector material

*El. Kanawati 2011, ** Mauborgne 2020, *** Ayllon 2020

Nuclear spectroscopic investigations also require knowledge of spallation cross sections from energies of a few tens of MeV to hundreds of GeV in typical rock- forming elements. The number of neutrons released in a spallation reaction is particularly important. Because of the wide variety of elements and energies in question, benchmarking experiments are particularly valuable [NCR10] for guiding the decision of physics simulations for GEANT4 and MCNP6. This data need overlaps with the needs of the radiation shielding and isotope production communities.

Another important data need is (n, γ) cross sections. While these are generally known with better precision than the prior two examples [Gla77], unexpectedly high cross sections are currently being identified [Gaf02] and high-capture cross section elements can be relevant for planetary nuclear spectroscopy measurements, even if the element is present at ppm concentrations and thus not directly detectable via nuclear spectroscopy measurements [Hor21].

4.6.5 Space Reactors

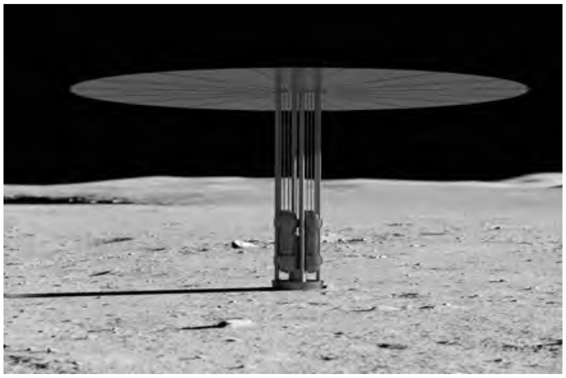

Figure 4.7: Illustration of a conceptual fission surface power system on the Moon which may potentially be used for the upcoming Artemis Mission [Fer16]

With the US returning to the Moon this decade, along with crewed missions to Mars later this century (see figure 4.7), NASA has resumed looking at nuclear options for propulsion, surface, and on-board power. Past efforts in nuclear thermal propulsion (Project Rover), nuclear electric propulsion (Project Prometheus), and surface power (Kilopower [Bra12], KRUSTY [How14]) have been conducted and form the basis of current research efforts. In addition to the existing reactor designs from those projects, new reactor designs (gas, liquid, and solid) and fuels are being explored for space applications. One critical aspect of reactors that will be used in space is the need for autonomous control, a need that places additional emphasis on uncertainty quantification of the nuclear data used in the design of these systems. The data needs for many of the advanced reactor concepts for terrestrial use are very similar to the needs for space reactor development, such as:

1. Fission product inventories, with accurate individual and cumulative yields;
2. Secondary radiation generation and deposition;
3. Cross sections for the assessment of irradiation damage that are not currently available in the ENDF libraries;
4. Reduction of uncertainties on fast neutron reaction cross sections on uranium isotopes.
5. Increased resolution in thermal scattering cross sections
    - Hydride moderator cross section (ZrHx and YHx over a range of stoichiometries)
    - In core materials (SiC and ZrC)
    - Uranium nitride parahydrogen (from cryogenic to high temperature)
    - Increased resolution in the epithermal energy region
    - Beryllium and Beryllium oxide
6. Uncertainty data – updated covariance data will allow for more accurate characterization of reactor uncertainty sensitivities
7. Testing Infrastructure – Space reactor technologies could benefit from pre-existing or new infrastructure for experimental testing and evaluation of nuclear data
8. High energy photonuclear reactions and photon sources can be further characterized to understand any impact to the reactor during idle, start up, or nominal operation

Though space and advanced terrestrial reactors share many common nuclear data interests, space reactors have unique size constraints and design criteria, and will operate in an entirely different radiation environment than their Earth-bound counterparts. These data needs address several areas of reactor development for space applications, including accident tolerant fuels, material effects under conditions of high temperature, shielding, and reliability.

4.6.6 Planetary Defense

Planetary defense is a field of research devoted solely to the purpose of preparing for a scenario where a near-Earth object, such as an asteroid, could potentially collide with the Earth. Though an asteroid impact similar to what caused the extinction of the dinosaurs is an extremely low-probability event, there are many other smaller asteroids that pose a threat and could cause extensive damage; a recent example is the 20 meter asteroid that exploded over Chelyabinsk, Russia in 2013. It is estimated that there are about 130,000 near-Earth asteroids that are greater than 100 m in diameter and only 20% have been accounted for and their orbits characterized [Pie20].

In the event that the Earth did need defending from an asteroid impact, the preferred mitigation mission would be a kinetic impactor, which is both the simplest and currently the most developed option in terms of technology [FLU20]. However, in the event that a kinetic impactor would be insufficient to prevent an asteroid impact, either from the asteroid not being in the correct size range or there not being enough time to deflect the asteroid's orbit, sending a spacecraft carrying a nuclear device to intercept the asteroid is an alternate option. A nuclear mitigation mission could be utilized two different ways, depending on the need. Upon detonation, the device would emit mostly x-rays and neutrons that would heat up and vaporize the illuminated surface of the asteroid, causing material to expand and be ejected. If the intended mission was to deflect the asteroid, the ejected material would impart a momentum push to the asteroid in the opposite direction, while keeping the bulk intact and altering the orbit enough to miss the Earth. If the intended mission was to disrupt the asteroid, the x-rays and neutrons would cause a shock wave to penetrate through the entire asteroid, breaking it into many small, fast moving fragments that would miss Earth by a large margin or vaporize in the atmosphere.

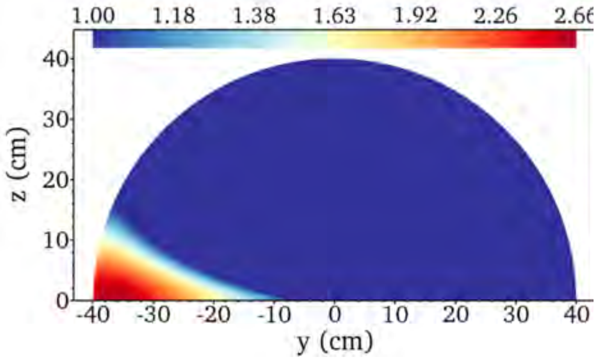

Figure 4.8: Energy deposition from a 50 kt yield neutron source visualized in an 80 cm SiO2 asteroid using MCNP. The color scale corresponds to the number of factors above the melt threshold the asteroid was heated. Dark blue indicates the material was not melted. (from [Bos20]).

Simulations with Nuclear Data and Uncertainties

Correctly simulating the energy deposition from the device's radiation and the subsequent ejecta while designing a mitigation mission would be essential to its success. Such simulations would require accurate cross sections of all interactions and reactions for neutrons at the energies around the output of a nuclear device for the elements that make up asteroids. Though the output neutrons have a variety of energies, the most probable energies are 14.1 MeV (from the $^{2}H+^{3}H$ fusion reaction), 2.45 MeV (from the $^{2}H+^{2}H$ fusion reaction), and 1 MeV (peak value of the fission spectrum Watt distribution for ^{235}U) [Bur20]. Asteroids are roughly composed of various stony materials such as silicates or hydrocarbons, metals such as iron or nickel, and potentially some ice, depending on its particular type [Dup20]. Those compounds predominantly include the elements H, C, O, Mg, Si, S, Ca, Fe, and Ni, though others are possible (see Section 4.6.4 above). Chondrites and other meteorite samples can be used to provide insight into variations in initial particle (including photon) interactions and energy deposition with such astronomical bodies.

Currently, the most efficient way to simulate the nuclear deflection/disruption of an asteroid is to first generate an energy deposition function from the radiation (such as in the figure 4.8 above) which, in the case of neutrons, would utilize Monte Carlo transport codes such as MCNP [Dun21] or Mercury [Tou16]. The energy deposition function could then be used to initialize a standard hydrodynamics code (which includes damage models) that would calculate the asteroid's reaction to the energy deposited by the radiation over longer time scales [Bos20, Shi18]. The most recent versions of MCNP and Mercury get their neutron cross section data from ENDF B-VII.1 and the Evaluated Nuclear Data Library (ENDL) respectively. An example of the type of nuclear cross sections used to calculate the deposition in Fig. 4.9 can be seen in Fig. 4.9. In part because the choice of a nuclear mitigation mission will likely be made after locating an incoming asteroid with little warning time, the properties of the asteroid itself will contribute the largest uncertainties when formulating the mission. Key characteristics such as the material composition, structure, rotation, and even the mass/size will likely be poorly constrained before a launch if minimal data on the asteroid has been collected.

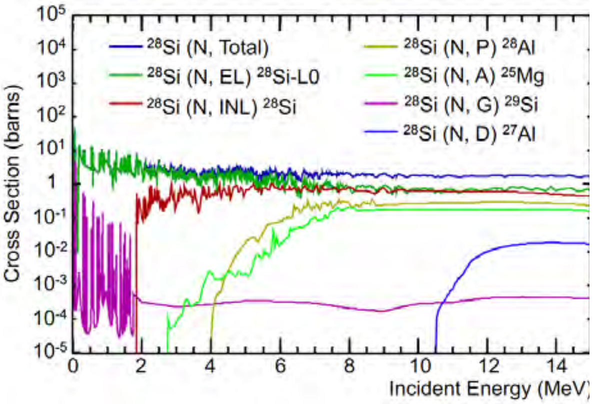

Figure 4.9: Neutron cross sections in ^{28}Si for reactions occurring an energies below 15 MeV [Fer16], Curves are taken from Ref. [Cha11].

Even if a full reconnaissance mission to the asteroid has been achieved beforehand and most properties are well characterized, simply changing which portion of the asteroid is illuminated by the device can still present an uncertainty. Creating a full picture of the sensitivities and uncertainties associated with the asteroid properties for a nuclear mitigation mission is an active work in progress for the members of the planetary defense community. However, many of the properties listed above will likely contribute greater uncertainty than the 25% arising from the nuclear data models. Even so, the data needs of planetary defense overlap significantly with the needs of planetary spectroscopy, which requires less than 5% uncertainty for neutron-induced cross sections in the energy range of interest. It is also likely that the asteroid surface compositions resulting from measurement efforts by those in planetary spectroscopy will inform the material characteristics for mitigation mission simulations, providing a two-fold benefit from more precise cross sections.

4.6.7 Space-Based Nuclear Detonation Detection

Another application of nuclear data that is highly relevant to national and global security is the employment of satellites to detect nuclear weapons detonation either on Earth, in the atmosphere, or in space. This continuous monitoring serves to verify that the countries party to the Limited Test Ban Treaty of 1963 and, later on, the Threshold Test Ban Treaty of 1974 are in compliance. This particular area represents a key nuclear data interest for the Defense Threat Reduction Agency (DTRA), which funds research for the purpose of countering weapons of mass destruction, as well as the Air Force Technical Applications Center (AFTAC), which hosts the U.S. Nuclear Detonation Detection System (USNDS) treaty-monitoring mission. There are currently two different space-based platforms that the detection systems occupy: the Space and Atmospheric Burst Reporting System (SABRS) and systems that ride along with our Global Positioning System (GPS) satellites in medium Earth orbit.

Depending on where the detonation occurred, the emissions that can be picked up will vary. If the detonation was in the air or on the Earth's surface, then the x-ray output from the resulting hot plasma of the nuclear detonation expands the air at a sufficiently high temperature to create optical light. In addition, the prompt gammas emitted from the nuclear reactions free some electrons, which rotate in the Earth's magnetic field and emanate pulses in the radiofrequency domain. If the detonation happens at high altitude or in space, then all of the x-rays, gamma rays (prompt and delayed), and neutrons can travel freely to the space-based detectors. If the detonation happens somewhere in the upper atmosphere, the resulting signals will probably feature some radiation from both categories, depending on where it happened.

The applicable energy and time domains for detecting the gamma rays and neutrons from a detonation via satellite cover a fairly large range. The gamma ray energies are in a range from 100 keV to 8 MeV. The prompt gammas arrive at early times (100 ns to 1 ms), whereas delayed gammas can arrive at up to 100 s. Neutrons are emitted with energies between 1 and 20 MeV and arrive roughly within the same time frame as the delayed gamma rays [Bur20].

The early time-delayed gamma rays that arrive within 100 μs to 100 ms and result from short-lived isomeric decays have significant uncertainties associated with their energies and half-lives. In particular, production estimates from ^{235}U, ^{238}U, and ^{239}Pu fission are important for calculating delayed gamma fluxes. There are also significant uncertainties on fission product yields (FPYs). There is a need for more incident neutron energies and more precise isotopic decay half-lives shorter than 0.5 s. Some experiments have been completed and others are underway with the hope of eventually measuring FPYs with decay times of order 1 s. In the case of a nuclear detonation in air, knowing the neutron cross sections with elements in the air, such as H, O, N, and C, may also be important for understanding the light output of the detonation.

In general, implementing an approach that better quantifies uncertainty (which is required for these studies) is of great interest. Two techniques under consideration are using uncertainties reported in ENDF or sampling the half-life and energy uncertainties via Monte Carlo methods.

4.6.8 Summary of Space-Based Needs

The range of nuclear data users whose work is based in space is a varied one. While the largest research areas are represented here, it is likely that some research areas within the field were left out. As the nuclear data community is just beginning to explore space applications , there is abundant need for further discussion. In the meantime, some key overlaps have already been noted.

For the purposes of space radiation protection, He-induced inclusive double differential light ion (p, ^{2}H, ^{3}H, ^{3}He, ^{4}He, n) cross sections at beam energies from 0.1 to several GeV per nucleon on targets of H, C, O, Al and Fe as well as total reaction cross sections for most GCR ion species on targets at beam energies above 1.5 GeV per nucleon are critical needs. These nuclear data weaknesses overlap with those of the isotope production and medical physics communities as well as the planetary spectroscopy community, which requires spallation cross sections from energies ranging from 10 MeV to hundreds of GeV in elements that form planetary surfaces.

The planetary spectroscopy community also needs precise ($n,n'\gamma$) cross sections for rock-forming elements between 0.1 and 50 MeV with less than 5% uncertainty. Though that is a significant request for the experimenters that generate nuclear data, these cross sections are also needed in safeguards and stewardship applications, homeland security applications, and planetary defense.

In terms of the other research areas, there is less overlap between the other space application users. The needs of the space reactor community will in many cases follow the needs of the nuclear energy, and advanced reactor communities. The nuclear data needs from the satellite-based nuclear detonation detection community overlap with many applications in their need for improved fission product yields and fission product decay data.

5 Conclusions and Acknowledgements

The six application areas discussed in this report are by no means a complete listing of all of the ways that nuclear data is needed for societal benefit. Notably absent are data needs in support of nuclear fusion, which recently achieved a milestone in the achievement of Lawson's criterion in an inertially-confined high energy density plasma [Abu22], ushering in potentially a new class of nuclear science studies in neutron-rich high energy density plasmas [Cer18] and renewing interest in fusion as potential clean energy source. Closely aligned with fusion is the materials damage, which was a topic at WANDA 2019 [Ber19a]. Other potential application areas on the horizon that depend on nuclear data include the development of high-precision quantum clocks based on the use of nuclear isomers, such as the first excited state of ^{229}Th [Thi19]. The unique aspect of the nucleus as the highest energy density system practically accessible makes the importance of nuclear data an evolving story and ensures that it will remain essential to new human endeavors into the future.

However, all of the applications listed in this report share a common requirement: the recruitment, retention and training of a skilled nuclear data workforce, which encompasses measurement, modeling and evaluation, is key need for all the topical areas discussed in this report. This includes not only staff trained in nuclear physics, but also nuclear chemistry and nuclear engineering. The need for a trained workforce is implied in the needs listed in all six application areas in section 4 and explicitly called out in specific subsections on basic science (4.1.1) and national security (4.4.3). Furthermore, the comprehensive list of recent sole USNDP accomplishments in section 2.1 and collaborative efforts in section 2.2 would not have been possible without trained personnel to carry them out.

The USNDP recognizes this need and has instituted numerous training opportunities both domestically (see section 2.2.5) and internationally (see section 3.1.1). This need is also recognized by one of the leading collaborators of the USNDP, the Office of Nonproliferation Research and Development (DOE/NNSA/NA-22), which five years ago funded the Nuclear Science and Security Consortium (NSSC)[44] which included a Nuclear Data Crosscutting area. The NSSC, which is now comprised of 9 university and 5 national laboratories, was renewed for an additional 5 years in FY22 with nuclear data being "promoted" from being a crosscutting area to being an integral part of the nuclear physics topical area. The NSSC academic partners include nuclear physics, engineering

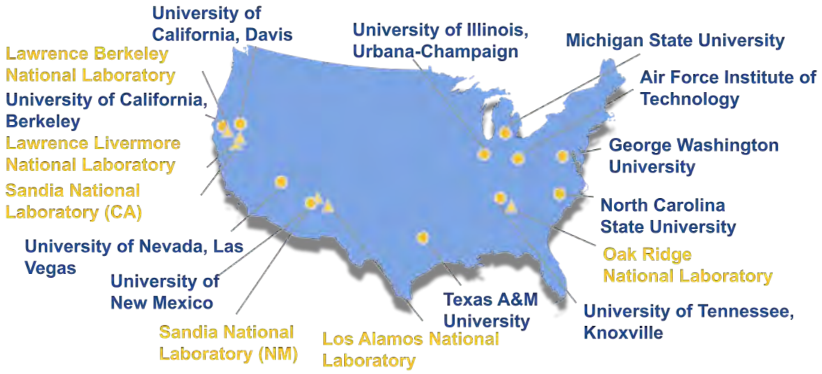

Figure 5.1: NSSC partners universities and laboratories

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[44] https://nssc.berkeley.edu

and chemistry groups and departments throughout the United States and recently hosted a nuclear data summer school (see section 2.2.5.2) in collaboration with the Peder Sather foundation at the University of California – Berkeley and the Norwegian Research Council. It is worth noting that the other two NA-22-sponsored consortiums as well as many of the Stewardship Science Academic Alliance programs also have students and faculty involved in nuclear data-related research. These workforce development activities will feature prominently in the second NSAC-ND report due at the end of January 2023.

While only a small number of nuclear science and engineering graduates will become nuclear data evaluators it is important that all of members of the field have an awareness of how their work feeds into the nuclear data pipeline. It is up to the members of the academic and research community to impart to their students, postdocs and early career staff an understanding of both the importance of nuclear data and the way that their work contributes to it so that they can partner with members of the USNDP and other relevant international organizations to make sure that the full fruits of their labor are realized.

Lastly, there was a notable development that occurred shortly before the release of this report that was particularly applicable to discussions of nuclear data. The White House Office of Science and Technology Policy (OSTP) updated U.S. policy guidance to make the results of taxpayer-supported research immediately available to the American public at no cost[45]. This memo calls out the importance of free and open access to tax-payer funded research, pointing to the accelerated pace of research that followed the onset of the CoVID-19 pandemic and the resulting policies and treatments that undoubtedly helped to save many lives. The memo lists 11 tasks that are meant to coordinate activities between different government agencies to ensure streamlined public access to federally-funded research that reduces barrier due to societal inequities and engages all governmental and non-governmental stakeholders.

The NSAC-ND subcommittee recognizes the value of open access to all nuclear data and notes that the robust mechanisms for nuclear data acquisition, compilation, evaluation and dissemination at the heart of the USNDP provides an implementation pathway for the goals listed in the OSTP memo. This report and the follow-on document planned for release in early 2023 should help guide efforts to ensure that nuclear data is made available to all users in a free and useful manner in accord with the goals of the OSTP memo and the betterment of humanity.

In closing the chair would like to acknowledge the efforts of the entire subcommittee and give special thanks to the members who listed at the top of Nuclear Data Needs Section 4 who contributed significantly to the various portions of the report. I would also like to thank my colleagues in the USNDP who provided input to the Accomplishments section: Shamsuzzoha Basunia, Jon Batchelder, Dave Brown, Aaron Hurst, Filip Kondev, Hye-Young Lee, Libby McCutchan, Eric Matthews, Michael Smith and Boris Pritychenko. I would also like to than Dr. Paraskevi Dimitriou from the IAEA for her contributions on International Collaborations (Section 3). Special thanks are due to Drs. Catherine Romano and Ramona Vogt for reading

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[45] https://www.whitehouse.gov/wp-content/uploads/2022/08/08-2022-OSTP-Public-Access-Memo.pdf

through the entire document both as a copy editor and contributor, and also for their years of service to the nuclear data community in general.

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