Proceedings for the Workshop on Applied Nuclear Data 2023

Amy E. Lovell[1], Bruce D. Pierson[2], Nathan Gibson[1], Jason Harke[3], Stephanie Lyons[2], Elizabeth McCutchan[4], Gencho Rusev[1], Sebastian Schunert[5*], Etienne Vermeulen[1], Andrew Voyles[6,7], Catherine Romano[8], Todd Bredeweg[1]

[1]Los Alamos National Laboratory
[2]Pacific Northwest National Laboratory
[3]Lawrence Livermore National Laboratory
[4]Brookhaven National Laboratory
[5]Idaho National Laboratory
[6]University of California, Berkeley
[7]Lawrence Berkeley National Laboratory
[8]The Aerospace Corporation
[*]Present address: Radiant Industries

LA-UR-24-28785
February 27 – March 2, 2023

Los Alamos
NATIONAL LABORATORY

TABLE OF CONTENTS

ABSTRACT

The Workshop for Applied Nuclear Data Activities (WANDA) took place from February 27 to March 2, 2023, in Crystal City, Virginia. The aim of the four-day meeting was to bring together nuclear data producers, users, and federal program managers to facilitate interagency collaboration on nuclear data needs and solutions. The workshop consisted of talks by federal program managers,g updates from the Nuclear Data Working Group (NDWG), five topical roadmapping sessions, the Nuclear Data Interagency Working Group (NDIAWG)-funded project reviews, and concluded with summaries of the roadmapping session recommendations. Over 160 attendees from headquarters, national laboratories, universities, industry, and international institutions joined the workshop, and these proceedings summarize the workshop, while highlighting important recommendations and outcomes.

1 Introduction

The 2023 Workshop for Applied Nuclear Data Activities (WANDA2023) is the seventh in a series of workshops bringing together the nuclear data community (data producers and users) to identify and prioritize nuclear data needs and to describe actionable strategies to address those needs. The first few iterations of this type of workshop included the Nuclear Data Needs and Capabilities for Applications (NDNCA) workshop in 2015 [1] and the Nuclear Data Exchange Meeting (NDEM) in 2016. After NDNCA, the Nuclear Data Working Group (NDWG) was founded [2] to facilitate cross-cutting collaboration between programs, made up of representatives designated by program managers with interest in nuclear data needs. These needs, priorities, and potential funding mechanisms were presented to federal program managers during NDEM after which the Nuclear Data Interagency Working Group (NDIAWG) was founded [3]. The NDIAWG is comprised of federal program managers who are interested in addressing nuclear data needs, with the goal to coordinate nuclear data funding between participating program offices. The NDIAWG is chaired by the Department of Energy (DOE) Office of Science, Office of Nuclear Physics (NP). A detailed timeline of nuclear data activities can be found in Fig. 1.

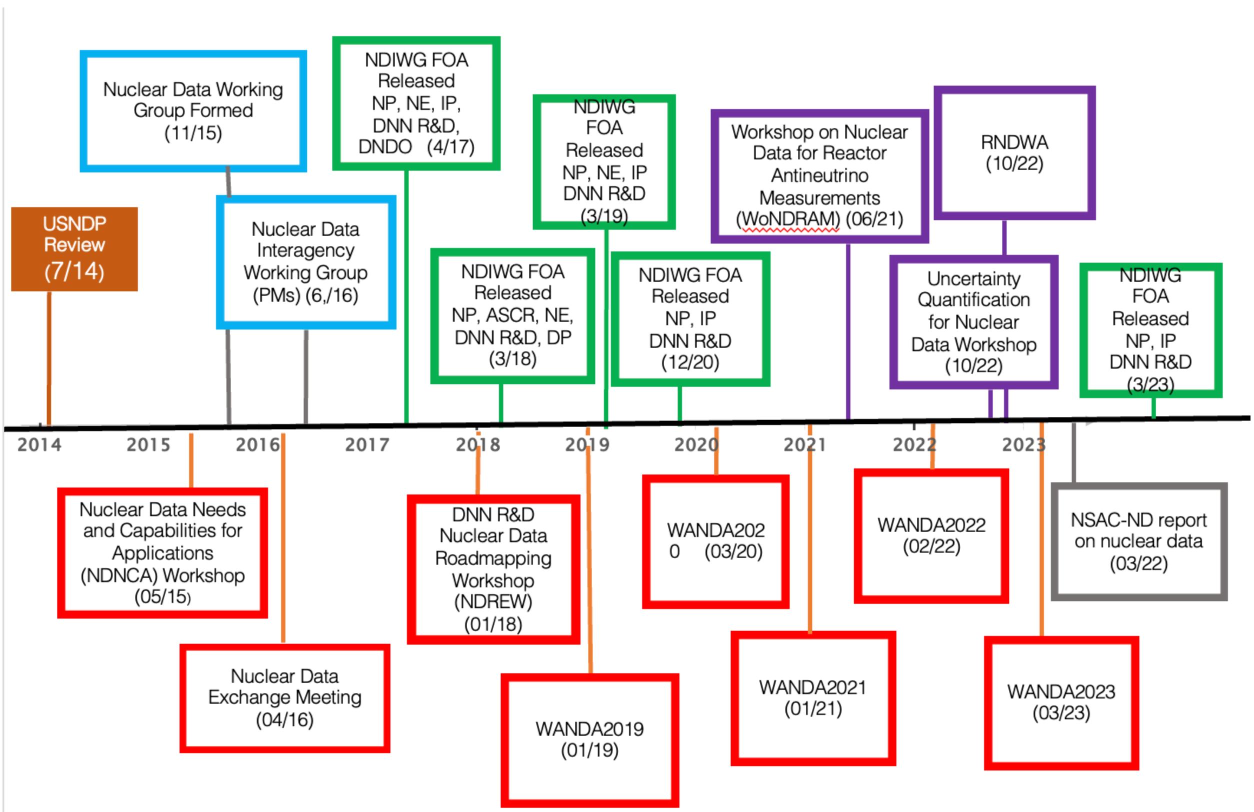

Figure 1 Timeline of NDWG and NDIAWG activities, credit C. Romano.

After NDEM, the first of a now-annual NDIAWG funding opportunity announcement (FOA) was released and managed by DOE NP. These FOAs are developed from the recommendations of the annual nuclear-data focused workshops. Since the release of the first NDIAWG FOA in 2018, over $60 million in nuclear data improvements have been funded that directly impact applied science. This level of effort was readily realized through a collaborative funding environment. Multiple projects have been funded for the following cross-cutting nuclear data topics:

- Reactor antineutrino source terms,
- Fission yields and their decays
- Neutron-induced secondary particles
- (α,n) reactions and secondary particles
- Inelastic and elastic scattering cross sections, and
- Infrastructure enhancements

A similar format has been followed for the WANDA meetings since 2018. The first day, federal program managers or their designated representatives give overviews of their nuclear data needs in an opening plenary session. In addition to these needs, the international nuclear data community is often represented. Additionally, to help lay the foundation for understanding the complexity of the whole process of creating nuclear data, a talk or discussion on the nuclear data pipeline is presented. This plenary session is then followed by either serial or parallel roadmapping sessions to discuss nuclear data needs and their cross-cutting applications.

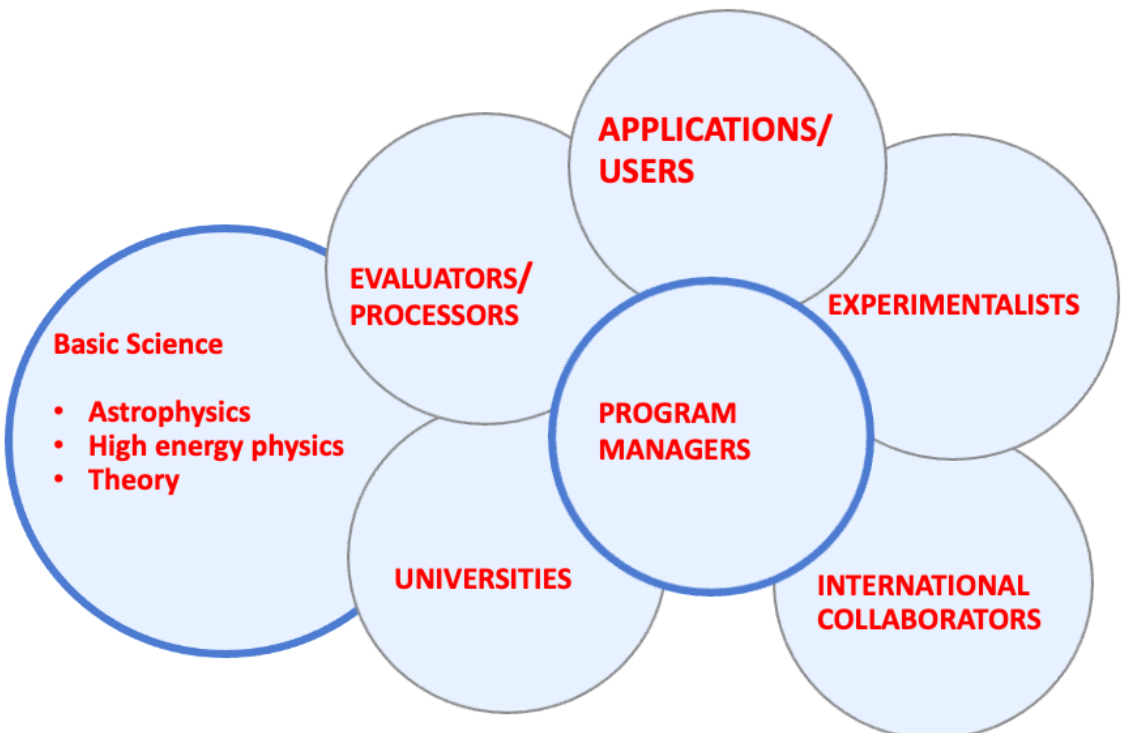

Figure 2 Interaction between federal program managers, nuclear data producers and users, universities, the international community, and the basic science community, credit C. Romano.

Recently, there has been a concerted effort to include more of the basic science community into the nuclear data environment. Although the applications of the two communities are often different, many of the data needs are similar, and many in the nuclear data community were originally trained in – and still work in – basic science. The collaboration of the communities brought together by the WANDA workshops is shown in Fig. 2.

2 The Goals of the NDWG and NDIAWG and Current Updates

As mentioned previously, the NDWG was founded in 2015 with the goals of facilitating communication, collaboration, coordination, and prioritziation of nuclear data development across multiple federal program offices, national laboratories, and industry. The NDWG membership is currently just under 50 members. Interested programs can each nominate up to two nuclear data/application experts from the national laboratories who represent the program or laboratory mission interest within the NDWG. This nomination and representation ensures that program-specific needs are communicated. In addition, each DOE and National Nuclear Security Administration (NNSA) national laboratory is able to nominate up to two individuals to represent their missions and communicate opportunities back to their home institution.

To facilitate these goals, the NDWG is responsible for determining the scope of the roadmapping sessions held during the WANDA workshops based on current nationla priorities, dunding agency mission goals and input from the greater nuclear data community. These roadmapping sessions gain consensus from the participants on cross-cutting nuclear data needs and actionable recommendations that will improve nuclear data for applications. These recommendations are recorded in proceedings such as this, and are used to guide the NDIAWG FOA topics. Proceedings from previous WANDA workshops can be found on the NDWG website [4], along with other nuclear data needs publications.

The NDIAWG is led by the Office of Science, Office of Nuclear Physics and open to all interested federal program managers across DOE, NNSA, NASA, NIH, DOD, and other funding agencies. Membership has grown to 17 agencies since 2018. The NDIAWG communicates regularly on nuclear data needs and coordinates planned rpojects. It realeases an annual nuclear data FOA aimed at creating cross-cutting funding opportunities that are co-funding across the NDIAWG agencies. These FOAs have been very successful at funding a wide variety of nuclear data projects, many of which are highlighted in a review session at the end of each WANDA meeting.

3 Plenary Sessions for WANDA2023

There were two plenary sessions for WANDA2023, Monday and Thursday mornings. On Monday morning, federal program managers talked about the nuclear data needs for their programs. Additionally, international collaborators discussed their programs and needs. An introduction to the "Nuclear Data Pipeline" was again given by Dr. Dave Brown from Brookhaven National Laboratory (BNL). On Thursday morning, NDIAWG FOA-funded projects were highlighted, with short talks from projects that started in fiscal year 2023 and longer talks from the other ongoing projects.

A selection of participants from WANDA 2023 are shown in the figure below. The attendees included federal program managers, nuclear data producers, users, international and industry partners. The website with the majority of the presented talks can be found on the WANDA 2023 indico page, https://conferences.lbl.gov/event/1067/.

Figure 3 Group photo from WANDA 2023

3.1 Interagency Nuclear Data Talks

Dr. Tim Hallman, the Associate Director for Nuclear Physics, gave the welcome talk for WANDA 2023. He overviewed continued efforts in nuclear data, including the recent FOAs put out by the NDIAWG and highlighted some possible non-traditional sources of nuclear data, including the Relativistic Heavy Ion Collider (RHIC) at BNL. He also overviewed the recent charge from the Nuclear Science Advisory Committee (NSAC) to establish a sub-committee "to assess challenges, opportunities, and priorities for effective stewardship of nuclear data". (It is worth noting that Lee Bernstein gave an overview of the NSAC sub-committee findings and reports.) Lastly, he went over recent diversity, equity, and equality initiatives, including the addition of Promoting Inclusive and Equitable Research (PIER) Plans in all Office of Science FOAs.

This talk was followed by one from Keith Jankowski, the Program Manager for Nuclear Data, who discussed the United States Nuclear Data Program (USNDP) and the NDIAWG. He went over USNDP challenges, including the quickly diminishing number of evaluators for nuclear structure information and described a funding opportunity in the works to address this issue. He also highlighted the growing membership of the NDIAWG, which added seven new agency members since 2020.

Several agencies highlighted their nuclear data needs, including:

- **The DOE Isotope Program** – cross sections (including neutron-induced, proton-induced, α-induced, γ-induced, and deuteron-induced) for medical and industrial isotope production, and stressed the need to perform similar measurements across multiple facilities to characterize targets.

- **Defense Nuclear Nonproliferation Research and Development Program** – scoping studies on neutron-induced emission, (α,n) reaction data, secondary γ-ray emission, non-actinide reaction networks; emphasized the need for higher-fidelity codes and capabilities and expanded data for energy ranges relevant for nonproliferation (e.g. 14 MeV neutrons). Additional investments are required for correlated neutron-γ emission probabilities, event generators such as CGMF/FREYA (fission) and MCIDI (γ-ray cascades), fission product yields for major and minor actinides, and nuclear data that impact reactor antineutrino spectrum calculations and measurements. For plutonium production detection, improved cross sections for actinides, fission products, and activation of structure materials are needed, along with fission product gamma emission energies and intensities. For near-field detection, the needs are radiative capture and inelastic scattering production data, correlated fission data evaluations, and stopping powers. For emergency response, improved gamma-production cross sections and radiative capture and inelastic neutron scattering data are needed. For safeguards, data are needed for spontaneous fission yields for ^{239}Pu and ^{240}Pu, multiplicity distributions for spontaneous fission, and neutron energy distributions. For ground-based nuclear detonation detection, x-ray and conversion electron branching ratios for select Xe isotopes are needed, along with half-life experiments to confirm accuracy. Finally, the nuclear data needs for forensics include short-lived fission products, activation products, and cumulative fission product yields for major and minor actinides.

- **Defense Threat Reduction Agency (DTRA)** – modeling and simulation tools, sensors and software to locate and identify threats, and technologies to monitor and characterize nuclear detonations.

- **Office of Experimental Science (OES)** – experimental measurements are a continued need due to the limit of first-principal theories for nuclear physics, and currently OES supports measurements in fission properties, fission product yields, reactions on unstable targets, and neutron scattering.

- **Advanced Simulation and Computing (ASC)** – accurate experimental data for evaluations, improved theory capabilities, robust uncertainty quantification, validation and verification, and modern processing and data structures, all to benefit the nuclear data pipeline.

- **Nuclear Criticality Safety Program (NCSP)** – cross section and other nuclear data on ^{233}U, ^{235}U, ^{238}U, ^{237}Np, ^{239}Pu, ^{240}Pu, Pb, Fe, ^{35}Cl, Zr, Hf, Ta, as well as thermal scattering laws.

- **Office of Nuclear Energy (NE)** – nuclear data for the unique materials needed in advanced reactors, including sodium, molten chloride or fluoride salts, lead, grafphite, UZr, UN, SiC, and stainless steel.

3.2 International Collaborators

Michael Fleming, Head of the Data Bank, discussed the nuclear data applications and needs of the Nuclear Energy Agency (NEA). The next stakeholder meeting will be held in 2023, the first since 2019, which will consider topics including advanced reactors/fusion, materials modeling, source facilities, waste and handing, and medical applications/isotopes. He discussed target accuracy requirements that have been updated through the Working Party on International Nuclear Data Evaluation Co-operation (WPEC). They are also working on more direct and automated links between data development and end users.

3.3 Nuclear Data Pipeline Talk

Dave Brown, from BNL, gave an overview of the nuclear data pipeline. The pieces of the nuclear data pipeline include experiment, theory and evaluation, data processing, transport codes, benchmarking, the end user, and sensitivities/uncertainty studies that provide feedback from the users to the rest of the pipeline. It is not uncommon that some end users do not understand the nuclear data that is included in their application codes or do not know the limits of the data, therefore it is particularly important to get the highest quality data to the end users. The pieces of the nuclear data pipeline are coordinated through the Cross Section Evaluation Working Group (CSEWG). The importance of all pieces of the pipeline were highlighted.

3.4 FOA-Funded Project Overviews

On Thursday morning, there was an overview of currently funded projects from past FOAs. These overviews were an informative view of the solutions to nuclear data needs that had previously been identified by the NDIAWG and prompted plenty of further discussion.

4 Highlights and Recommendations from the Roadmapping Sessions

Detailed session summaries written by the session co-leads are found in the appendices.

4.1 Gamma-ray Strength Functions and Level Densities

The session contained focused discussions on specific research applications of gamma-ray strength functions and levels densities, for example, Hauser-Feshbach calculations (Monte Carlo or deterministic) and neutron-capture cross sections calculations, astrophysical network calculations, radiation transport simulations, calculations of the gamma-ray heat in reactors, and the reactor antineutrino problem. This session focused on:

- Current nuclear data gaps in astrophysics
- Conduct a roadmapping discussion identifying actionable work to address current gaps.

The nuclear data needs that were identified by the community and future recommendations were:

- Development of an Evaluated Statistical Properties library/database
    - Preferred gSF/NLD models based on reaction of interest
- Understand the underlying nuclear structure that drives gSF behavior (e.g. low-energy upbend, pygmy resonances, M1 enhancements, etc.)
- Determine the dependency of gSF & NLD on deformation, mass, neutron/proton number and integrate these dependencies into predictive models/codes
- Determine/understand the limitations of the Brink-Axel hypothesis
- Development of targeted experiments to resolve theorical calculation disputes for key nuclei
- Can determined trends be used to inform ML/AI algorithms to advance predictive capabilities?

4.2 Fission Product Yields: Where We Are, Where We're Headed

Significant investment into improved measurements and theory combined with both national and international collaboration currently leading to the first US re-evaluation of fission product yields on the 30th anniversary of England & Rider's release of ENDF-349. The enhancements in the fidelity and quality of fission product yield measurements and theory as a function of incident neutron energy was a dormant art before this investment. This session will review the historical needs that drove this investment to re-assess fission product yield data, their applications, and user data needs to identify what next steps in this focal area should be. Emphasis will be placed on the value of this data on reactor decay heat calculations, reactor fuel inventory estimates, and national security needs. This session focused on:

- What steps have been accomplished thus far addressing these needs?
- What applied needs remain unmet?
- What future steps are needed to close the gap on past, current, and future needs for improved fission product data?

The community identified the following nuclear data needs and made the following recommendations:

- We need realistic target uncertainty guidance from users to help guide experimental efforts when determining fission product yields.
- Make efforts to include covariance uncertainties when performing measurements and providing data to theorists so they can include covariant uncertainties when modeling fission product yields.
- Branching ratios are a problem in many isotopes. The nuclear data is likely incorrect in many circumstances which can be seen when comparing FPYs determined for a single isotope from its emitted gamma-rays.
- Care must be taken when modeling is applied to map fission product yields across incident neutron energies. Specifically, the ranges from thermal to fission spectrum neutrons and then up to 14 MeV incident neutrons.
- Rabbit systems coming online at multiple facilities will enable shorter FPYs to be measured and this will help correlate independent fission product yields to cumulative fission product yields. This will help constrain theory and allow experimental constraints to be applied to measurements, ie: independent yields should add to cumulative for a mass chain.
- The experimental and theory community should be more tightly coupled with NNDC evaluator and database community.

4.3 Isotope Production

The isotope production landscape has changed significantly over the last four years, both because of the war in Ukraine as well as additions from new commercial suppliers in the medium energy proton range and with electron accelerators. This session checked in with the 2018 speakers for a status update and an assessment of the changes in needs across the isotope production field. This session focused on:

- Status of isotope production data at the labs & universities
- What has been achieved since 2018
- Where do we go heading forward for Isotope production in a changed landscape?
- What are the needs to improve robustness of measurements?

The community identified the following nuclear data needs for isotope production:

- Cross sections for charged particles, including for protons up to about 200 MeV and other light ions up to about 30-50 MeV, with a fidelity goal of less than 5%; this information should be stored in a reliable, evaluated repository.
- The spectra of Meitner-Auger emitting radionuclides should be measured.
- The structure of near-stability isotopes should be measured to produce higher fidelity data, including decay data such as lifetimes and branching ratios.
- The ability to train and retain experts in creating targets, especially high-purity radioactive targets with well-defined thicknesses.
- Accurate charged particle stopping powers.
- Traineeship and graduate programs, which provide a pathway for students, should continue to be funded.
- Expanding the use of universities for producing small quantities of emerging and "bespoke" radionuclides for R&D.

4.4 Processing and Preservation

This bi-modal session will start with a discussion about expanding data availability and the rapidly evolving computational landscape. New computing architectures and simulation approaches require changes in nuclear processing and formatting to support new methods. Discussions about data preservation will follow in the afternoon. Sophisticated datasets are seldom mined for all their richness and often analyzed with a focused goal and then shelved. This is inefficient, both intellectually and financially. A newly issued OSTP memorandum will require data underlying federally funded research to be made “freely available and publicly accessible by default at the time of publication.” This session will focus on:

- What does the future of nuclear data processing look like?
- How do we address data curation, preservation, and sharing?
- What improvements are necessary to completely preserve modern datasets?

From the processing half of the session, the following technical areas were identified as requiring further investment:

- Adapting to new evaluated representations and formats,
- Making use of nuclear data effectively on high performance computers,
- Creating robust and well-maintained tools for processing beyond criticality, including quantities such as:
  - Depletion and decay heat,
  - Energy deposition and materials damage,
  - Thermal scattering and unresolved resonance processing,
  - Photonuclear and charged particle transport, and
  - Fusion systems and isotope production,
- Propagating nuclear data uncertainties from evaluation to application, and
- Improving consumer-facing tools for interacting with data.

From the preservation half of the session, the following topics were highlighted as requiring further discussion

- What is the cost increase for an experiment from the archiving requirement and who bears this cost?
- What are reasonable embargo periods for data?
- What aspects of an experiment need to be preserved?
- Can data be developed in a common format to allow some uniformity amongst similar experiments?
- For NNSA laboratories, how will data undergo review and release procedure

5 Conclusions and Next Steps

WANDA2023 was very successful in bringing together nuclear data producers, evaluators, users (including those from national labs and universities), and federal program managers to discuss cross-cutting nuclear data needs and the effort required to address those needs. Over 170 people were in attendance at WANDA2023 over the course of the week, and this report overviews the presentations and discussions that were had during the meeting, as well as addressing the recommendations of the community for nuclear data needs for gamma-ray strength functions and level densities, fission product yields, isotope production, and nuclear data processing and preservation.

Following other non-technical discussions stemming from previous WANDA meetings, there is a continued desire to broaden the reach of WANDA, both to more federal programs (outside of the few who typically contribute to the annual FOAs) and to more students and university contacts. There has been a growing participation in the WANDA meetings (although total attendance was lower in 2023 compared to 2022 because of the return of the in-person meeting), particularly from university faculty and students. Ways to increase this participation are still under discussion, and there will be a strong push for a poster session for students, postdocs, and early career faculty/staff at WANDA2024.

Due to the delayed writing of this report, at this time, WANDA2024 has already taken place. During the summer of 2023, a new WANDA co-chair was nominated and elected, and planning was well under way. A renewed federal interest in fusion science led to the targeted focus on this topic in the planning of WANDA2024, similar to space science applications being heavily prioritized during WANDA2021. For WANDA2024, plans for a poster session were included from the beginning.

6 References

[1] L.A. Bernstein, D. Brown, A.M. Hurst, J.H. Kelley, F.G. Kondev, E.A. McCutchan, C.D. Nesaraja, R. Slaybaugh, and A. Sonzogni, *Nuclear Data Needs and capabilities for Applications Whitepaper*, No. LLNL-CONF-676585, https://bang.berkeley.edu/events/ndnca/whitepaper (2015)

[2] Catherine E. Romano, *The Nuclear Data Working Group: Accomplishments and Future Plans*, Oak Ridge National Laboratory (2017)

[3] Nuclear Data Interagency Working Group/Research Program, DOE National Laboratory Announcement Number: LAB 17-1763, https://science.energy.gov/~/media/grants/pdf/lab-announcements/2017/LAB_17-1763 (April 26, 2017)

7 Acknowledgements

The organizers would like to thank Lisa Felker and Stacy La Pineda for their exceptional effort in handling the meeting logistics, both before the meeting – for the first in-person meeting since the beginning of the COVID-19 pandemic – and during the meeting. They would also like to thank Isabel Hernandez, Joseph Gordon-New, Soren Cheng, Maksat Kuatbek, Chad Lani, and Stefania Dede for their service as rapporteurs during the workshop.

Support for WANDA2023 was provided by the NDIAWG.

This work was performed under the auspice of U.S. Department of Energy by Los Alamos National Laboratory under Contract 89233218CNA000001, Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344, and Lawrence Berkeley National Laboratory and the U.S. Nuclear Data Program under contract DE-AC02-05CH11231. Pacific Northwest National Laboratory is operated by Battelle for the U.S. Department of Energy under Contract DE-AC05-76RL01830. This work was additionally was supported by the Office of Experimental Sciences Campaign 4, National Nuclear Security Administration, US Department of Energy through Los Alamos National Laboratory.

8 Acronyms and Abbreviations

Acronym	Definition
ASC	Advanced Simulation and Computing
BLIP	Brookhaven Linac Isotope Producer
BNL	Brookhaven National Laboratory
CRP	Coordinated Research Project
CSEWG	Cross Section Evaluation Working Group
DANCE	Detector for Advanced Neutron Capture Experiments
DFT	Density functional theory
DICER	Device for Indirect Capture Experiments on Radionuclides
DMP	Data management plan
DOE	Department of Energy
DTRA	Defense Threat Reduction Agency
EB	External bremsstrahlung
ENDF	Evaluated Nuclear Data File
ENSDF	Evaluated Nuclear Structure Data File
FAIR	Findable, Accessible, Interoperable, ReUsable
FAM	Finite amplitude method
FOA	Funding Opportunity Annoucment
FPY	Fission Product Yield
FRIB	Facility for Rare Isotope Beams
FY	Fiscal year
GENESIS	Gamma Energy Neutron Energy Spectrometer for Inelastic Scattering
GNDS	Generalized Nuclear Database Structure
gSF	Gamma-ray strength function
HIPPO	Horizon-Boradening Isootpe Production Pipeline Opportunties
IB	Internal bremsstrahlung
IAEA	International Atomic Energy Agency
INL	Idaho National Laboratory
IP	Isotope Production
IPF	Isotope Production Facility
KERMA	Kinetic energy released in materials
LANL	Los Alamos National Laboratory
LANSCE	Los Alamos Neutron Science Center
LBNL	Lawrence Berkeley National Laboratory
LET	Linear energy transfer
LLNL	Lawrence Livermore National Laboratory
MAE	Meitner-Auger electron
MiND	Micro-caorimeters for Nuclear Data
NCSU	North Carolina State University
NDIAWG	Nuclear Data Interagency Working Group

Acronym	Definition
NDWG	Nuclear Data Working Group
NEA	Nuclear Energy Agency
NNSA	National Nuclear Security Administration
NLD	Nuclear level density
NP	Nuclear Physics
NSAC	Nuclear Science Advisory Committee
OES	Office of Experimental Science
OSTI	Office of Science and Technology
PET	Positron Emission tomographys
PFNS	Prompt fission neutron spectrum
PID	Persistent IDentifiers
PNNL	Pacific Northwest National Laboratory
PuRe	Public Reusable Research
QA	Quality assurance
QRPA	Quasi-random phase approximation
R&D	Research and Development
RHIC	Relativistic Heavy Ion Collider
SPECT	Single-photon emission computed tomography
TAMU	Texas A&M University
TENDL	TAYLS Evaluated Nuclear Data Library
UBA	Univeristy of Alabama, birmingham
UIN	University Isotope Network
USNDP	United States Nuclear Data Program
UWM	University of Wisconsin, Madison
WANDA	Workshop for Applied Nuclear Data Activities
WPEC	Working Party on International Nuclear Data Evaluation Co-operation

Appendix A Detailed Roadmapping Session Summaries

In this appendix, we provide the detailed summaries of each of the roadmapping sessions that were written by the session co-leads.

8.1 Gamma-ray Strength Functions and Level Densities

The gamma-ray strength functions and level densities session is summarized in detail below and was organized by:

- Stephanie Lyons, PNNL
- Gencho Rusev, LANL

The WANDA 2023 Session on Gamma-ray Strength Functions and Level Densities was organized with an introductory talk, nine contributed talks, and two discussion sections. The introductory and contributed talks covered both experimental and theoretical efforts including: an overview of the applications of the statistical model, sensitivity of calculated cross sections to gamma strength functions and level densities and their uncertainties, and experimental and theoretical methods to measure and calculate these quantities.

The gamma-ray Strength Functions (gSF) and the Nuclear Level Densities (NLD) are building blocks of statistical model calculations, such as for calculating reaction rates where no experimental data is available. The gSF describes probability that a gamma-ray will be emitted from an excited state within the nucleus. Within statistic model codes, such as TALYS [Kon2008], there are typically several gSF options that are available to use when performing calculations. The NLD is defined as the number of levels expected per MeV within the nucleus. Again, there are typically several different options within the model codes for this parameter such as the Fermi Gas Model and Constant Temperature Model. Therefore, while we can obtain the discrete levels for many nuclei close to stability from evaluated databases, such as ENSDF, statistical model properties (gSF and NLD) describe the excitation energies beyond the discrete states in the quasi-continuum and continuum. However, without experimental benchmarks to help define accurate model parameters, calculations can be “tuned” using the variety of options for these underlying physical parameters, which can lead to orders of magnitude of variation within the result.

gSF and NDL are key to reaction modeling and indispensable for applications because the statistical model is implemented in codes used for the evaluation of nuclear data. The cross-section calculations are highly sensitive to gSF and NDL as well as the gamma-ray emission from excited states. In addition, the cross-section calculations use an optical model, which is known to be accurate for nuclei near the valley of stability but may not describe more exotic regions of the nuclear chart. There is a strong demand from applications, such as neutron-capture cross sections, reaction network calculations, fission gamma-ray spectra, data evaluation, etc., to extrapolate data and benchmarks for gSF and NLD to neutron-rich and deficient nuclei.

8.1.1 *Improving a theoretical understanding:*

Many applications require (n,n’), (n,2n), (n,g), and (n,n’g) reaction rate information. The reaction rates for these cross-sections are typically evaluated using Hauser-Feshbach calculations that rely on optical models, NLDs, and gSFs. While the optical model near stability is well studied and includes uncertainty quantification [Pru2023], newer microscopic versions are under development. As already described, calculated cross-sections may be highly sensitive to the NLD and gSF parameters and therefore calculations can be unreliable without adequate constraints. Figure 4 shows the significance of the NLD and gSF uncertainty on reaction rate calculations. The NLD is shown to have higher impact on nuclei close to stability (red regions), whereas the gSF has a higher impact farther from stability (blue regions) [Nik2020].

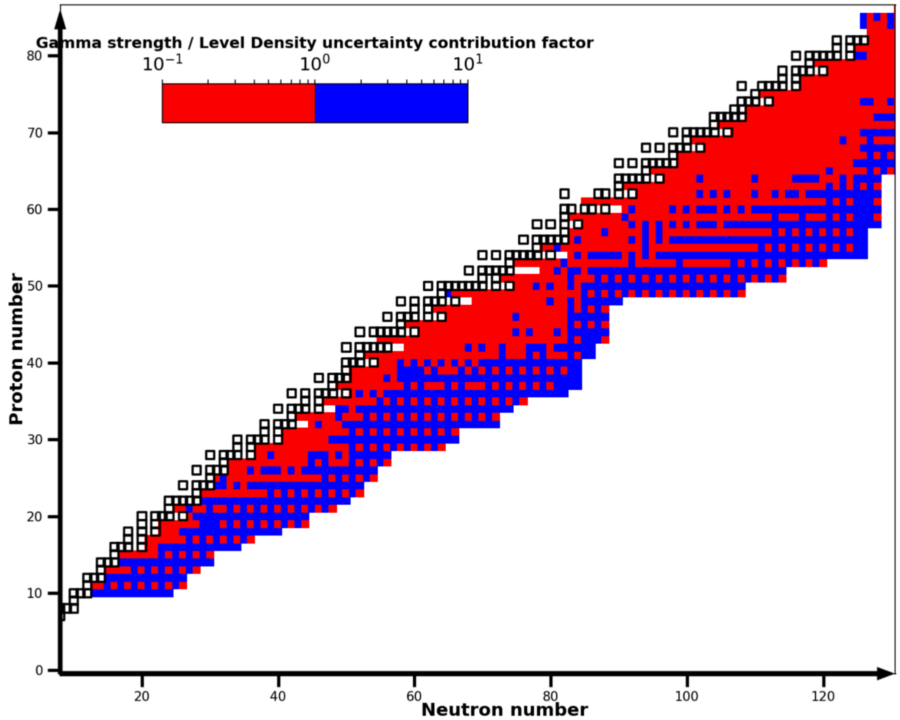

Figure 4. Table of isotopes, whether the gSF or NLD model dominates in the contribution to the variation of the reaction rate. The color bar values greater than 1 (blue) correspond to the gSF dominating, while values less than 1 (red) correspond to NLD dominating the uncertainties. Figure from Nikas et al. (2019).

At present, a variety of compilations, databases, as well as direct and indirect constraints are available for evaluators to use. The Reference Input Parameter Library (RIPL-3) and Photon Strength Function Database are common starting points, with adjustments being made to reproduce the desired quantities. Some constraints that are used are the discrete-level density, resonance spacing parameter (D0), and the radiative width (<Γγ>). However, measurements of D0 and Gg are only available for stable isotopes. Gathering experimental constraints for statistical properties for nuclei beyond stability requires the use of indirect measurement techniques, which are described further in the next section. However, there are experimental limitations which, therefore, require an advanced theoretical understanding of the underlying nuclear structure and reaction theory. There are several experimentally observed phenomena, such as the low-energy upbend [Sei2017, Ren2016, Wie2012] and scissors dipole resonance [Kro2012], that could be theoretically determined through further study. Figure 5 shows some of the gSF

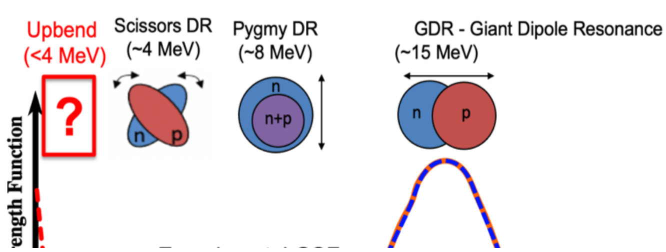

Figure 5. Gamma-ray Strength Function phenomenon relative to the Standard Lorentzian Function used to describe the Giant Dipole Resonance. Several observed phenomena are shown along with the typical observed signature. (Courtesy of A. Ramirez)

features that has been observed through experimental determinations of the gSF. It demonstrates the deviation at lower energies from the Standard Lorentzian Function typically used to describe the Giant Dipole Resonance. How might these features stemming from resonances that are tied to structural components be implemented within model calculations?

Recent advances in nuclear theory could enable the development of further predictive power of statistical quantities. Shell model calculation developments have provided microscopic predictions for NLDs and gSFs [Kar2020, Gor2023]. Performing informed truncations of the model space and leveraging the increased capabilities of modern computers has increased the reach of shell model calculations. For example, the moments method was developed to reduce the computational need to compute and diagonalize the Hamiltonian over the full model space of interest [Sen2016]. The moments method should be applicable to any model space for which an effective shell model Hamiltonian is available. The challenge for this technique is in the implementation, as it would be a complex process to insert the moments methodology NLD calculations into tables or reaction codes. Additionally, as stated, it requires an effective shell model Hamiltonian to be defined, which for more exotic nuclei would require further development.

Theoretical models of electromagnetic processes are also required to make reliable predictions and interpret experimental results that look at photon data, which touches almost every aspect of nuclear physics. Part of the broader framework of nuclear density functional theory (DFT) is linear response theory and quasi-random phase approximation (QRPA). Linear response theory is currently the only approach that predicts electromagnetic observables across the entire nuclear chart [Sch2015]. Using perturbation operators for characteristics of the various physical processes, there are two methods available: direct calculations, requiring a large, dense diagonalizable matrix, or the finite-amplitude method (FAM), which solves for the strength function directly [Avo2011, Nak2007]. While FAM is computationally far less expensive than performing the full diagonalization, it doesn’t offer direct access to the excited levels or wavefunctions that fully describe the interaction. Combining these methods with QRPA methods, that have been the cornerstone of photon data and beta-decay evaluations for many years [Mar2016, Mol2019, Nom2020], would provide the capability to compute the linear response fully and consistently across the nuclear chart. This improvement could significantly improve uncertainty quantification for evaluations.

Further theoretical development to provide deeper understanding of the underlying nuclear structure/reaction theory and how it impacts the gSF and NLD is needed. The development should address specific questions and identify relevant experiments to benchmark against. The theory should provide a microscopic understanding of the gSF, explain the gSF dependence on deformation, mass and neutron numbers, and study the limits of the statistical model assumptions. The theory should also study the impact of deformation to NLD and the NLD dependence on the spin and parities of the states. It is also important the reaction models to describe non-statistical effects in addition to the statistical. These improvements should be validated or benchmarked with targeted experimental efforts.

8.1.2 *Advancements to determine statistical properties:*

In order to further nuclear theory developments for statistical properties, a variety of experimental methods, both new and established, are required to provide necessary validation and benchmarking data. Much of the required (n, n’), (n, 2n), (n, γ), and (n, n’γ) reaction rate information that is necessary for many applications cannot be directly accessed by traditional experimental method, and therefore is determined by statistical calculations that are not validated near the region of interest. These calculations are also used for nuclear data evaluations, making the benchmarks critical to establishing reliable databases for use in a variety of applications.

There are several established approaches to determining the necessary parameters to describe the NLD and gSF. Traditional methods of neutron-capture and neutron-transmission experiments can access the neutron resonance parameters at the neutron-separation energy and nuclear resonance fluorescence can be used to determine gamma strength at lower energies. Current state-of-the-art instrumentation exists for these methods at Los Alamos National Laboratory. The Detector for Advanced Neutron Capture Experiments (DANCE) [Rei2004] and Device for Indirect Capture Experiments on Radionuclides (DICER) [Sta2022] can be used to determine neutron capture and transmission rate, respectively, which can then be used in simultaneous R-Matrix calculations to provide necessary data to determine NLDs and gSFs. Neutron resonance parameter measurements can provide average resonance spacing for several different spins to provide an understanding of D0 and $\langle \Gamma\gamma \rangle$. These measurements can be used to test or constrain NLD assumptions that are used in indirect techniques, such as the Oslo Method. The NLD can also be determined from particle evaporation spectra. The particle evaporation technique probes the NLD over larger spin and excitation energy intervals compared to neutron resonance data and is a completely model independent method. Results demonstrate consistency with neutron resonance models [Voi2012] for some nuclei and contain large disagreement with others [Voi2019]. Understanding the reason for this disagreement can improve accuracy of level density modeling.

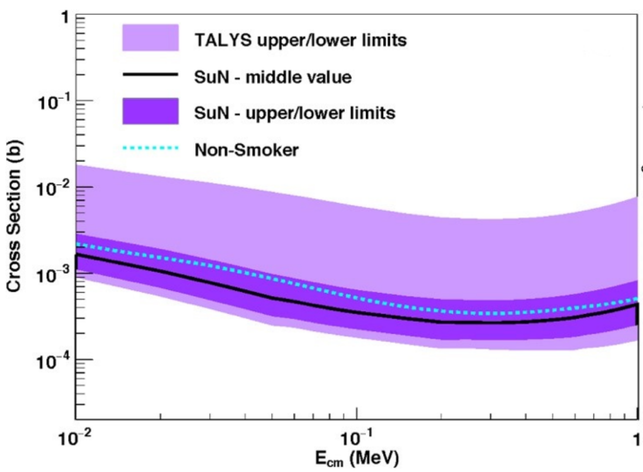

Figure 6. The $^{68}Ni(n,\gamma)^{69}Ni$ cross section uncertainty constraint (dark purple) compared to the uncertainty from Hauser-Feshbach statistical calculations (light purple) and Hauser-Feshbach code Non-Smoker [Spy2017].

In recent years, several techniques focused on the determining (n, γ) cross-sections for short-lived nuclei have emerged. As both reaction participants (isotope of interest and the neutron) do not make suitable targets, indirect techniques have been developed to provide the much-needed data to improve predictions from theoretical calculations. The surrogate [Ciz2007, Esc2012] and β-Oslo methods [Spy2014, Lid2016, Lar2018] will be described as examples, but are just two of the many existing indirect techniques. The surrogate technique substitutes the reaction of interest with an alternate, easier to experimentally access reaction that populates the same compound nucleus [Esc2012]. It is expected that the formation and decay of the compound nucleus are independent of each other to the first order, so the information gained from observations of the compound nucleus decay also provides information for the reaction of interest. Recent work has been done to establish (d,pγ) reactions as a viable surrogate for (n,γ) reactions [Esc2012]. The method was validated using the ^{95}Mo(d,p) reaction as a surrogate for ^{95}Mo(n,γ) [Rat2015, Rat2019].

Another indirect reaction method is the β-Oslo method [Spy2014, Lid2016, Lar2018]. This technique uses the β-decay of short-lived radioactive nuclei to populate high-lying excited states in the compound nucleus of interest. The subsequent de-excitation is measured in a segmented total absorption spectrometer that is sensitive to both individual γ–rays and the total energy emitted. Analysis of these data enables extraction of the NLD and gSF [Spy2016]. These quantities are then used to constrain the Hauser-Feshbach calculations and have been shown to reduce the cross-section uncertainty by orders of magnitude, as shown in Figure 6 [Lid2016]. The β-Oslo method requires several assumptions, which are actively being worked towards resolving. One area that has recently been improved is the normalization of the gSF. The novel analysis method, or Shape Method, uses a pair of states with the same J^π in the compound nucleus to iteratively scale or stitch together a series of data points from various initial energies to create an independent normalization for the gSF. Further efforts to compare the resultant reaction rate determinations from the surrogate method and β-Oslo method are needed as the two techniques offer different advantages which can be used to further our understanding the NLD and gSF across the nuclear landscape and help understand potential systematic uncertainties within each technique.

Research and development efforts are necessary to improve our understanding and the morphology of NLD and gSFs across the nuclear chart. These statistic properties are the backbones of statistical cross-section codes that used for nuclear data evaluation and employed in a variety of applications. Sufficient improvements will require both theoretical improvements as well as targeted experimentation to validate and benchmark those improvements. Systematic studies of these properties as a function of a variety of other nuclear properties such as deformation, mass, and neutron/proton number should be performed to better understand how these properties evolve through critical regions of the nuclear chart such as shell-closures, mid-shell closures, regions of shape co-existence. These types of comprehensive studies will enable thorough and integrated predictive capabilities to advance our capabilities in nuclear data evaluation and provide the most accurate cross-sections for applications.

Recommendations for future work:

- Development of an Evaluated Statistical Properties library/database
    - Preferred gSF/NLD models based on reaction of interest
- Understand the underlying nuclear structure that drives gSF behavior (e.g. low-energy upbend, pygmy resonances, M1 enhancements, etc.)
- Determine the dependency of gSF & NLD on deformation, mass, neutron/proton number and integrate these dependencies into predictive models/codes
- Determine/understand the limitations of the Brink-Axel hypothesis
- Development of targeted experiments to resolve theorical calculation disputes for key nuclei
- Can determined trends be used to inform ML/AI algorithms to advance predictive capabilities?

8.2 Fission Product Yields: Where We Are, Where We're Headed

This session was comprised of two, half-day sessions, broadly focused on the past, present, and future of fission product yield nuclear data and their applications. The session leads were

- Jason Harke, LLNL
- Sebastian Schunert, INL

Sessions II and III took place on Tuesday February 28th, 2023, lasted from 8:00 am to 17:00 pm, and included two discussion slots of about 1 hour each. The overarching theme of the session was to connect users and suppliers of fission yield data and to spur discussion that can be used to drive future funding decisions. This theme was motivated by the observation that the importance of fission yield data in the nuclear engineering practice is often not well communicated to the suppliers of nuclear data. Conversely, users of nuclear data are unaware of (1) what data is available and at what quality and (2) how fission yield data is measured and what uncertainties are attainable. Bringing the two groups together has led to a fruitful discussion on priorities for fission yield research that addresses the needs to advanced reactor engineering and nuclear security.

The session was roughly broken into two sub-sessions with the morning sub-session focusing on nuclear engineering applications – especially from the advanced reactor community, and the afternoon sub-session focusing on measurement, modeling, and data processing for fission yield data.

8.2.1 *Morning session*

Overview of LWR and Advanced Reactor Fuel Forms - Dr. Sebastian Schunert (INL)

Dr. Schunert introduced a taxonomy of reactor types and distinguished them by simple metrics: fuel form, moderator, coolant, spectrum, power density. Four reactor concepts (pressurized water reactors, sodium fast reactors, gas-cooled pebble bed reactors, and molten-salt fueled reactors) were described in detail. The importance of fission product yield data for nuclear reactors was highlighted by 4 examples: reactivity effects via Xenon pit, fuel-cladding chemical interaction, TRISO fission product retention, and decay heat.

Q/A:

- What is the most pressing need for advanced reactors? Answer: decay heat calculation, which can be brute force calculated with ORIGEN, but a decay heat standard is missing for most reactors.
- Concern of DPA calculations was voiced, stopping powers are poorly understood so DPA estimates are inaccurate.

Fission Product Yields: SCALE/ORNL Perspective - Dr. Jesse Brown (ORNL)

Dr. Brown highlighted the need for accurate fission product yield data for the SCALE code ORIGEN (Oak Ridge Isotope Generation). ORIGEN is a general-purpose code for tracking isotopic inventories that is utilized for reactor operations, spent fuel storage/handling, structural material activation, and fuel cycle analysis. Dr. Brown emphasized that fission yield data are paramount for computing decay heat after reactor shutdown. The accuracy of ORIGEN's predictions is determined by the accuracy of its data. For fission product yields, ORIGEN uses energy dependent data (thermal fission, fast fission, high energy fission) and yields are interpolated using the mean energy of neutrons causing fission. ORIGEN was validated against radiochemical assay experiments. The importance of this validation study is (1) ORIGEN can be used to validate fission yield data, and (2) validation highlights the need for covariance data.

Q/A:

- The plan of moving covariance data into ENDF was discussed.
- The validation methods for downstream codes like ORIGEN were discussed.

Importance and Needs for Fission Product Yields in Molten Salt Reactor Chemistry and Corrosion Modeling - Dr. Mauricio Tano (INL)

Dr. Tano focused on the impact of fission product yield data on modeling and simulation of molten salt fueled reactors. He emphasized that fission products play a fundamental role in the chemical behavior and corrosion of molten salt fueled reactors. Uncertainties in fission product yields significantly reduce the precision with which we can predict the redox behavior of fuel salts, the fission product concentration in the off-gas system, and the corrosion behavior. Dr. Tano notes that "data-informed experiments to reduce FP yield uncertainties are needed for improving the chemical behavior predictions of MSRs."

Q/A:

- What accuracy on FY data is needed for chemistry analysis? Presenter answered 10%.
- The fission yield uncertainties used for the presentation were determined using a simplified model.

"Accident Source Terms" (virtual presentation) - Dr. David Luxat

Dr. Luxat presented on the importance of fission product yield data for severe accident codes like MELCOR. Among other functions, MELCOR is used to predict radiological consequences of severe accident scenarios in light water and advanced reactors. Fission product yields are essential to compute the source term for MELCOR. MELCOR computes the fission product transport from the fuel into coolant, moderator and structural material and ultimately into the environment. Dr. Luxat emphasized that fission product transport is a highly nonlinear process that is influenced by solubility of fission products in liquid pools, fission product deposition on structures, and interaction of fission products. Therefore, uncertainties in fission product yields are much more problematic than for linear models. The radiological consequences of fission product release into the environment are a function of the fraction of the inventory released to the environment, the abundance in the reactor inventory, the half-life, and the radiobiological importance of particular nuclides. The radiological consequences are not obvious and require careful analysis.

Importance and Needs for FPY for fluid properties in MSRs (virtual presentation) – Dr. Theodore Besmann

Dr. Besmann's talk focused on molten-salt fueled reactors where fission products are present in the fuel-salt coolant during operation. Fluid properties (collective term for thermodynamic state and transport properties such as thermal conductivity) are essential for predicting the performance of molten-salt fueled reactors, but they depend strongly on fission products in the fuel salt. Dr. Besmann emphasized that it is essential to determine in which phase (gas, liquid, precipitate) a fission product is present for designing off-gas systems and assessing potential radiological source terms. Uncertainty in nuclear data creates uncertainty in the thermodynamic state of the system (e.g., the precipitation temperature and vapor pressure). As an example, 50% difference in molar fraction is shown to lead to an order of magnitude difference in vapor pressure predictions for some components. Vapor pressure is an important quantity in accident source term characterization in MSRs.

How Integral Benchmarks Benefit Fission Product Data via Data Calibration – Dr. Daniel Siefman

Dr. Siefman focused on how post irradiation examinations that are documented as benchmarks can be used to calibrate fission product yield data. The ideal set of benchmark data calls for a well characterized neutron source, a well characterized target, high precision fission product analysis, and a computational model with evaluated uncertainties that affect fission product production. Dr. Siefman proposes Marginal Likelihood Optimization for the data adjustment process because it decrease the influence of inconsistent integral parameters on the adjustment.

Q/A:

- The lack of experimental data for calibration of fission product yield was noted. Comments agreed that a lot more work needs to be done in this area. INL was mentioned as a place to perform this work.
- Characterization of neutron spectra was briefly discussed. Fast systems have extremely well-known neutron spectra, but data does not seem to be available.
- The appropriateness of activation foil measurement of neutron spectra for epithermal and thermal neutrons was discussed. Are activation foils and deconvolution enough or are new techniques required?

Covariance requirements in SCALE and effects for NRC – Dr. Will Wieselquist

Dr. Wieselquist emphasized the quest to quantify uncertainty for any best estimate computed with the SCALE code system. This maxim requires that nuclear data – including fission product yields – contain well quantified uncertainties. However, the joint probability distribution functions for nuclear data are not available, and instead only mean and some covariances are provided. As of ENDF/B-VIII.0, energy correlation of fission product yields, correlation among fission product yields and with decay data are missing. Dr. Wieselquist highlighted key data needs for the nuclear regulatory commission: any data with safety implication, data improvements must not deteriorate predictions for LWR fleet predictions, robust uncertainties for everything, no uncertainties present in thermal scattering laws and activation data. A smell test for covariance data is proposed. If there is a high probability that a realization is non-physical and/or inconsistent, then something is probably wrong, and it should be addressed.

IAEA activities on Fission Yield and expected outcomes" (virtual) – Dr. Roberto Capote

Dr. Capote gave an overview of fission product yield activities that the IAEA is involved in.

- First, he highlighted the coordinated research project on evaluation of fission yield of major actinides. The main scope of this project is **^{252}Cf(sf), n + ^{235,238}U**, **n + ^{239,241}Pu**, including energy dependence. This project contains an evaluation, theory, validation, and dissemination component.
- The TUNL-LANL-LLNL fission product collaboration investigates neutron induced fission of major actinides at 6.5 MeV, short-lived fission products from neutron-induced fission of ^{235,238}U, fission product yields from photon-induced fission of ^{240}Pu and neutron-induced fission of ^{239}Pu as a function of incident energy, and energy dependent fission product yields from neutron induced fission.
- The CEA/Cadarache-LPSC-ILL collaboration on the Lohengrin recoil detector produced new preliminary results on ^{235}U(n_{th},f).
- ^{252}Cf spontaneous fission yields at the FRS ion catcher (GSI).
- Measurement of independent fission product yields with SPIDER (LANL).
- CEA/NNL new evaluation for JEFF-4 was mentioned and technical details were provided
- A progress update on the United Kingdom fission yield data base was provided.
- A progress update on the ENDF reevaluation of fission product yield that is based on the combination of experimental data and model calculations via Kalman filter optimization.
- Benchmarking fission yields with beta decay data (and vice versa) performed at IFIC, CSIC – University of Valencia and ATOMKI Debrecen compares decay heat as a function of time for ^{235}U and ^{239}Pu computed with JEFF 3.1.1, JEFF 3.1.1+TAS with experiments by Tobias and Dickens. Sensitivity of burn-up, decay heat and anti-neutrino spectra to FPYs are highlighted.

8.2.2 *First discussion session*

The first topic discussed was the energy dependence of fission product yields. The question was brough up what the energy dependence means exactly. It was then noted that the 500 keV is mostly from assessment of Godiva, but other voices in the audience maintained that a typical fission spectrum is implied. The JEFF community representative noted that the JEFF community does not consider the energy values meaningful: "In the Robert Mills contribution to FYs, cumulative experiments were performed, and results were tuned to some fast reactor spectrum. There is no 400-500 keV mono-energetic spectra, that's physical nonsense." Dr. Wieselquist noted that NRC requested more energy resolution on fission product yields, and he said that interpolation is not performed between FY curves in different reactors, but a single curve is selected that fits the reactor best. It is unknown if 3 points are enough and maybe we need 10. A compromise was proposed to do some in-between energy step at around 100 keV. This should be sufficient for most applications because fission spectra do not change that much. An additional guidance is to clarify the meaning of energy dependence for fission yield and communicate that to users of nuclear data.

The second topic was cumulative versus independent fission yields. First, the definition of cumulative and independent fission yields was discussed. Big difference on uncertainties and how they are handled in ENDF and JEFF were mentioned. Reactor physics only cares about independent yields. The need for new measurement techniques and revision of existing measurements (best estimate and uncertainty) was discussed.

The third topic that was discussed is how accurate fission product yields have to be. The question was directed to Dr. Tano on what the needs for MSRs are. The uncertainty level required for MSRs was quoted as 0.1% for useful analysis. Experimenters responded that this level of accuracy is hard if not impossible to obtain. In general, there is no good guidance on what the uncertainty on fission product yields needs to be for downstream nuclear engineering applications. A sensitivity analysis should be performed that give guidance what the required uncertainty on FPYs should be for advanced reactors.

The fourth topic was that the audience agrees that the Rabbit needs to be put in working order at NSERC.

The fifth topic was that Thorium fission yields are unknown but required. There is an evaluation effort at MARCOS and LANL for thorium yields.

The sixth topic was salt irradiation analysis. It was asked if there have been salt irradiation experiments. It was noted that INL would be a suitable place to do it, but INL representatives did not have information if salt irradiation has happened.

Summary from the morning session:

1. Accurate fission product yields are important for a variety of reactor applications:
    - Decay heat
    - Molten salt fueled reactors: thermodynamic state & corrosion behavior
    - Fuel-cladding chemical interaction for sodium fast reactors (fuel lifetime limit)
    - Source term calculation/fission product retention
2. There is a need for a prioritized list of important fission products and how accurate we need to know them.
3. Need for providing and handling covariances/uncertainties of FPs
4. Need for targeted integral experiments for fission product yield benchmarking and calibration.
5. Energy dependence of FP yields (at least in part) driven by NRC request to ORNL's SCALE code

8.2.3 *Afternoon session*

FPY needs and requirements for libraires – Dr. Alejandro Sonzogni

The presentation largely focused on inconsistencies in databases and conflicting entries. Of note were ENDF uses Maeck's data where JEFF does not and that ENDF and JEFF FPYs don't agree within their uncertainties.

Major points made during the presentation to the community:

- Compatibility is an issue depending which library is used
- There is a need to maintain fission yields on a continuing basis and keep compatibility.
- Need to measure the Maeck data for validation.

- Using Maeck's data significantly influences correlations.
- ENDF calculates decay heat by average energy and not via the spectrum.
- Some calculations are based on theory and cannot be reproduced.
- Need new fission product yield measurements.
- Wants to reproduce ^{102}Y and ^{104} Nb.

LANL FPY theory and evaluation – Dr. Amy Lovell

Dr. Lovell provided an overview of fission product yield theory and evaluations and identified several areas that need improvement. A theme was a more complete understanding of experimental results so they could be reliably used to help theory and evaluations.

Using the fission fragment decay model for the calculations we have a lot of interesting input that further constrains the results. Energy dependance from thermal to 20 MeV which is taken into account in the models.

Modeling needs include:

- Need to know fission probabilities of multi-chance fission
- Fission fragment initial conditions
- Disentangle detector response from physics
- Properties of neutron-rich nuclei
- Optical model
- Level density
- Discrete levels
- Nuclear mass

Experimental inaccessibility hinders the models since the necessary info is not easily accessible. Theory and evaluation scientists need:

- Complete, curated databases
- Updated decay data (consistency from independent to cumulative FPY)
- Validation and benchmarking methods
- Correct/consistent documentation from experiments

Reasonable agreement with minimal tuning between the code and the experimental data.

- Need to understand the following to be able to make comparisons between models/predictive codes and experimental results.
- Fission fragments initial conditions are needed (hard to get, fission is quick so we get that after the fact through models)
- What assumptions are used?
- Detector disentanglement?
- Detailed uncertainties from experiments.

Microscopic fission models: State of the art and future opportunities – Dr. Nicholas Schunck

Microscopic fission models: use of nuclear density functional theory

- There are five different methods to do this
- Need to combine some methods to provide better description of the initial conditions and use as input to other models for better results.

Systematic calculations of fission product yields across the mass table for applications such as astrophysics or nuclear forensics:

- Neutron-induced fission: programmatic applications
- Spontaneous fission: programmatic and fundamental science (super heavy elements and astrophysics)
- Delayed fission: fundamental science (astrophysics)

● Longer term developments:

- A unified theory of fission that includes dissipation, fluctuations and collectivity is still needed
- Uncertainty quantification and propagation
- Use of machine learning? – built on top of the theory to facilitate the calculations (not redoing physics)
- We are predicting but also fitting on some instances
- Forward first – then go back and see what all the constraints are

Outlook

- More work to combine method to increase fidelity
- Systematic calculations of FPY across the mass table
- Unified fission theory
- Dissipation
- Fluctuations
- Collectivity
- Uncertainty quantifications and propagation

FREYA and Fission Yields – Dr. Ramona Vogt

Dr. Ramona Vogt gave a detailed update of the status of the FREYA code. FREYA covers the compound nucleus through beta decay.

Event-by-event is efficient for fission since there are so many outcomes. FREYA can be adapted to meet the needs of phenomena being studied (ie: cumulative fission yields).

Can be put into transport codes since its quick

FREYA can be used to determine:

- Branching ratios
- $T_{1/2}$
- Beta decay
- Nuclear mass
- FREYA is capable of working on cumulative yields with the introduction of beta decay
- physics

FREYA is adept at studying:

- Neutron emission
- Photon emission
- Neutron-photon correlations
- Spin related effects and correlations

FPY measurements at TUNL – Dr. Mathew Gooden

Where we started investigating yields:

- Energy dependency that appears in critical assembly data
- Discrepancies between assemblies

- For fission products there is no data between 2 MeV to 14 MeV
    - Goal was to fill in as much of the region as we could

● Can we get better than 20% spread in measurements for Nd?

TUNL – photofission – Dr. Calvin Howell

Dr. Howell gave an overview of recent photo-fission measurements and results from research at Triangle-University Nuclear Laboratory.

Used for cargo scanning
· Including fission and gamma induced neutrons
- Photofission for active interrogation purposes

· Uses HIGS and Time of flight to separate gammas from neutrons
· Can't measure cross-sections below 1 MeV
· Extrapolates from 1 MeV down
- Challenge is to push PFNS data analysis down to a minimum En of about 0.5 MeV

Differential Measurements of Prompt and Delayed Neutrons on
- Uranium-235
- Uranium-238
- Plutonium-239

FPY Beta-gamma branching ratios – Dr. Kay Kolos

Needs detailed info on decay for models
· Gamma intensity is used for FPY calculations and has error propagation
· Many long-lived isotopes have 3-30% uncertainties for the gamma intensity
· nuCaribu will open up for short-lived FP

Needs:
- Fission-product decay data
- γ-ray intensities
- Improvement on the FPYs evaluations
- new fission yields measurements → still poor beta decay information
- nuCARIBU → new opportunities for measuring short-lived fission products

Uranium gamma data needs for microcalorimetry at the IAEA NML – Dr. Geonbo Kim

High precision quantification with microcalorimetry.
· Great resolution below 300 keV
· Missing peaks in Ge detection of ^{233}U
· Can possibly be used to determine enrichment
· Large/unknown errors for $^{235}U/^{236}U$
· Need to improve nuclear data for safeguards
Questions
How tolerant is it the detector.
Not made to be in a radiation beam / us shaping time
Describe SOFIA
Talk later

Useful for auger elections and coincidence
No problem for measurements
How segmented is the detector system, 0.5 kg detector but loss of resolution
Detector can be biased, usually is not but can change the range to include/exclude auger electrons

SLFPY measurements at NCERC – Dr. Jeremias Garcia-Duarte

Need more study of the short-lived FF:
Branching ratios may be inconsistent in the nuclear databases
Need more work determining these branching ratios
Short lived fission product yields
Different isotopes after the fission – halflives microseconds to days
The results in the report are from the 50's – new campaign to measure SLFPY

Applications of Fission Product Yields & Other Nuclear Data at TerraPower – Dr. Tommy Cisneros

Fast spectrum needs
· There is salt corrosion and FPY are needed to better understand the process
· At high burnup there is FP crowding
· How does the salt properties change w/ added FP
· Better data will allow for more protection and estimates for dose rate of workers
· Need delayed neutron migration throughout the system
· ^{35}Cl(n,p) high priority needs
Develop a fast spectrum molten salt reactor – design experimental test reactor

- Get to grid scale high burnup reactor
- Uranium fuel – operate on the fast spectrum – low burnup – not too many fission products
- Need to develop the technology to work with fission products in the salt
- Uranium enriched salt – fuel polishing anticipated
- Need to be able to guarantee we have the ability to remove heat and continue operation
- Physical properties might change
- Data needed for estimation of the dose rate on workers and more protection
- ^{35}Cl(n,p) very very high in priority for data

Nuclear data needs for Plutonium accounting using microcalorimeters – Dr. Dan Becker

Want a non-destructive technique – gamma ray spectroscopy – germanium detectors

- Pixelated devices with good efficiency and excellent energy resolution
- Optimize the thermometer and the absorber independently based on requirements
- Need better reference data – not purely laboratory instruments
- You have to know the branching ratio to get the relative content of these elements
- Uncertainties in the branching ratio is the main issue for both detectors
- Specific gamma rays we need better branching ratios

Summary :

- Branching Ratios uncertainties limit isotopic analysis using gamma spectroscopy to ~ 1 % accuracy
- We've identified top candidates where better values would be useful
- Highest priority are absolute measurements of the "anchor" BRs

Maybe use conversion electrons to help with the branching ratio?
Would the efficiency of seeing the conversion electrons vs the x-rays be different?

Maybe we could exploit the knowledge of conversion electrons in some way?

Session III Discussion:

- We can do experimental covariances – what kind of experimental covariances can the experiments provide and what are we(theorists) looking to provide after? What do want the theorists to do?
- In the fission products there are no covariances in ENDF
- There is a compilation of covariances for actinides, simple derivation, what would you want for modeling?
- Need individual experimental yields then turn them to covariances
- In reactor physics we go to solve - make a lot of approximations – you lose a lot in the process – need high process computers – too many isotopes – physical meaningful results, how do we get them from simulations? Benchmark? One very high-performance model and use as a benchmark
- For reactor physics, too much to simulate, too many starting points. How many till you trust your low fidelity calculations? – need better data!
- Look at recent activity in the libraries – prioritize with the request evaluation ENSDF
- What does the uncertainty mean? (regarding the uncertainties they are requesting) If 10% is good enough?
- Uncertainty from 12% - 5% would be good, for plutonium we need below 0.5% uncertainty (is that feasible with the experiments?)
- We need a fast rabbit!!!! No color preference
- How do we share info between the communities? Put together a listserv – email Dave Brown! (NNDC) Or use twitter – ENSDF gives the new things coming in – companion database takes paper by paper and gets it in the correct format
- Updates in NNDC – twitter
- Branching ratios – the cross section uncertainty?
- Correlation measurements – is there any insight in any momentum state? Predictions? Constraints? Capability of correlations between fission fragments and neutrons? Not yet
- Cross sections, extreme lowest precision needed – need more reasonable goals, tuning the uncertainties to more attainable results
- With decay data measurements we can do it but it's hard with a neutron cross section
- Try to quantify this – but titanic undertakings
- Managing expectations so people don't give up… don't ask a theorist (in-jest)
- Sensitivity study needed

8.3 Isotope Production

The isotope production roadmapping session followed from a history of similarly themed sessions on isotope production and targetry. The session leads were:

- Etienne Vermeulen, LANL
- Andrew Voyles, UCB/LBNL

8.3.1 *General Session overview:*

Domestic isotope production is an incredibly dynamic landscape, changing to reflect advances in production pathways, as well as demand from research, clinical, and industrial applications in both the public and private sectors. Beyond what is normally seen, this field has changed significantly over the last several years, both because of the war in Ukraine as well as additions from new commercial suppliers in the medium energy proton range and with electron accelerators. This session aims to check in for an updated production assessment of the status of isotope production data at national labs & universities from the 2019 WANDA Isotope production session, determine what has been achieved since then, and combine this status update with an assessment of the changes in needs across the modern isotope production field. A particular emphasis for this session is on production capabilities and infrastructure and identifying what instrumentation and nuclear data needs are required to address the current needs of the field.

8.3.2 *Detailed summary section:*

Radioisotopes, together with surgery and chemotherapy, provide targeted diagnostic and treatment options in the battle against cancer. Historically, the vast majority of clinical applications of radionuclides have focused on diagnostic applications to locate and image the site of disease, namely, single-photon emission computed tomography (SPECT) and Positron Emission Tomography (PET), both of which rely on a steady supply of radionuclides on a national (and international) basis. In recent years, production of radionuclides for therapeutic applications have gained significant attention for their apparent efficacy in treating advanced disease — ^{177}Lu [Fend16] and ^{225}Ac [Krat16] having gained some of the most attention for applications in beta therapy and targeted alpha therapy, respectively. Beyond medical applications, domestic isotope production efforts are responsible for meeting the increasing supply demands of various stable and radioisotopes for research, industrial, and national security applications.

All of this research and work is built upon a network of trained personnel, students, and infrastructure, including accelerators, target fabrication, radiochemistry, and distribution. Domestically, much of this network is made up of the DOE Isotope Program's production and development sites, consisting of Argonne, Brookhaven, Idaho, Los Alamos, Oak Ridge, Pacific Northwest, and Savannah River National Laboratories, the Y-12 National Security Complex, University of Missouri, and the University Isotope Network (UIN), currently consisting of University of Alabama – Birmingham, University of Missouri, and University of Washington. Outside of the DOE Isotope Program (IP) portfolio, a number of other institutions are key collaborators for IP R&D, including University of Wisconsin – Madison, FRIB / Michigan State University, Duke University, Washington University – St. Louis, University of Utah, Texas A&M University, University of California – Davis, University of California – Berkeley, and Lawrence Berkeley National Laboratory. To this end, speakers were selected to cover as broad of a range as possible from amongst these institutions, with an emphasis on ensuring representation of each of the different production approaches used domestically, and focusing on highlighting the capabilities and needs of those facilities which have recently joined the DOE IP UIN.

This same focus on infrastructure and capabilities-related nuclear data needs was the primary goal of the corresponding session in WANDA 2019, with the relevant recommendations detailed in the final summary report [Bern19]. Given the vital role that domestic isotope production efforts play, it is imperative to perform an updated assessment of the extensive nuclear data needs for this work, in all portions of the nuclear data pipeline. As such, this session has provided a status update on the 2019 recommendations, as well as an updated assessment and recommendations for the highest-priority nuclear data needs for the current domestic isotope production landscape. Through this assessment, we wish to answer two guiding questions: where do we go heading forward for Isotope Production in a changed landscape, and what are the needs to improve robustness of measurements?

Status Update from WANDA 2019

A major focus of WANDA 2019 was the basic, yet important task of bringing together the users and producers of nuclear data from both the national labs, as well as universities – DOE IP, Argonne, Brookhaven, Lawrence Berkeley National Laboratories, and University of Wisconsin – Madison, University of California – Berkeley, Central Michigan University, University of Washington, Rutgers University, and Johns Hopkins Medicine were represented by the speakers. The overall goal for this year was to improve data for established isotopes, develop excitation functions for emerging ones and ensure that the gaps in the current body of data that is available are filled. To do so, each production site provided an overview of what production capabilities they offered, as well as an outline of their needs to meet upcoming production goals. Likewise, for those sites which utilize radioisotopes for applications, a list of relevant nuclear data shortcomings, "wish lists", and gaps was compiled.

Several high-level priorities were identified, with recommendations for funding proposed in the final report. Most broadly, all sites are in need of either improved or first measurements of production cross sections for established and emerging radionuclides. This includes excitation functions for production via charged particles (both protons and other light ions), fast neutrons, and photonuclear reactions (including activation cross sections for converter materials). Much work has been published since then (particularly for energetic protons), and the body of cross section data continues to grow as IP research groups perform targeted measurements where data are needed, with photonuclear cross section measurements at ANL having expanded significantly since 2019. This recommendation is not a need which can be fixed immediately but requires persistent, sustained effort to continually measure high-priority cross sections for the application community, until better predictive tools are available. One success story on this front is that of the TREND collaboration [Fox21a, Fox21b], which was formed as a result of NDNCA/WANDA [Bern15] and is still measuring high-priority cross sections across the full range of proton energies accessible within the DOE IP system. Likewise, the previous year's session identified a clearly articulated need to generate an evaluation of high-energy charged particle induced reactions important for radioisotope production, either as part of ENDF or through the creation of a new application-specific library for IP users. In recent years, the IAEA has led a Coordinated Research Project, "Nuclear Data for Charged-particle Monitor Reactions and Medical Isotope Production" (F41029), to accomplish this [Herm23, Engl19], but the recommended cross sections they provide are a statistical average of a down-selected subset of data from EXFOR [Zerk18], rather than a formal nuclear data evaluation guided by physics models. The user community continues to request such an evaluated database for isotope production, and despite calls for such an effort in every year of WANDA to date, no such effort has yet been funded. Given the required scope for the project, it is imperative that a funding model be identified, likely including interagency support, given the cross-cutting needs and benefits it would offer. As research groups continue measuring production cross sections to enable such an evaluation, it is important that the groundwork be laid as soon as possible. Development of additional target fabrication capabilities and training in this work was also identified as a high-level need, one which is still outstanding, and was a focus area for WANDA 2020 [Roma20]. Likewise, an improvement in charged-particle stopping powers was brought up by multiple parties and even had its own session at WANDA 2019. Despite this, and the renewed importance of this topic for space applications (which has been covered as a topical session for several WANDA workshops since then), no significant efforts have yet been carried out to address this need. Finally, given their role both for therapeutic and theranostic applications, the need for improved clinical dosimetry, and measurements of the electron spectrum for Auger electron-emitting radionuclides was brought up as a repeated need. This is still an outstanding issue, and one with some early results presented in the current year's workshop.

Summary of current needs

Cross Sections

Far and away, the most universal nuclear data need for the isotope production community is an expansion of cross sections for the production of medically relevant (and other) emerging and established radionuclides, as well as beam monitor reactions, a topic which has been highlighted in nearly every year of WANDA to date, as well as the NDNCA precursor workshop. Unlike many other nuclear data needs, the need for cross sections presents far more of a broad scope need, given the wide variety of incident beams and energies used by the isotope production community. This is additionally compounded by the fact that, unlike many other application areas, isotope production has needs for not just cross sections for the channel of interest, but nearly all other energetically accessible channels as well, for the purposes of quantifying the production of *all* impurities and/or contaminants. In many ways, the nuclear data community and funding needs to treat the needs of IP in the same approach as data needs for reactor burnup/depletion or astrophysical/stellar nucleosynthesis applications – efficient, economical, and reliable isotope production has a functional need for "everything" in terms of reaction channels, not just the channel of interest. For stable isotope production cross sections, the use of in-beam, prompt-gamma spectroscopy measurements appear to be one compelling option, especially if traditional tools for quantifying stable isotopes (such as ICP-MS) are not available.

A comprehensive list of reactions was captured by Dr. François M. Nortier (Meiring) in 2017, which formed the basis of DOE IP's funding of nuclear data in the intervening years, but these capture only one subset of domestic IP needs, a list which is continually evolving. In general, several broad sets of cross section needs have been identified in this year's assessment, encompassing the overall field. Energetically speaking, energy-differential cross sections are needed for reactions induced by charged particles (protons up to ~200 MeV, but particularly above 30 MeV, and light ions [up to at least ^{7}Li] up to ~30-50 MeV/u), neutrons (both primary and secondary neutrons created through primary reactions), and photonuclear reactions (both for production as well as reactor heating). Photonuclear data are becoming increasingly important, as the potential of intense electron-linac bremsstrahlung sources appear to be growing in role within the IP landscape for novel production pathways. There are primarily data gaps for emerging radionuclides, particularly for reactions using enriched isotope targets. However, a wide variety of research and industrial isotopes require cross sections as well, as well as for exploring alternative pathways of established medical radionuclides. In performing measurement campaigns, <5% uncertainty in cross sections has been recommended as a general fidelity goal, both for informing production modeling, though different facilities and applications will have varying sensitivities by necessity. As cross section data are needed for accurate prediction of isotope production, cross sections for any and all impurities (unwanted isotopes co-made with the desired ones) are also required to be reported, as this helps define the problem space, inform shipping/shielding requirements, and guide modeling and evaluation. It is important to note that contaminant radionuclides have been the primary focus historically, but current needs also require cross sections for the production of stable isotopes as well. This is particularly relevant where high specific activity production is needed, as any stable isotope production of the product element will compete with labeling of the desired product. Increasingly, as production takes place on heavy element targets at 100 MeV+ energies, measurements and modeling of (p,f) have become a vital need, as the fission products will create significant issues for meeting QA standards in production. Similarly, the stacked-foil approach [Fox21a, Fox21b] has been shown to be an invaluable tool in producing cross section data over a wide range of energies, and the Curie [Morr20] toolkit developed by Dr. Jon Morrell offers a convenient set of spectroscopy and irradiation planning tools to assist in the interpretation of such datasets. However, the 100+ MeV measurements by the TREND collaboration have made it clear that the substantial secondary neutron flux seen at these high-energy accelerator facilities not only is a concern for safety and impurity co-production but will incorrectly suggest an enhanced cross section above approximately 100 MeV for reaction channels which can alternatively be populated by (n,2n)/(n,3n), in addition to the (p,xn) route via the primary proton beam.

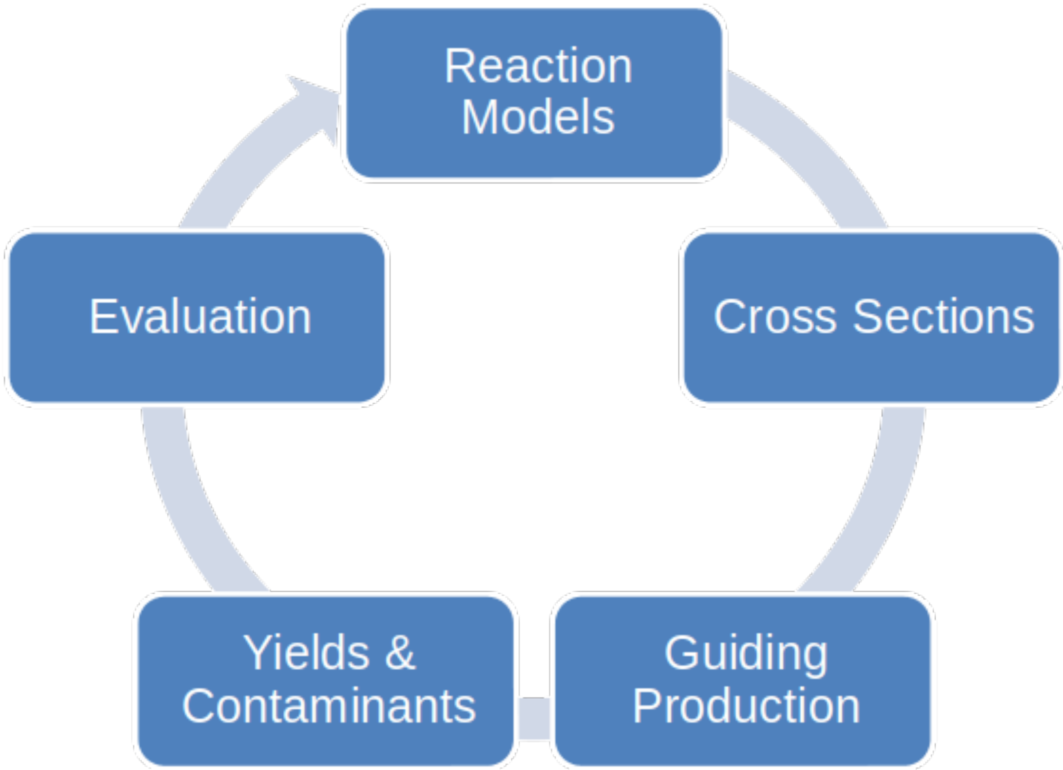

Figure 1: Nuclear data needs for production cross sections follow a set of circular dependencies. Predictive capabilities for estimating unmeasured reaction cross sections require robust and evaluated cross section and yield data, but the process of reaction evaluation requires these same predictive codes. Supporting cross section measurements is thus indispensable in improving our predictive capabilities.

A full list of reactions in need of additional cross section data is an ever-changing task, and one that cannot be fully captured in this summary. However, several radionuclides were mentioned in discussions as high-priorities, and should be considered for facilities which could support such measurements: cross sections are needed for production of ^{43,47}Sc, ^{44,45}Ti, ^{56}Ni, ^{134}Ce, ^{149,54,155,156}Tb, ^{193m}Pt, and ^{203}Pb, fission cross sections and yields for ^{232}Th(p,f), and ^{238}Np(n,f), ^{229}Th(n,f), inelastic scattering cross sections for ^{117m}Sn(n,n’), ^{195m}Pt(n,n’), and neutron capture cross sections for Cm(n,g) and Cf(n,g). This recommendation is not a need which can be fixed immediately but requires *persistent, sustained effort* to continually measure high-priority cross sections for the application community, until better predictive tools are available. The need for improvements in these predictive tools was the focus of WANDA 2021 [Kolo22] and likewise presents a persistent example of ongoing work needed by the community. However, as these data gaps are filled in by IP-motivated measurements, high-fidelity campaigns to measure all visible channels will prove a significant boon in improving these predictive tools.

In addition to the cross section data themselves, a more fundamental need by the users of the IP community is a *reliable and evaluated repository of production data*. The majority of users in the isotope production community are not nuclear data experts, and most not even nuclear physicists, but generally chemists. As a result, many might not know of or be able to use the EXFOR database [Zerk18] to retrieve production data, let alone more complex nuclear data tools offered by the NNDC and IAEA. Better examples of what the community more often uses are the TENDL database [Koni19] or the IAEA’s Charged-particle cross section database for medical radioisotope production [Herm18]. However, neither of these are ideal, nor are they truly evaluated by data experts in the same way by which ENDF is generated – the former is an extremely complete library (though it only supports incident neutrons, gammas, and charged particles up to alphas) but is essentially a global optimization of the TALYS [Koni12] modeling code to EXFOR data, and the latter is a simple moving average of downselected EXFOR data for reaction channels selected by the members of the IAEA CRP who participate in the project. The ideal repository needed by the IP community would be a new library or database, offering evaluated recommendations of cross section data, not only for the channels of interest but all relevant impurity and stable channels as well. Such a library would need to offer the full set of experimental data in addition to the recommended values but presented in both format and structure tailored towards nuclear data *users*, rather than evaluators or generators. In addition to the recommended cross section data, such a library should also have integrated tools to calculate stopping power, production yields, specific activity, cold metal yields, radionuclidic purity, and dose rate estimates to assist in shielding and shipping. Such a library would need to be accessible, transparent, and flexible to updates and requests – a library designed with the user's utility in mind. Such a library has been desired by the community for many years and has been requested by federal funding agencies as well. However, no momentum yet exists for such a project, and its success hinges upon not only providing persistent funding to support the expansion and update of the database, but to also train and retain the data experts needed to carry out such a persistent effort. Given the benefit that this would also produce beyond just the IP community, an interagency funding model might be a suitable way to address this fundamental need and help better integrate the nuclear data and isotope production communities.

Finally, a common theme throughout the discussions of this session made it clear that the community desires a "request list". In such a system, IP users in need of new or improved cross section or decay data could submit a request ticket, leading to a continuously-updated, community-driven list of data needs, in addition to the normal feedback gained through conferences, workshops, and the like. The ENSDF library uses such a system whereby users can request updated evaluations or point out issues and has been massively successful in guiding needs for evaluation in the structure community. To host such a request list would require no funding, and the LBNL/UC Berkeley Nuclear Data Group has taken the initiative to launch such a feedback mechanism via the new Isotope Production Nuclear Data Issues website [Nucl23]. This project is now publicly accessible and will generate a compiled list of cross section and decay data needs, which could be trivially cross-referenced against the range of facilities capable of performing measurements (which have been updated and captured through this year's WANDA session), to determine which facilities may be best suited to carry out the measurements. While the measurements themselves necessarily require funding, this community-driven list will be an invaluable tool to present to DOE IP, the Nuclear Data Interagency Working Group, or any other agencies looking to see what the current nuclear data needs are when preparing funding calls.

Meitner-Auger Therapeutics

Meitner-Auger electron (MAE) emitting radionuclides have demonstrated significant potential for therapeutic applications, due to the high radiotoxicity derived from the high linear energy transfer (LET) of low-energy electrons emitted by certain decays, as well as their potential to spare healthy tissues due to the short range of these electrons [Filo21]. However, there are a number of nuclear data needs that may be standing in the way of their widespread clinical use. R. W. Howell made a point that Meitner-Auger therapeutics will necessarily require a supply of high-specific activity radioisotopes, because the cell killing mechanism requires several 100s to 1000s of decays, depending on the location of the drug in the cell. Because of this, so-called "alternative" production pathways, such as alpha-induced reactions, may be required to achieve the desired specific activities (likely using carrier-free synthesis methods) needed to establish clinical efficacy. These production pathways are often lacking in experimental cross section data, necessary for production planning. At a high level, there are several major data needs impacting the calculation of patient dose from an MAE emitting radionuclide: the electron spectrum per decay, its radiological half-life, the secondary decay radiation emission spectra (chiefly, bremsstrahlung), the stopping power and matter interactions of all decay radiation, and biological uptake and clearance patterns. The first three are primarily nuclear data needs, numbers 3 and 4 have cross-cutting needs with the atomic data needs mentioned in previous WANDA reports [Bern19], and the latter two are primarily biological needs; all will be explored in more detail here.

Current preclinical evaluations are often hampered by the low specific activities in many potential production pathways — it is widely anticipated that wider access to R&D quantities of high-specific activity MAE emitting radionuclides will facilitate more studies, leading to clinical trials for emerging candidates. This has been bolstered by work in recent years which has demonstrated that targeting of the cellular membrane, rather the cytoplasm or organelles, may have increased therapeutic efficiency for radionuclides where nucleus/DNA targeting is challenging [Poug08]. This is particularly exciting to the rapid rise in recent years for the efficient production of synthetic antibodies for targeting of specific disease sites, which will be necessary to adapt these MAE radionuclides to a wider variety of therapeutic applications. In addition, there is a growing focus on the photon spectrum associated with MAE emitting radionuclides, which has two primary components: external bremsstrahlung (EB) produced as electrons and beta particles traverse tissue; and internal bremsstrahlung (IB), which arises during the beta decay process itself. Minimal photon yield for an MAE is key to minimizing patient dose, and the contribution from IB has not currently been accounted for in any of the Monte Carlo transport codes used for calculating dose from MAE emitting radionuclides.

Additionally, a great deal of experimental work remains to be done to measure both the emission (energy) spectra and the multiplicity of Meitner-Auger electron emitters per decay. While the direct vs. indirect therapeutic effects from an MAE emitting radionuclide are obviously dependent on the energy of a given emitted electron, in general, the efficiency of a potential candidate radionuclide depends most simply on the total number of electrons emitted per single decay event. P. Stollenwerk emphasized that the very low energy electrons arising from the N- and O-subshells, less than 500 eV and perhaps even below 18 eV, are of the greatest importance for understanding Meitner-Auger electron dosimetry. These data, in particular, are often the least available, none are available providing electron multiplicities, and there are many discrepancies seen between the relative intensities (of the various emissions) and the current state-of-the-art theoretical predictions, which currently lack any sufficient accuracy for the emission of N- and O-subshell electrons in the MAE cascade. Conventional measurements of conversion electron spectra have primarily been accomplished using surface barrier and cold silicon detectors, but the dead layer on these conventional semiconductor detectors precludes the direct measurement of the full MAE spectrum. In these cases, the produced radionuclide samples for study may be accelerated and implanted directly into a silicon detector, but these measurements are extremely sensitive to the detector response and stopping power of the low-energy electrons, which itself is an outstanding data need [Alot18]. However, due to stopping powers, this approach cannot be used for measuring MAE spectra for $Z>40$ radionuclides, which lack any measurements whatsoever — all decay information in these cases is based on theoretical models with limited accuracy. As a new approach to these measurements, a “cylindrical mirror analyzer”, utilizing decaying isotopes in the gas phase, was presented showing superior resolution to other methods. While this tool offers excellent resolution for MAE multiplicity, the finite number of electron detection pads creates very poor spatial resolution, and poor energy resolution as a consequence. Discussion emphasized the potential for micro-calorimeter detectors to perform high-resolution spectral measurements, which may also aid in this issue. The Argonne group is actively at work increasing this energy resolution through expanded detection pads and MCP detectors. An upcoming NA-241 supported conference on micro-calorimeters for Nuclear Data (MiND 2023) may be a good venue for highlighting these needs [Mind23]. Given that the Isotope Production community’s expertise in radionuclide production and target fabrication will be necessary for the wider deployment of micro-calorimeter detectors, there is an obvious cross-cutting benefit for both communities here. A more fundamental issue with theoretical and the limited experimental spectra is that all of them represent the spectrum from a decaying free atom. However, all targeted radionuclides achieve specificity through chelation and linkage to a targeting molecule. Given the atomic nature of the MAE spectrum, it is obvious that the atom’s local environment (i.e., integration into a molecular structure) will have a major impact on the resulting spectrum. To date, no measurements of the complexed or radiolabeled molecules have been made, creating an additional knowledge gap compounding on top of our already completely theoretical MAE spectra. This has massive clinical impact and necessitates MAE spectral measurements for both free atoms, as well as in labeled molecules to understand the significance of this impact.

While there are many proposed candidates for MAE therapeutic applications [Filo21], spanning a wide range of lifetimes, masses, and decay spectra, the community has lacked a common set of priorities for R&D. In September of 2022, the IAEA hosted a committee to prioritize emerging candidates for clinical applications and establish a set of criteria for evaluating the potential of each candidate. In short, these are 1) the energy and multiplicity of MAE's per decay, 2) the photon/electron ratio per decay, 3) co-emission of conversion electrons and/or beta particles, 4) normal tissue toxicity, 5) radiological half-life, 6) targetry availability for production, 7) established separation chemistry for high specific activity, and 8) targeting vector availability. While numbers 6 through 8 are technical challenges being addressed by the IP community, numbers 1 through 3 and 5 represent the nuclear data needs discussed already. It is worth noting that while nuclear data for lifetimes are generally adequate, measurements are needed with higher precision for some of the shorter-lived MAE radionuclides, due to the direct impact this has on dosimetry. A review article on this criteria is currently in preparation by the committee, but they have already released a list of recommendations for the priority radionuclides to further R&D: ^{58m}Co, ^{64}Cu, ^{67}Ga, ^{71}Ge, ^{77}Br, ^{99m}Tc, ^{103}Pd, ^{103m}Rh, ^{107}Cd, ^{111}In, ^{119}Sb, ^{123}I, ^{125}I, ^{125m}Te, ^{135}La, ^{155}Tb, ^{161}Tb, ^{165}Er, ^{180}Ta, ^{189m}Os, ^{191m}Os, ^{193m}Pt, ^{193m}Ir, ^{195m}Pt, ^{197m}Hg, ^{201}Tl, ^{231}Th, ^{237}U, and ^{239}Np. Of these, ^{71}Ge, ^{155}Tb, ^{161}Tb, ^{165}Er, ^{180}Ta, and ^{193m}Pt were ranked as the highest priorities.

Structure & Decay Data

While nuclear structure and decay data are generally quite good near stability, i.e. for most medically-relevant radionuclides, it was demonstrated during this session that there are still some key gaps affecting isotope R&D and routine operations. A. Renné shared ongoing work at the ATLAS/GAMMASPHERE instrument to measure fusion-evaporation reactions on ^{157}Gd, which highlighted the need for improved gamma-cascade modeling and data and which also highlighted gaps in decay schemes for relatively close-to-stability isotopes. These improvements would enable alternative means to measure production cross sections, particularly for isotopes which are either stable, or do not have decay schemes conducive to other measurement techniques (such as stacked targets). The IP community has a strong connection to the near-stability discrete structure community - both are reliant upon accurate low-lying level schemes for the interpretation of prompt measurements, which are emerging at LBNL as a way to measure production cross sections for stable and long-lived products, which make up a significant fraction of the total residual product cross section at high beam energies. In addition, we recommend that for groups performing such in-beam measurements for IP-relevant cross sections, that the addition of prompt (n,x) coincidence measurements in such studies be included through pulse-shape discrimination organic scintillators, as the neutron spectra (as function of angle and energy) are invaluable in understanding, constraining, and improving our reaction models. While nuclei far from stability often get the most attention currently for high-energy and astrophysics applications, near-stability structure is often claimed as "having been done years ago." However, the current suite of applications (including IP) often demand higher-fidelity data than the most recent structure evaluations offer. More generally, the IP community requires improved decay data for lifetimes and decay radiation branching ratios (both particularly so for isomers), and improved branching ratios for the population of excited and isomeric states.

Additionally, S. Lapi emphasized the importance of developing good calibration standards for devices known as "dose calibrators", which are routinely used in the medical community to accurately dispense radioisotopes for human use. Errors in the nuclear decay data used in generating these calibration standards, or in the algorithms used by these devices to quantify activity, could have grave consequences.

This becomes particularly important when considering theranostic strategies, in which multiple isotopes may be injected into a patient simultaneously.

Radioactive Targetry

The fabrication of high-purity targets with well-defined thickness is essential for virtually all basic and applied nuclear science. The isotope production community is particularly beholden to this need, as high purity (both isotopic and trace metal) enriched isotopes and preparation of well-characterized thin targets are needed to conduct the cross section measurements discussed above, as well as the fabrication of thick production targets capable of surviving the multi-uA beam currents used in high-power production facilities. The ability to fabricate and characterize targets has waned over the last two decades due to the retirement of trained professionals, such as John Greene at the Center for Accelerator Target Science at Argonne National Laboratory, together with the lack of opportunities for early career staff. Target fabrication is becoming something of a dying art, especially given how reliant it is upon the passing along of firsthand experience and process knowledge. Currently, the National Isotope Development Center (NIDC) at Oak Ridge National Laboratory has maintained a robust, but extremely expensive target fabrication capability. However, the ability of NIDC to fabricate radioactive targets is far more limited. Los Alamos National Laboratory has developed a limited repertoire of low-activity radioactive targets [Kuvi22]. However, these and other radioisotope targetry capabilities are generally limited in scope and tailored around internal mission needs for research groups at labs/universities. The U.S. Nuclear Data Program has also recognized this need and has also highlighted the need for target fabrication capabilities to support applied nuclear science as a high priority in the recent Nuclear Science Advisory Committee's Nuclear Data Subcommittee reports [Bern22, Bern 23].

Training and retaining expertise and competency in the scientists who carry out this research is particularly relevant as the field begins to make use of radioactive targets, which recently revealed the largest neutron capture cross section ever seen [Shus19]. New detector systems, such as HotLENZ [DiGi21] and DICER [Stam22] at LANL offer the chance to use radioactive targets to measure neutron-induced data not accessible using radioactive beam facilities such as FRIB. Combining radioactive target fabrication with the isotope production capabilities already present within the IP community could open the door for an entirely new research program within NSD. This would allow for production of relatively short-lived isotopes, which can then be turned into radioactive targets in support of applied research programs, or for truly unique isotope production capabilities. As much as production cross section data are limited, the library of measured cross sections for radioactive targets pales in comparison. Given the fact that the IP community has extensive experience working with highly radioactive irradiated targets, there is a unique opportunity to leverage these skills to support the IP and astrophysics communities by producing relatively short-lived isotopes, which are turned into radioactive targets to be used at the same facilities they are produced at.

This need for target fabrication was discussed heavily in this year's WANDA session and has made it clear that additional training, expertise, and fabrication facilities are needed to support the IP field, as well as other application areas. These general needs and recommendations are presented here, but a deeper assessment of these needs will be explored in WANDA 2024.

Stopping Power Calculations

While not strictly *nuclear* data, the accuracy of charged particle stopping powers was mentioned as being significantly important to a number of members of the isotope production community. During production with charged particles, the beam energy must be precisely known throughout the stack of irradiated materials in order to predict production yields and radiopurities. For facilities like the Brookhaven National Lab (BNL) Brookhaven Linac Isotope Producer (BLIP) or the Los Alamos National Lab

(LANL) Isotope Production Facility (IPF), the optimum energy range for production may be as little as 10% of the incident beam energy. Because production cross sections may vary by orders of magnitude over this energy range, even small errors in stopping powers may compound to significant errors in predicted vs actual isotope yields.

For nuclear data experiments, the issue is similar. As discussed previously, the dosimetry of Meitner-Auger emitting radionuclides is most strongly dependent upon the stopping power of the <500 eV electrons in these spectra. Similar needs also exist for alpha- and beta-therapy candidates, though the state of these data is in a better state relative to the paucity of data for the lowest-energy electrons. Additionally, the cross section data upon which the isotope production community heavily relies must be made with a precise determination of the beam energy. Fortunately, measurement techniques such as stacked-target activation can make up for errors in stopping power using the activity ratios of isotopes produced having well-known cross sections [Voyl21, Grav16]. However, the fact that this approach is consistently needed to correct for errors in stopping power calculations only highlights the fact that improvements are needed for the beams and energies relevant to isotope production.

This need is one of the worst-kept secrets affecting all areas of Isotope Production: target design, measurements of both cross sections and yields, ***and also patient dosimetry***. Existing stopping power models were tuned well enough in the past, but current applications demand a higher fidelity. As discussed in previous WANDA years, this need is cross-cutting with space applications, dosimetry/shielding, and semiconductor application areas.

University Connections

In recent years, the DOE Isotope Program has significantly expanded the role of universities in routine production, and R&D. The university isotope network of production sites has recently expanded to include Texas A&M University (TAMU), the University of Alabama, Birmingham (UAB), and the University of Wisconsin, Madison (UWM). There are many universities currently engaged in research and development related to novel isotope production pathways and new technologies. Indeed, while the national labs often receive the spotlight within IP, universities make up a significant share of domestic production efforts. Universities are an essential tool for early R&D, development of radiochemical separation protocols, and leading the translation from mCi-scale production towards labeling, small animal studies, and early clinical/pre-clinical applications. A majority of presenters during this session highlighted some form of university engagement, including the recent IP funded training effort “Horizon-Broadening Isotope Production Pipeline Opportunities” (HIPPO) [Hipp23]. It is anticipated that university involvement and training efforts will continue to grow to meet the many data needs identified during the session.

In addition, it is clear that students (both graduate and undergraduate) are leading the vanguard in many areas of IP R&D. Not only are they leading many of the IP-relevant nuclear data measurements, but the Isotope Production community is a great training pathway for young scientists through connections with the national lab system. The various traineeship programs, in addition to research towards a graduate degree, represent an incredible pathway for workforce development of the IP field and one which we recommend is continued to be funded, as universities make for fantastic “incubators” for the next generation of leaders in the field.

Finally, it was discussed that given the expenses of purchasing radioisotopes through NIDC, local universities (particularly with access to small accelerators or research reactors) present a viable option for clinical/pre-clinical researchers looking for alternative sources of radionuclides for their studies. Given that most such facilities operate on a recharge cost model, developing connections with local (or nearby) universities may allow for researchers to obtain R&D quantities of emerging radionuclides, at a fraction of the cost of developing their production through the DOE IP sites. Not only would this facilitate additional clinical/pre-clinical work, but further develop student exposure to potential connections for employment after graduation.

8.3.3 *Summary & Conclusions*

Since the last WANDA Isotope Productions session in 2019, a number of measurements that were previously given a high priority have been performed, and we have seen improvements in experimental capabilities across the sites. There have been a number of exciting developments in spectroscopy capabilities, particularly for Meitner-Auger electron emitters. Several "alternative" production pathways have been considered and experimentally investigated. These developments have proven essential in the ability of the Isotope Program to respond to emergent radiopharmaceutical development, as well as to supply chain disruptions caused by the COVID-19 pandemic and the war in Ukraine. However, each speaker identified a multitude of remaining nuclear data needs, the resolution of which will be essential to the mission of the Isotope Program. There are still significant gaps in measured nuclear reaction cross sections, and there is a need for improved predictive tools. Structure and decay data gaps still need to be addressed, most importantly for Meitner-Auger emitting radionuclides. The "art" of targetry is a continual need on both the experimental and production sides of isotope production, requiring training of the next generation. Atomic stopping power calculations and tabulated data are currently too low in accuracy for production applications. And finally, the connection between the Isotope Program and universities has proven to be of great value, and these connections will be invaluable to closing the identified gaps in nuclear data.

8.3.4 *Bibliography*

[Alot18] Alotiby, Mohammad, et al. "Measurement of the intensity ratio of Auger and conversion electrons for the electron capture decay of 125I." Physics in Medicine & Biology 63.6 (2018): 06NT04.

[Bern15] Bernstein, L, et al.. Nuclear Data Needs and Capabilities for Applications. No. BNL-108491-2015-IR. Brookhaven National Lab.(BNL), Upton, NY (United States), 2015.

[Bern19] Bernstein, Lee, et al. Final report for the workshop for applied nuclear data activities. No. LLNL-PROC-769849. Lawrence Livermore National Lab.(LLNL), Livermore, CA (United States), 2019.

[Bern22] Bernstein, Lee, et al., "First Report of the Nuclear Data Subcommittee of the Nuclear Science Advisory Committee." United States: N. p., 2022. Web. doi:10.2172/1890079.

[Bern23] Bernstein, Lee, et al., "Second Report of the Nuclear Data Charge Subcommittee of the Nuclear Science Advisory Committee." United States: N. p., 2023. Web. https://science.osti.gov/-/media/np/nsac/pdf/docs/2023/NSAC-ND_Report_2_031923.pdf

[Dewa18] Dewaraja, Yuni, et al. "Impact of internal bremsstrahlung on Y-90 SPECT Imaging." (2018): 577-577.

[DiGi21] DiGiovine, B., et al. "A holistic approach to the optimization of neutron beam transport at the LANSCE facility." NIM A: Accelerators, Spectrometers, Detectors and Associated Equipment 1013 (2021): 165631.

[Engl19] Engle, Jonathan W., et al. "Recommended nuclear data for the production of selected therapeutic radionuclides." Nuclear Data Sheets 155 (2019): 56-74.

[Fend16] Fendler, Wolfgang P., et al. "177Lu-PSMA-617 therapy, dosimetry and follow-up in patients with metastatic castration-resistant prostate cancer." Nuklearmedizin. Nuclear Medicine 55.3 (2016): 123-128.

[Filo21] Filosofov, Dmitry, Elena Kurakina, and Valery Radchenko. "Potent candidates for Targeted Auger Therapy: Production and radiochemical considerations." Nuclear Medicine and Biology 94 (2021): 1-19.

[Fox21a] Morgan B. Fox, Andrew S. Voyles, Jonathan T. Morrell, Lee A. Bernstein, Jon C. Batchelder, Eva R. Birnbaum, Cathy S. Cutler, Arjan J. Koning, Amanda M. Lewis, Dmitri G. Medvedev, Francois

M. Nortier, Ellen M. O’Brien, and Christiaan Vermeulen, Measurement and modeling of proton-induced reactions on arsenic from 35 to 200 MeV. Physical Review C, 104 (2021) 064615.

[Fox21b] Morgan B. Fox, Andrew S. Voyles, Jonathan T. Morrell, Lee A. Bernstein, Amanda M. Lewis, Arjan J. Koning, Jon C. Batchelder, Eva R. Birnbaum, Cathy S. Cutler, Dmitri G. Medvedev, Francois M. Nortier, Ellen M. O’Brien, and Christiaan Vermeulen, Investigating high-energy proton-induced reactions on spherical nuclei: Implications for the preequilibrium exciton model. Physical Review C, 103 (2021)

[Grav16] Graves, Stephen A., et al. "Nuclear excitation functions of proton-induced reactions (Ep= 35–90 MeV) from Fe, Cu, and Al." Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 386 (2016): 44-53.

[Herm18] https://www-nds.iaea.org/medical/

[Herm23] Hermanne, A., et al. "Evaluated and recommended cross-section data for production of radionuclides with emerging interest in nuclear medicine imaging. Part 1: Positron emission tomography (PET)." Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 535 (2023): 149-192.

[Hipp23] https://cyclotron.tamu.edu/hippo/

[Kolo22] Karolina Kolos, Vladimir Sobes, Ramona Vogt, Catherine E. Romano, Michael S. Smith, Lee A. Bernstein, David A. Brown, Mary T. Burkey, Yaron Danon, Mohamed A. Elsawi, Bethany L. Goldblum, Lawrence H. Heilbronn, Susan L. Hogle, Jesson Hutchinson, Ben Loer, Elizabeth A. McCutchan, Matthew R. Mumpower, Ellen M. O’Brien, Catherine Percher, Patrick N. Peplowski, Jennifer J. Ressler, Nicolas Schunck, Nicholas W. Thompson, Andrew S. Voyles, William Wieselquist, and Michael Zerkle, Current nuclear data needs for applications. Physical Review Research, 4 (2022) 021001.

[Kon12] A.J. Koning and D. Rochman, "Modern Nuclear Data Evaluation With The TALYS Code System", Nuclear Data Sheets 113 (2012) 2841

[Koni19] A.J. Koning, D. Rochman, J. Sublet, N. Dzysiuk, M. Fleming and S. van der Marck, "TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology", Nuclear Data Sheets 155 (2019) 1

[Krat16] Kratochwil, Clemens, et al. "225Ac-PSMA-617 for PSMA-targeted α-radiation therapy of metastatic castration-resistant prostate cancer." Journal of Nuclear Medicine 57.12 (2016): 1941-1944.

[Kuvi22] Kuvin, Sean Andrew, et al. "Direct measurement of Ni 59 (n, p) Co 59 and Ni 59 (n, α) Fe 56 at fast-neutron energies from 500 keV to 10 MeV." Physical Review C 105.4 (2022): 044608.

[Mind23] https://conferences.lbl.gov/event/1243/

[Morr20] https://jtmorrell.github.io/curie/build/html/index.html

[Nucl23] https://nucleardata.berkeley.edu/ipndi/

[Poug08] Pouget, Jean-Pierre, et al. "Cell membrane is a more sensitive target than cytoplasm to dense ionization produced by auger electrons." Radiation research 170.2 (2008): 192-200.

[Roma20] Romano, Catherine E., et al. Proceedings of the workshop for applied nuclear data: Wanda2020. No. ORNL/TM-2020/1617. Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States), 2020.

[Shus19] Shusterman, J.A., Scielzo, N.D., Thomas, K.J. et al. “The surprisingly large neutron capture cross-section of 88Zr”. Nature 565, 328–330 (2019). doi:10.1038/s41586-018-0838-z

[Stam22] Stamatopoulos, Athanasios, et al. "DICER: a new instrument for nuclear data for nuclear security." Journal of Radioanalytical and Nuclear Chemistry (2022): 1-5.

[Voyl21] Andrew S. Voyles, Amanda M. Lewis, Jonathan T. Morrell, M. Shamsuzzoha Basunia, Lee A. Bernstein, Jonathan W. Engle, Stephen A. Graves, and Eric F. Matthews, Proton-induced reactions on Fe, Cu, & Ti from threshold to 55 MeV. The European Physical Journal A, 57 (2021) 94. https://doi.org/10.1140/epja/s10050-021-00401-2

[Zerk18] Zerkin, V. V., and B. Pritychenko. "The experimental nuclear reaction data (EXFOR): Extended computer database and Web retrieval system." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 888 (2018): 31-43.

8.4 Processing and Preservation

The processing and preservation session was really split into two sub-sessions, one on the future of nuclear data processing and the other on the preservation of nuclear data. These sub-sessions were organized, respectively, by:

- Nathan Gibson, LANL
- Elizabeth McCutchan, BNL

8.4.1 *The Future of Nuclear Data Processing*

Nuclear data processing is the manipulation of evaluated nuclear data for use in an application code. At its simplest, this could be the insertion of a single number (e.g., a half life) into a simple script (e.g., computing activity of a sample of a given mass). Typically, though, processing is considered to be a much more significant step with codes like NJOY, FUDGE, AMPX, and NDEX serving large-scale transport codes. Processing steps include but are not limited to resonance reconstruction, energy grid refinement and linearization, Doppler broadening, computing redundant quantities (e.g., energy deposition, gas production, average scattering cosines, distributions in alternate reference frames), re-formatting. Processing also includes application-specific steps like multigroup collapse for deterministic transport, sampling for ensemble-based uncertainty quantification, and the collection of complete libraries of application-formatted data files.

This sub-session explored what the future of nuclear data processing entails through examining the status and reasons for continued investment in the four major US-based code efforts and by looking at four specific examples of further processing needs. Discussion, although very brief, highlighted additional areas of interest.

Major US-Based Processing Code Efforts

NJOY

Dr. Wim Haeck of Los Alamos National Laboratory introduced the NJOY code. Dating back to the 1970s, NJOY is the most well-known processing code and, with a major overhaul in 2016, is now open-source. While NJOY2016 is still considered the production version of the code and is being updated to support data changes with each new evaluation, a ground-up re-write using the moniker NJOY21 is in process. The goals of this new effort are to allow the code to be more flexible, giving users the ability to use pieces of the code for specific needs rather than only supporting end-to-end processing, to move away from close coupling with the ENDF format, and to address knowledge management concerns. To this last point, with the retirement of the original leaders of nuclear data processing, teaching a new generation all the subtle details of processing will help to avoid mistakes from creeping into this crucial piece of the nuclear data pipeline.

FUDGE

Dr. Caleb Mattoon of Lawrence Livermore National Laboratory introduced the FUDGE code. FUDGE was also relatively recently open-sourced and is a modernized take on processing. Rather than simply supporting the transformation of data for insertion into an application code, FUDGE is also intended to be an evaluator tool. It provides many operations needed by evaluators and also provides one of the most robust checking tools currently available. As part of the development of this code, a new nuclear data format, the Generalized Nuclear Database Structure (GNDS), has been developed and is now an international standard. GNDS allows for a more flexible and more easily computer-readable storage for nuclear data, and the ENDF project has already begun releasing new evaluations in this format. The EMU tool, built on top of FUDGE, is a uncertainty toolkit and is discussed later in this report.

AMPX

Dr. Jesse Brown of Oak Ridge National Laboratory introduced the AMPX code. AMPX is the primary nuclear data processing tool for the SCALE code suite, and, like NJOY and FUDGE, was recently open-sourced – a real theme of this discussion. AMPX uses a modular code structure to support a wide variety of codes and applications in SCALE and currently is able to meet the needs of these codes. However, there were several areas identified that warrant further investment, including formal decay library generation, a more streamlined API for accessing data, speed, and user interfaces.

NDEX

Dr. Jason Thompson of Naval Nuclear Laboratory introduced the NDEX code. Although the newcomer to this discussion, NDEX has a long history of co-development with the Monte Carlo code MC21 and has reached a significant level of maturity. NDEX originally was a supplement to NNL's processing via NJOY, creating data files in a desired file format and with some in-house implementations of important physics. Currently, NDEX is endeavoring to be a standalone processing code and is seeing rapid progress being made. NDEX features advanced algorithms for unresolved resonance treatment, thermal scattering, Doppler broadening, photon scattering, and charged-particle slowing down.

Impact of Advanced Computing Architectures on Nuclear Data Needs

Dr. Paul Romano of Argonne National Laboratory gave a talk focusing on data needs related to advanced computing architectures. It has now become clear that we are living in the age of GPUs, with this technology winning out over various other options over the last several years. Benefits of GPUs are seen not only in the largest supercomputers in the world but also in smaller clusters available to large portions of the scientific community.

With respect to nuclear data, the primary practical difficulty of porting to these architectures is the use of complex, nested data hierarchies. The polymorphism programming paradigm is not well-suited for use on GPUs, which motivates the need for different approaches to memory layout. One approach is to provide more "uniform" outputs from processing codes, such that all angle/energy distributions are given similarly, but this is at the cost of higher memory footprints. Another approach is the use of parametrized forms of distributions, perhaps aided by machine learning.

To this last point, the latest computer architectures provide a strong incentive to use less memory and more FLOPs. This motivates the increasing use of on-the-fly algorithms and model-based physics. Some existing examples include the windowed multipole formalism for the resolved resonance range and fission event generators.

Nuclear Data for Depletion in SCALE

Dr. Jordan McDonnell of Oak Ridge National Laboratory presented a specific example of nuclear data processing needs: depletion calculations in ORIGEN. Currently available depletion data libraries combine nuclear data of a wide variety of observables, including half lives, branching ratios, reaction Q-values, reaction data, fission product yields, energy deposition, and particle emission data. These typically are not available from a single source and thus require expert curation to assemble, and the libraries are typically very far from being in sync with the latest ENDF and ENDSDF releases, with currently default data coming from ENDF/B-VII.0 and ENDF/B-VII.1. Depletion and related simulations also require data not included in these databases, relying on the JEFF/3.0-A activation library.

Tools are needed to enable the adoption of newly available data in an easier manner. While local expert curation cannot be avoided without something like an additional focused CSEWG committee, a smoother pipeline to combine data from various sources would be most welcome. A deeper connection to the ENDSF database could provide richer data, including additional metastable states and decay schemes. ORIGEN, along with nearly all other similar computational tools, does not provide for sensitivity and uncertainty calculations. As richer uncertainty data becomes available, including with the new fission product yield evaluation stemming from previous NDIAWG funding, there is a desire to measure the impact through these sorts of codes. Finally, adopting new data more quickly requires serious validation efforts.

Self-Consistent Energy Normalization for Quasistatic Reactor Calculations

Dr. Jason Thompson of Naval Nuclear Laboratory gave a presentation, originally authored by Dr. David Griesheimer and others for the ill-fated PHYSOR2020 conference, of another specific nuclear data processing need related to energy deposition. During reactor depletion calculations, the rate of depletion is closely tied to energy release and a normalization is used to relate computed depletion rates with realistic changes in inventories. Energy is deposited directly through fission and through other reaction mechanisms captured in the quantity KERMA (kinetic energy released in materials).

In the case examined here, a common assumption for the energy rebalance factor for thermal reactor applications was found to break down for faster-spectrum reactors, where a significant fraction of fissions are caused by above-thermal neutrons. Improperly balancing the energy will cause an incorrect rate of isotopic depletion.

In further discussion, this work highlights a major need in nuclear data processing, as the corresponding need is slowly being addressed in the ENDF library. That is, as ENDF fills out previously missing secondary particle distributions, processing codes must be able to accurately compute heating information from them. This must be combined with sensitivity toward the application, where subtle details about how the data is used must inform the data provided.

Covariances and Uncertainty Propagation

Dr. Kyle Wendt of Lawrence Livermore National Laboratory gave a talk about processing concerns for uncertainty propagation, including an overview of the EMU tool he developed. The EMU tool is built on top of FUDGE for generating random realizations of nuclear data from the tabulated covariance information.

Because covariances in ENDF are not given with distribution information, when generating realizations for ensemble-based uncertainty studies, a distribution—typically a multivariate normal—must be assumed. This is never accurate in reality, as quantities such as cross sections can never be negative, and normal distributions cannot be formulated without negative tails. However, pragmatic approaches can be taken, where one alters the assumed distribution slightly to get only physically meaningful samples. This motivates larger studies of understanding how much data is lost from missing distribution information and improved ways of tabulating evaluated uncertainties.

The available covariance data in the ENDF library is incomplete, and there is desire for an improvement in coverage. While generation of missing data does not necessarily fall into the theme of processing, processing codes can enable and help to understand the effect of the gaps. Also, while it is often clear which nuclides have uncertainty information and which do not, it can be a bigger challenge to interpret results when nuclides have incomplete information, perhaps only for certain channels in certain energy ranges. In other discussions at WANDA and at the previous NDUQWM venue, a desire for a new "medium-fidelity" covariance library to fill in gaps was highlighted as a significant need in the field. Processing codes have a role to play in using this data and helping users interpret it.

Other Discussion

While the current status and several needs related to nuclear data processing were explored, the discussion session largely highlighted additional areas where processing is important and improvements can and should be made. These areas include specifics of on-the-fly methods, processing and formatting beyond typical evaluations, thermal scattering support, materials damage calculations, data for fusion energy, feedback loop between processing and evaluation, multigroup methods, specific needs for photonuclear applications, etc. There was also discussion of the need of consumer tools for non-experts to interact with nuclear data. While many tools exist, including the JANIS web application and modern extensions to FUDGE and NJOY, further focus in this arena is warranted.

Summary of Nuclear Data Processing Needs

This short session was a great introduction of the topic of nuclear data processing to the WANDA venue. Perhaps the greatest need identified is continued attention to explore how the community and funding sources can work together to make improvements in this piece of the pipeline. While programmatically-driven funding (e.g., Advanced Scientific Computing Program, Nuclear Criticality Safety Program, and Navy Nuclear Propulsion Program) supports most of the current development, this session highlighted that so many more programs benefit from the infrastructure provided by processing codes and processing expertise to perform simulations with any new piece of nuclear data.

The current status of codes highlighted two themes of current development. First, by moving to an open-source model, we are now able to engage the wider community in new ways and interact more easily outside individual labs. This is intended to improve the pace of development, the transparency of the quality assurance approaches, and the ability for others to work in niche areas. Second, knowledge management is a vital issue at the heart of each effort. We are currently reaping the benefits of the work that a previous generation, including leaders like Bob MacFarlane, Red Cullen, Nancy Larsen, and Cecil Lubitz, set for us. But without continued investment, the expert knowledge required to ensure ongoing quality is at risk. This sentiment has driven existing programmatic funding, but coupled with the new open-source approach, there are opportunities to look for new ways of addressing the issue.

The following technical areas were identified as requiring further investment:

- Adapting to new evaluated representations and formats,
- Making use of nuclear data effectively on high performance computers,
- Creating robust and well-maintained tools for processing beyond criticality, including quantities such as:
  - Depletion and decay heat,
  - Energy deposition and materials damage,
  - Thermal scattering and unresolved resonance processing,
  - Photonuclear and charged particle transport, and
  - Fusion systems and isotope production,
- Propagating nuclear data uncertainties from evaluation to application, and
- Improving consumer-facing tools for interacting with data.

8.4.2 *Nuclear Data Preservation*

Reproducibility, verification, and repeatability of scientific results are pillars of scholarly research. These pillars can only be achieved if scientific results are properly preserved and made publicly accessible. Currently, data preservation and data sharing are not well integrated into the nuclear data pipeline. To lay the groundwork for incorporating data preservation strategies into the nuclear data process, this sub-session explored the opinions and concerns of the community on data preservation. Some initial questions that were raised to the speakers and audience were:

- What steps does the community need to take to make data "FAIR" (Findable, Accessible, Interoperable, and ReUsable)?
- What tools can be developed to enable more uniform and centralized methods for sharing and preservation of data?

- Can we leverage data preservations efforts from other scientific fields?

Note this subsession on data preservation was timely, considering DOE has designated 2023 as "The Year of Open Science".

Overview of US Data Preservation

Dr. Jin Wu of Brookhaven National Laboratory opened with an overview of data preservation efforts. Data shared and analyzed by many teams of scientists worldwide has now become routine in many fields. In 2014, NASA began sharing data through their initiative Data.nasa.gov. Their Open Innovation site harvests data across several organizations and now offers access to more than 40,000 data sets. In High-Energy physics, data from CERN's Large Hadron Collider are made available for public access, along with analysis codes and virtual machines, which are prepared to begin analysis of data immediately under most operating systems. These data curation and sharing initiatives are guided by the so-called FAIR principles which propose that data be, to the greatest degree achievable, (1) Findable, with a globally unique identifier and rich metadata, (2) Accessible through a standard protocol, (3) Interoperable with as much standardization as possible, and (4) Reusable with rich provenance metadata. Through these principles, the greatest re-usability of data can be achieved, to the benefit of both researchers and funding agencies. The current status of experimental low-energy nuclear physics data sets does not meet FAIR principles, with data sets scattered (both in many laboratories and using a variety of storage media), not well-documented and typically not accessible over a network. This "self-curation" by individual research groups lacks uniformity and results in a situation where data discovery and reuse are often difficult or impossible. Dr. Wu advocated for a centralized repository for low energy nuclear data that would directly support data management and FAIR data requirements of funding agencies. Such a repository would have numerous benefits to the community, including guidance for future experiments, validation of results, data mining of byproducts of experiments and training for students and junior scientists.

Data ID Services

Drew Huitt from Office of Science and Technology (OSTI) provided an overview of the services offered by OSTI. The mission of OSTI is to advance science and sustain technological creativity by making R&D findings available and useful to DOE researchers and the public. OSTI offers two venues for searching their collection of scientific and technical information, through OSTI.GOV and the DOE Data Explorer. Dr. Huitt focused on persistent identifiers (PIDs) which are digital identifiers that are globally unique, persistent and machine resolvable with an associated metadata schema which identifies an entity in perpetuity. DOI's are an example of a commonly used PID. The community was encouraged to assign DOI's to datasets, which has several advantages, including making the data FAIR, visible, reusable, citable and searchable. PIDs are not limited to datasets but can be assigned to a number of objects including data, software, text documents, awards, people and organizations, hence providing the opportunity to link all essential aspects of a research project. Through the DOE Data ID Service, OSTI works with researchers to develop a robust metadata description of a dataset and assign a DOI. Collaboration with OSTI to develop DOI's was strongly encouraged.

Public Access Policy and Data Management Plans

Dr. Michael Cooke, Senior Technical Advisor for the DOE office of the Deputy Director for Science Programs provided the DOE perspective on public access and data management. Current public access policy is set by a 2013 OSTP public access memo which led to the development of a 2014 DOE Public Access Plan. Requirements of the plan include free public access to federally funded publications following a 12-month embargo period and the requirement of data management plans (DMPs) to accompany receipt of federal grants and contracts. Updated guidance for DMP's was issued early 2022 which provided researchers with suggested elements of a DMP and guidance for DMP reviewers. Dr. Cooke highlighted the fact that Public Reusable Research (PuRe) Data Resources form one of the three pillars of the Office of Science Enterprise. The topic which garnered the most discussion was a new 2022 OSTP Public Access Memo which builds on the 2013 memo and requires immediate access to federally funded research. Some highlights of the memo include removing the 12-month embargo on publications to provide immediate access and additionally requiring that the data underlying the publications similarly be made immediately accessible. An additional requirement will be the use of PID's for all aspects of research output, which tied nicely with the Data ID services talk by Dr. Heuitt.

openNP

Dr. Adrien Matta of GANIL introduced the openNP project. OpenNP is a new open data initiative being pursued within several European Nuclear Physics Laboratories and is designed to organize and facilitate access to data from laboratories across Europe. In this initial phase, OpenNP will focus on cataloging data sets (experimental, simulated and theoretical), along with associated metadata and tools. OpenNP is a collaborative approach to data preservation. Each aspect of an experiment, from the accelerator and detectors, to the DAQ, analysis, etc, is assigned to an individual within the collaboration. This automatic aggregation approach to data preservation helps to integrate open data practices into the everyday workflow and increases the visibility of each member of the collaboration. The data catalog which OpenNP aims to develop will allow for improved experimental planning and potential re-use of data from existing datasets. Longer term goals for OpenNP include synergy with data lake efforts to store and preserve datasets and the incorporation of analysis and simulation capabilities into the software platform.

Case Study from LANL

Dr. Matthew Devlin of Los Alamos National Laboratory (LANL) presented a laboratory perspective on data archival. This case study involved the Chi-Nu detector at LANL with data measured on prompt fission neutron spectra (PFNS) for ^{239}Pu,^{235}U, and ^{238}U totaling 45 TB in size. Data archival was built into the funding as the collaboration recognized early in the experimental planning the need to properly preserve a 12+ year project with a total cost of more than $20 M. For this particular experiment, the data analysis uses nuclear data in the form of a response matrix. Thus, careful data preservation would allow the data to be reanalyzed with future ENDF/B libraries which could contain improved nuclear data input. Dr. Devlin emphasized that storing the data was the trivial aspect of the data preservation. Foresight into knowing each important detail of the experiment that would make the data useful to another user in the future is challenging if not impossible for all potential use cases.

Discussion

The discussion session was able to reach consensus on a few aspects of data preservation. However, giving the infancy of the concept of data preservation and data sharing, the large number of questions and concerns which were raised in the during the discussions clearly highlights the need for subsequent dialog on this topic.

A few key takeaways emerged from the resulting discussion.

There was overall consensus that raw data preservation and sharing was not necessary at this time. Arguments against storage of raw data included the overall cost, needs for redundancy which further increase cost and that such data would be virtually impossible for someone other than the original experimenter to decipher.

There was additional consensus that preservation of all aspects of an experiment should be a process which occurs throughout the lifecycle of the experiment. Attempting to document the research after the fact would incur additional time and likely miss important aspects of the experiment.

Finally, there was modest consensus that the community requires a central repository for data preservation. This opinion was somewhat motivated by cost considerations; establishment of a central repository would reduce the burden on individual institutions to develop their own data preservation platforms. Additionally, there were suggestions to try and develop common data formats that would facilitate data sharing and reuse amongst similar types of experiments.

There were also several concerns about data preservation raised throughout the course of the discussion session. The most discussed item was the "cost" of data preservation. There are two costs which would come with a data preservation requirement. The first is the cost of the data storage itself and the need to implement redundancy. These costs can vary depending on the required latency for the data retrieval. Of greater concern was the time that researchers will need to spend in order to preserve each aspect of the experiment. Additional questions ensued on whether or not this extra effort could be incorporated into the funding proposal and would funding agencies be providing additional funds to cover data preservation efforts.

Another open question concerns the embargo period on the data, that is the time between when the experiment is completed and when it can be made available to the public. This interval will certainly need to be decided on through discussions with the community. It will need to be a balance between providing the researcher with sufficient time to analyze and publish the portion of data of interest to the original proposed experiment with a reasonable time frame for users who need the data for their specific application. One example which was raised was the lengthy time between experiment and incorporation into EXFOR for data collected at nTOF at CERN.

Summary of Nuclear Data Preservation Needs

Data preservation is an important piece which is currently missing from the nuclear data pipeline. The greatest need relating to nuclear data preservation which emerged from this session was for additional dialog and conversations on how this community can begin the initial steps toward FAIR data storage and sharing. These conversations should not be limited to the nuclear data community, as other fields have made significant process in data preservation which can be leveraged to develop a data preservation platform which meets the needs of this community.

The following topics were highlighted as requiring further discussion

- What is the cost increase for an experiment from the archiving requirement and who bears this cost?
- What are reasonable embargo periods for data?
- What aspects of an experiment need to be preserved?
- Can data be developed in a common format to allow some uniformity amongst similar experiments?
- For NNSA laboratories, how will data undergo review and release procedures