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ABSTRACT

On February 28 – March 4, 2022, the Nuclear Data Interagency Working Group (NDIAWG) hosted the 5-day virtual Workshop for Applied Nuclear Data Activities (WANDA2022) to facilitate interagency collaboration on nuclear data for applications. This year's focus was nuclear data for space applications, but also included photon reactions and transport, reactions on unstable nuclei, and data adjustment topics. The annual WANDA workshops are planned by the Nuclear Data Working Group (NDWG) with the goal of assembling users and producers of nuclear data to provide input to identify and prioritize nuclear data needs and to suggest solutions to address those needs. The workshop consisted of talks by agency program managers, six topic-focused road mapping sessions and a review of NDIAWG-funded projects. More than 350 attendees represented national laboratories, universities, and federal agencies, as well as international organizations and industry. The proceedings presented herein summarize the workshop's content, highlight important outcomes, and document attendees' recommendations.

INTRODUCTION

WANDA was initiated by the NDWG to bring nuclear data producers, evaluators, and users together with appropriate program managers and stakeholders to communicate and prioritize nuclear data needs for applications. The primary objective of WANDA is to discuss nuclear data priorities, determine where needs overlap in associated program areas, and recommend a national plan to address these high-priority needs. The prioritized nuclear data needs are communicated to the research community and to the federal agencies that may be impacted by nuclear data deficiencies so that they can take appropriate action to meet mission requirements.

WANDA 2022 was the sixth in a succession of meetings that started in 2015 with the Nuclear Data Needs and Capabilities for Applications (NDNCA) [1] meeting. Three years later, the Nuclear Data Roadmapping Enhancement Workshop (NDREW) [2] was held and set up an annual event which became the WANDA series [3-5], starting in 2019. WANDA is planned by the Nuclear Data Working Group (NDWG) [6], formed in 2015 following the NDNCA meeting to facilitate cross-program collaboration on nuclear data. The NDWG supported by the Nuclear Data Interagency Working Group (NDIAWG) which meets quarterly and is open to all interested federal program managers. The NDIAWG is chaired by the Office of Nuclear Physics in the DOE Office of Science (DOE-NP) to coordinate nuclear data efforts between participating program offices. Many of the nuclear data priorities are based on outcomes of the WANDA workshops and identified in proceedings such as this one. DOE-NP leads the release of an annual NDIAWG Funding Opportunity Announcement which allows participating NDIAWG member programs to fund nuclear data of interest, providing a unique mechanism of cross-agency collaboration.

The core of the WANDA meeting is a group of topical breakout sessions led by subject matter experts. Each WANDA meeting identifies cross-cutting nuclear data needs for users in the United States. Twenty-three nuclear data projects, directly tied to session topics of previous meetings, have been funded through the NDIAWG FOA since 2018, demonstrating the success of the WANDA meetings and the NDIAWG collaboration. Furthermore, numerous new collaborations have been formed, new nuclear data is becoming available to the users, and new researchers are joining the community effort in nuclear data production. Future WANDA workshops will continue increasing mutual awareness and understanding of different stake-holder segments of the nuclear data community.

THE NDWG AND THE NDIAWG

The NDWG was formed in 2015 after the NDNCA workshop with the goal of facilitating communication, collaboration, coordination, and prioritization of nuclear data efforts across multiple program offices, the national laboratories, universities, and industry. The group is composed of nuclear data and applications experts nominated to represent program or national laboratory mission interests. Each interested program office can nominate up to two laboratory researchers to represent their mission interests, to ensure that program-specific needs are communicated, and collaborative opportunities are leveraged. Additionally, each DOE and National Nuclear Security Administration (NNSA) national laboratory is invited to nominate up to two individuals to represent their laboratory's mission and communicate back opportunities.

The NDWG is responsible for organizing the annual WANDA workshops that inform the topic areas called out in the annual NDIAWG FOA. The NDWG solicits input on mission-driven nuclear data needs and determines the topics for the WANDA roadmapping sessions. The workshops are designed to be an open forum to collect recommendations from the larger science community and to document that input.

The NDIAWG is led by the Office of Science, Office of Nuclear Physics (NP) and is open to all interested federal program managers across DOE, NNSA, and other federal agencies. The NDIAWG communicates regularly on nuclear data needs and planned projects. It releases a cooperative NDIAWG FOA each year to facilitate co-funding of cross-cutting nuclear data projects. Those offices that cannot participate directly in the FOA coordinate their funded nuclear data projects with the NDIAWG.

WANDA 2022 PROGRAM

WANDA 2022 was held virtually on February 28 – March 4, 2022. It was comprised of nuclear data needs talks by managers of domestic and international agencies, six roadmapping sessions (summarized in Appendix A), and an update on the NDIAWG-funded projects. The agenda of the workshop and slides from the presentations can be found at https://conferences.lbl.gov/event/880/.

WANDA 2022 topics were focused primarily on nuclear data for space applications. With the rise of industry's interest in space, the increase in satellite deployments, and NASA's ambitious goals, the NDWG and NP reached out to the space community to better understand their nuclear data needs. The resulting roadmapping session topics are listed below, and topics 1 – 4 are focused on the space mission.

1. Nuclear Data for High Energy Ion Interactions and Secondary Particle Production
2. Neutrons as Secondary Particles and Their Interactions with Matter
3. Photon Reactions and Transport
4. Stopping powers, energy deposition and dose
5. Nuclear Data adjustments and Impact on Applications
6. Reactions on Unstable Nuclei

The following are summaries and recommendations of the WANDA2022 roadmapping sessions. Detailed descriptions are in Appendix A.

1. Nuclear Data for High Energy Ion Interactions and Secondary Particle Production

Understanding the harmful effects of galactic cosmic rays (GCRs) on space exploration requires a substantial amount of nuclear data. Specifically, the interaction of energetic GCR charged particles with spacecraft materials generates secondary radiation that, through energy deposition, can harm astronauts and electronic systems. By identifying the gaps in our knowledge of the relevant nuclear data and identifying ways to fill those gaps — with measurements, compilations, evaluations, dissemination, reaction modeling, sensitivity studies, and uncertainty quantification — the safety and viability of space exploration can be improved.

Recommendations:

1. The community modeling interactions of cosmic rays with matter could strongly benefit from utilizing advances in nuclear reaction theory by the RHIC community for modeling reactions important for GCR secondaries.
2. Adopti uncertainty quantification (UQ), sensitivity analyses, machine learning (ML) approaches, and high-performance computing (HPC) resources to better model highly complex space systems with proper uncertainty propagation to improve sensitivity studies.
3. Cross section measurements with high energy ions using the STAR detector at RHIC are a high priority. This is time critical because the accelerator will shut down in 2025 to begin preparations for EIC construction.
4. Additional beam time for appropriate measurements at other facilities to produce the required data.
5. Cross section databases at GSI and at NASA exist but these two are not necessarily complete and it is not clear how they will be maintained in the future. Therefore, borrow approaches from the nuclear data community for the compilation, dissemination, archiving, and management of nuclear data at cosmic ray energies to consolidate the data and allow for future archiving. (Note that the appropriate energies for GCRs are well above those used by the nuclear data community at this time.)

6. Arrange a meeting between those currently working in space applications, such as at NASA and others, with those modeling hadron transport in heavy-ion collisions to initiate communication to the benefit of both communities.

2. Neutrons as Secondary Particles and Their Interactions with Matter

The space radiation environment, consisting of galactic cosmic rays, solar energetic particles and trapped belt radiation, creates a unique secondary neutron environment through interactions of those radiations with materials in that environment, including spacecraft and habitat shielding, planetary surfaces, and others. Because of the wide range of particle species and energies, secondary neutrons range in energies from thermal to several tens of GeV via interactions with protons and heavy ions ranging from several MeV to several GeV/nucleon. Secondary neutrons add to the overall risk of exposure to humans and electronics, and in thickly shielded scenarios are a significant portion of that risk. On the other hand, secondary neutrons are a benefit in the field of planetary nuclear spectroscopy through the activation of elemental components of the planet surface as well as direct detection of secondary neutrons from GCR and solar energetic particles (SEP) interactions in the soil. During this session, several data needs were identified to better understand the neutron environment in space, including:

1. Secondary neutron cross sections from heavy ion interactions above several hundred MeV per nucleon, especially in the 1 – 10 GeV per nucleon range.
2. Cross sections for He interactions above 250 MeV per nucleon.
3. Double-differential cross sections beyond 90 degrees in the laboratory system.
4. Cross sections for neutrons below 2-5 MeV
5. (n,n’γ) data with:

   - Interactions over a wide range of targets (H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni)
   - Incident neutron energies from threshold (0.1 to 1 MeV) up to 50 MeV
   - Cross sections with less than 5% uncertainty
   - Emphasis on targets currently with greater than 20% uncertainty (H, O, Na, Mg, and S)

3. Stopping powers, energy deposition and dose

Well-benchmarked charged particle stopping powers (e.g., dE/dx) are critical for a wide variety of applications ranging from modeling single event effects (SEE) and human dosimetry calculations for space exploration; fission and fusion materials damage; Ion Beam Therapy (IBT) and optimized isotope production; and the modeling of detectors for basic science, national security, nuclear nonproliferation. Needs for specific applications have been well-documented at several Workshops for Applied Nuclear Data Activities (WANDA) including WANDA 2019 (materials damage); WANDA 2020 (detector modeling); WANDA 2021 (space applications, and most recently in a dedicated session at WANDA 2022. The topic was also listed as a cross-cutting nuclear data initiative in the final Nuclear Science Advisory Committee – Nuclear Data Charge subcommittee report.

Several key data needs related to stopping powers were highlighted:

1. The IAEA supports a stopping power database (https://www-nds.iaea.org/stopping/), and additional measurements and modeling are needed for heavy projectiles (Li to U) and complex molecules (plastics and oxides).
2. New work is needed to explore the role of machine learning (ML) and deep neural nets in estimating the stopping power for compounds where there are no pre-existing experimental data.
3. Improved alpha-particle stopping powers for nuclear safeguards are needed for UF6, PuF4, UO2:2.5H2O as well as U, Pu and Am oxides and carbides.

4. Shielding for electronics in space applications requires improved stopping power data for heavy-ion recoils in wide-bandgap semiconductors such as SiC, GaN and Ga2O3, as well as other materials such as GaAs, SiGe, and HgCdTe and elements of Cu, Ag, W, Ti, Ta, Sn and Pb.
5. Improvements in (p,x) and (n,x) cross-sections and the recoil spectra in many materials are needed.
6. Better experimental data for H and He stopping powers in High Energy Density Plasmas (HEDP) are important for fusion energy and stewardship science applications
7. Ion Beam and targeted alpha particle therapies require improved aqueous media stopping powers as well as secondary neutron production rates.

4. Photon Reactions and Transport

Historically, neutron induced reactions have been the focus of the nuclear data community, transport codes and their user community. But today, photo-nuclear reactions are becoming an important tool for understanding nuclear physics, producing important medical isotopes and for scanning material (e.g., cargo, special nuclear material) for distinct isotopes. During this session, important photo-nuclear experimental, theory, data evaluation, transport code and validation benchmark needs where presented and discussed.

The following high-priority needs emerged out of session presentations and discussions:

1. Develop experimental capabilities to address multi-neutron emission cross sections at energies beyond the giant dipole resonance (GDR).
2. Validate the accuracy of photonuclear data for photon energies less than 10 MeV for actinides and other common materials.
3. Measure photonuclear reaction production cross-sections of isotopes useful for nuclear medicine diagnostics and therapeutics, including reactions such as (ɣ,n), (ɣ,p), (ɣ,2n) and (ɣ,pn) at ɣ-ray energies in the GDR region (~1-40 MeV).
4. Develop photonuclear reaction theories in three areas, (i) the photo-absorption cross section, to which microscopic theories may be applied, (ii) the pre-equilibrium photonuclear reaction, and (iii) the photo-fission reaction.
5. Measure correlations between prompt fission neutrons or photons, and fission fragments properties, in particular the yield and total kinetic energy (TKE) as a function of incident photon energy.
6. Work towards a more complete evaluated photonuclear library with covariance data in a proper format.
7. Improve photon scattering physics in transport codes.
8. Create more benchmarks to validate photonuclear data and model physics used in transport codes.

5. Nuclear Data adjustments and Impact on Applications

Adjustment is key for nuclear data users as it combines the knowledge from a general-purpose nuclear data library with that of the user domain encompassed in integral experiments. Adjustment can lead to better understanding of safety and economical bounds on application quantities. It can also motivate the need for future measurement campaigns and theory developments to better constrain application quantities, and thus helps in guiding funding streams. While adjustment has been undertaken by some nuclear data users, others need guidance and tools to undertake adjustment for their application domain. During this session, several stumbling blocks were identified concerning integral data, the general-purpose library, and the needed tools and databases. High-priority needs were distilled out of these discussions.

Summary of recommendations:

1. Various users need cross-cutting tools that support and undertake adjustment.
2. Nuclear data covariances must be complete and reliable for a broad user group. I.e., reliable and well-tested covariances must be available for all relevant isotopes, observables (including also fission yields, angular distribution, thermal-scattering law) and a broad energy range.
3. Work is needed to stringently assess the quality of mean values and uncertainties of various existing integral experiment responses along with correlations between experiments.
4. Many integral responses should be stored in one easily-accessible database of past experiments. Along with that, users need an easily-accessible database of sensitivities, and tools to compute them, for various integral responses as a function of all pertinent nuclear data observables.
5. Users need cross-cutting tools to (1) identify existing and (2) design optimized new experiments representing their applications.
6. A mini-workshop targeted on adjustment for users and nuclear data practitioners is needed to better inform users on general-purpose libraries, available tools and databases.

6. Reactions on Unstable Nuclei

The Session for Reactions on Unstable Nuclei was divided into two sub sessions. One was the direct measurements on nuclear reactions with unstable nuclei and the other was the indirect methods to study reactions on unstable nuclei. These two sessions were followed by a dedicated discussion to solicit the community inputs for progressing our understanding of reactions on unstable nuclei.

Summary of recommendations:

1. The Importance of more measurements for the reactions on unstable nuclei is emphasized to improve the status of our knowledge and help constrain theoretical models; these data support a range of applications needs.
2. Various experimental efforts are being invested in developing new techniques, new capabilities, and new facilities to enable new nuclear reaction data with unstable nuclei via direct and/or indirect measurements. These experimental developments are novel and challenging, often requiring collaboration across different areas of expertise – e.g. mechanical and electrical engineering, nuclear physics, radiochemistry, and computational science. Opportunities for including technical contributors beyond nuclear science are needed to drive further innovation in this area.
3. With the difficulties in fielding the measurements with unstable nuclei, a system to share radioactive targets and special instruments amongst different facilities would enhance the completeness of nuclear data by studying multiple reaction channels simultaneously.
4. Predictive powers of reaction models are challenged by limited constraints and large uncertainties away from stability. Improved theory capabilities are needed for both reaction and integrated structure/reaction activities. Theory advancements will also support growing evaluation needs.
5. To effectively improve evaluation libraries, which lack in reactions on unstable nuclei, experimental, theory, and evaluation communities need to work closely for timely release of experimental data and sharing of theoretical efforts and progresses. Additional evaluators in both nuclear reactions and structure are needed to take on the increasing number of nuclei to be examined.

NEXT STEPS

The development of a new NDIAWG FOA is underway. Based on feedback from attendees, WANDA2023 will maintain the same format in a larger venue due to the increasing year-over-year attendance. There is interest to expand university participation, and the addition of a student poster session is recommended.

The NDWG updated its charter and is expanding its membership to include new federal agency representatives. Outreach and education with the broader community is ongoing.

A focused workshop on uncertainty quantification is in planning for early in FY23 to address uncertainty quantification methods and documentation for nuclear data. A need for improved data covariances has been identified across multiple applications. The goal of the workshop is to identify and prioritize activities for the next five to ten years in shared white paper.

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APPENDIX: SESSION SUMMARIES

APPENDIX A. NUCLEAR DATA FOR HIGH ENERGY ION INTERACTIONS AND SECONDARY PARTICLE PRODUCTION

1. Background and Introduction

The wide range of energies (up to ~TeV) and species (Z ~ 1 – 28) of Galactic Cosmic Rays (GCRs) make it very challenging to determine all of their potential effects on spacecraft and astronauts. However, this wide variety of particle characteristics produces overlaps of space research with many areas of nuclear science, including spallation sources, isotope production, ion beam analysis, fusion reactions, nucleosynthesis, fission reactors, and more. These overlaps can be exploited to better understand how to shield space missions most effectively from the effects of GCRs.

The flux and elemental composition of GCR "primaries", which are well-characterized as functions of energy, serve as the foundation for studies of their interaction with matter. Our atmosphere provides a protective barrier against direct effects of GCR primaries on Earth-based systems (and humans). The showers of particles (*e.g.*, pions, muons, neutrinos, electrons, gamma rays) generated via collisions of GCRs with nuclei (*e.g.*, ^{14}N) in the atmosphere are overwhelmingly harmless, with only a small fraction reaching the Earth's surface.

Above the atmosphere, however, the GCRs provide a serious impediment to the safety and viability of space exploration. Damage from GCR primaries can be serious, especially the 1% of primaries heavier than He, because damage scales as Z^2. Additionally, GCR primaries interact with spacecraft materials (*e.g.*, Al structures, polyethylene and composite shielding) to generate a complex cascade of secondary radiations (light ions, neutrons, gamma rays) which can further harm astronauts and disrupt or disable electronic systems. Shielding to reduce the GCR flux also serves as a target that can increase the secondary flux. Because of the wide variety of possible shielding materials and thicknesses, modeling is essential to determine the sensitivity of the secondaries (both flux and composition) to different shielding configurations, as well as to determine the subsequent harmful impact of those secondaries on electronic systems and humans.

The relevant space modeling efforts include simulations of the transport of primaries through materials to determine the flux and composition of secondaries, the stopping of secondaries in electronic systems and tissue, and the resulting damage from the deposited energy.These simulations inform the overall design of spacecraft to optimize shielding configurations given all relevant constraints (*e.g.*, weight, volume, dose limits). They require, as input, nuclear reaction cross sections, secondary particle emission energy and angle, and stopping powers.

2. Current status and Nuclear Data Gaps

The sections below detail the current the state-of-the-art and the relevant nuclear data gaps for experimental measurements, compilations, databases, disseminations, reaction models, sensitivity studies, and uncertainty quantification relevant for space science. It also covers end-user applications including transport simulations, studies of effects on electronics and humans, and spacecraft design. Areas of space research that can most benefit from cross-disciplinary collaborative research efforts are emphasized.

2.1. Experimental Facilities

In the US there are experimental facilities that carry out nuclear measurements for space research, such as the Radiation Effects Facility at Texas A&M University (TAMU); the Berkeley Accelerator Space Effects (BASE) facility at Lawrence Berkeley National Laboratory (LBNL); the NASA Space Radiation Laboratory (NSRL) at Brookhaven National Laboratory (BNL); the Single Event Upset Test Facility (SEUTF) at BNL; and the new FRIB Single Event Effects (FSEE) test facility at Michigan State University (MSU).

There are other accelerators in the US that have so far not been utilized for space research, including: the ATLAS facility at Argonne National Laboratory (ANL); the Relativistic Heavy Ion Collider (RHIC) at BNL; the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Laboratory (JLab); the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL); the Los Alamos Neutron Science Center (LANSCE) and Weapons Neutron Research (WNR) Facility at Los Alamos National Laboratory (LANL); and the Tevatron at Fermilab National Accelerator Laboratory (FNAL). Finally, there are three accelerators that have been recently decommissioned – the K500 and K1200 cyclotrons at MSU and an SC360 Cyclotron at Provision in Knoxville, TN.

In Europe, 9 accelerators in 7 countries have been used for space research. These include: the Heavy Ion Facility (HIF) and Light Ion Facility (LIF) at the Université Catholique de Louvain (UCL) in Louvain-la-Neuve, Belgium; the RADiation Effects Facility (RADEF) at the Accelerator Laboratory at the University of Jyväskylä, Finland; the G4 facility at the Grand Accélérateur National d'Ions Lourds (GANIL) in Caen, France; the Heavy Ion Synchrotron SIS18 at the Gesellschaft fur SchwerIonenforschung (GSI) Helmholtz Centre for Heavy Ion Research in Darmstadt, Germany; the INFN Southern National Laboratory (LNS) in Catania, Italy; the Holland Proton Therapy Center in Delft, the Netherlands; the KVI Center for Advanced Radiation Technology (KVI-CART) facility at the University of Groningen in the Netherlands; the CERN High energy AcceleRator Mixed field facility (CERN CHARM) at CERN in Geneva, Switzerland; and the Proton Irradiation Facility (PIF) at the Paul Scherrer Institute (PSI) in Switzerland.

Each of the facilities listed above have different maximum beam energies and intensities, detector stations, number of hours available for users, and specializations. What they have in common, however, is that the requests for beam time from users significantly outstrips the availability. The space electronics effects community, for example, has requested twice the available beam across the relevant US facilities in FY22; that factor is expected to grow even larger in the coming decade. It is possible that a portion of this demand could perhaps be met by repurposing existing accelerators that have become dormant, such as the K500 and K1200 cyclotrons at MSU or the Provision SC360 Cyclotron in Knoxville, TN.

Understanding the effects of GCRs with the highest (well over ~GeV) energies is important to the Space Radiation Protection community. However, with no measurements at projectile energies over 3 GeV/u, simulations of these effects lack an empirical foundation. Higher-energy measurements are also required to understand electronic effects in the latest circuits whose size is greater than the range of ions from nearly all accelerators used in these studies so far. There is, however, a possibility to fill this critical nuclear data gap by using beams from the Relativistic Heavy Ion Collider (RHIC) at BNL. A beam time proposal was recently made to bombard C, Al, and Fe targets with He, C, Si, and Fe ions at energies from 3 – 50 GeV, and to detect the light particle production (the "secondaries") with the STAR detector. This measurement, however, would have to be completed in the next few years before the conversion of RHIC to the Electron-Ion Collider (EIC) project begins.

An additional capability needed for space research accelerator measurements is a larger beam size to support electronics testing. Traditional accelerators have beam spot diameters that are capable of irradiating one chip at a time, and rastering and defocusing techniques now enable some of the facilities mentioned above to irradiate batches of chips. However, by irradiating large, complex subsystems all at once, the laboratory measurements more realistically reproduce the GCR damage inflicted in space. The special approaches needed to obtain wide beam diameters while keeping uniform beam density could be implemented at accelerators carrying out space-based research.

2.2. Databases, Disseminations, Compilations

At present, the primary means of dissemination of nuclear reaction cross sections measurements relevant for space research is via literature publications. There are, however, two compilations of this valuable data. The first is an online GSI - ESA - NASA database that contains 1786 data points from 110 peer-reviewed publications. The second is NUCDAT, a private data collection that contains 50,000 entries. The coverage of relevant ions, bombarding energies, and targets in these databases is a small fraction of the data needed for effective modeling.

It should be noted that both of these collections were compiled independently from the major nuclear data organizations (*e.g.*, the IAEA Nuclear Data Service or the US National Nuclear Data Center). The international standard reaction databases for nuclear reaction data, EXFOR (compilations) and ENDF (evaluations), have limited applicability for space research, as they are focused on neutron-induced reactions below 14 MeV. They do, however, contain some cross sections up to 200 MeV and a few charged-particle induced reactions. Finally, the OECD NEA Shielding Integral Benchmark Archive and Database (SINBAD) has some integral cross section information that is useful, such as a set containing measurements of 100–800 MeV/u He, C, Ne, Ar, Fe, Xe, and Si ions bombarding C, Al, Cu, and Pb targets.

There are also a number of specialized databases within the space electronics effects community, including (in the US) collections at NASA Goddard Space Flight Center (GSFC) and NASA Jet Propulsion Laboratory (JPL), and (in Europe) the Electronic Data Sheets at the ESA. A number of factors have, unfortunately, impeded the coordination between these different collections, including the different systems measured, proprietary data, security, formats, and funding to initiate and (especially) maintain a more unified data library.

The current disjoint collections of nuclear and electronic effects data sets for space research could benefit tremendously from the decades of experience in the nuclear data community in establishing, curating, combining, and disseminating data sets. By linking these datasets together and creating new customized collections, the nuclear data community could greatly improve access to the existing data that are so critical for simulations in space research studies. This effort would also be invaluable to guiding future experimental work, as gaps in the measurement data could be more easily accessed.

2.3. Reaction Models

Because *all* the relevant cross sections will never be measured, nuclear reaction models are critical for simulations that transport GCR primaries through spacecraft materials and predict the flux and composition of secondaries. Results of these transport simulations are subsequently utilized in electronic effects, human effects, and spacecraft design simulations. Nuclear reaction models are also essential to predict the yield, and therefore determine the viability of, accelerator-based measurements of reactions important for space research.

The space research community has had some successes with phenomenological nuclear reaction models. One notable example is the Double Differential Fragmentation model (DDFRG) which has been fine-tuned to agree with measurements in the NUCDAT collection mentioned above in section 3.2. Other models include NUClear FRaGmentation (NUCFRG), which uses an abrasion–ablation formalism, and the self-consistent Relativistic Abrasion–Ablation FRaGmentation (RAADFRG) code. Semi-empirical parameterizations (*e.g.*, Hybrid Kurotama, Kox-Shen) have also shown reasonable agreement with some datasets, and a number of such formulations have been collected and put online in the GSI-ESA-NASA database mentioned above.

For energies ranging from 0.1 – 1 GeV/u, most of the terms in reactions models (*e.g.*, pre-equilibrium, de-excitation, evaporation, intra-nuclear cascade, fission…) are reasonably well understood, but more data are needed to fine tune these models. However, the state-of-the-art models of the highest energy reactions in the space community lag recent work being done in the relativistic heavy-ion collision (RHIC) community. While the former conceptualizes heavy ion reactions in terms of abrasion, ablation, and coalescence, the latter embraces models that build up hadronic reaction products from quarks and gluons. A good example of such a RHIC-related model is the Ultrarelativistic Quantum Molecular Dynamics (UrQMD) model; this model predicts the yields of protons and neutrons measured at RHIC from the bombardment of Be and Au targets with 15 GeV protons. The utilization of this, and other, RHIC codes for predicting the yield of secondaries resulting from GCR transport through spacecraft materials would, when combined with additional higher-energy data, significantly advance the simulations needed to make space exploration safer.

2.4. End-User Applications

Some of the most critical end-user applications in space research are radiation transport simulations, electronics and human effects studies, and spacecraft design. Below we detail the current the state-of-the-art and relevant nuclear data gaps for each, with an emphasis on cross-disciplinary collaborative research efforts that can best impact space exploration.

2.4.1. Radiation Transport

Modeling the transport of GCRs through spacecraft materials is needed to characterize the flux and composition of secondaries. The space science community has invested 30 years of development in 3DHZETRN (3D High charge(Z) and Energy TRaNsport), a suite of deterministic (*i.e.*, non-Monte Carlo) codes that numerically solve the Boltzmann transport equation in three dimensions. With NUCFRG as its core nuclear reaction model, 3DHZETRN can calculate GCR-induced radiation levels for a variety of simple shielding configurations. This code, which is orders of magnitude faster than Monte Carlo (MC) transport codes, has been extensively benchmarked in simple slab geometries, with results comparing favorably with three-dimensional MC calculations. It should be noted, however, that MC codes can simulate the complex shielding geometries that more realistically represent those used in spacecraft.

Other transport codes from the space community include HETC-HEDS, SHIELD, and COMIMART-MC. Related code systems include OLTARIS (On-Line Tool for the Assessment of Radiation In Space), a web tool using HZETRN and NUCFRG to study the effects of space radiation for on spacecraft, humans, and electronics, and PLANETOCOSMICS (ESA) that uses GEANT (described below) for transport.

Transport simulations are also used throughout nuclear and particle physics, for applications ranging from accelerator shielding to thick-target isotope production to detector characterizations and calibrations to deciphering integral measurements. Some popular particle transport codes include FLUKA, PHITS, Geant4, and MCNP. These Monte Carlo (MC)-based codes have built-in nuclear reaction models, optimized over different energy ranges, and some have options to adjust model parameters to the problem at hand. In many cases, users only need to specify the geometry of the "target" and the input radiation field, and the code package handles all the transport calculations. These transport codes have been validated through extensive comparison with integral experiments, with some primarily at lower energies (*e.g.*, MCNP, Geant4) and others at higher energies (*e.g.*, FLUKA, PHITS).

In an alternative approach, the RHI community has extensive capabilities to simulate the production of light ions resulting from heavy ion collision. While the RHI codes are often used to extract QCD parameters from the central collision region, some (*e.g.*, the UrQMD model described above) already have the capability to predict yields of light particles. With some adaptation, other RHI codes may be helpful for modeling the interactions of the highest energy GCRs with spacecraft materials.

Finally, it may be advantageous for the space transport community to investigate the use of advanced computing approaches (*e.g.*, cloud computing, grid computing, machine learning, acceleration with graphical processing units (GPUs). Higher computing power can enable more and more complex systems to be modeled to a higher degree of spatial and energy resolution. An example of one such approach (GPU acceleration) for human effects research is discussed below.

2.4.2. Electronics and Human Effects

The secondaries generated by transport of the primary GCRs through spacecraft materials can disrupt and disable electronic systems and harm astronauts. Understanding these effects requires extensive modeling benchmarked by experimental measurements. For both human effects and electronics effects, modeling with higher spatial fidelity is needed. In electronics, the ~sub-micron size of the smallest features of the new, high-density systems is pushing a need for improved predictions of the species, angles, and energies of the produced secondaries. Such information, when combined with ion stopping power, enables MC-based codes like MRED to track these ions and their energy deposition within a chip. However, higher energy measurements are needed to probe the full physical range of the newest larger circuit elements and subsystems.

The push for higher spatial resolution in human effects modeling is driven by the need to more precisely inventory the damage that GCRs inflict at the sub-cellular level. Advances in ion-beam therapy for cancer patients on Earth are driving innovations that can benefit space effects research. An example is the development of a custom kernel for a nuclear reaction that includes terms for intranuclear cascade, particle evaporation, and non-elastic Barashenkov and Glauber-Gribov cross sections. This model shows very good agreement with measurements of, for example, 200 MeV protons bombarding ^{16}O targets. Planned improvements to this approach include expanding the physics models to accommodate ~GeV energies and heavier ions and shrinking the spatial resolution of the model (when combined with transport through human tissue) by a factor of 10^2 - 10^3. In order to achieve such improvements, the kernel will be ported to GPUs to enable the use of high performance computing (HPC) resources. A first effort to port the existing kernel has already resulted in transport simulations running 200 times faster than an equivalent simulation with Geant4. When coupled to tissue-damage codes as described below, this effort has the potential to significantly improve the fidelity of models predicting sub-cellular damage in humans resulting from bombardment by GCRs, and therefore to eventually improve the safety of human space exploration.

Two noteworthy studies of tissue damage involve coupling Geant4 to biological simulations. One is the Geant4-DNA code, a low-energy extension of Geant4 that enables studies of the cellular radiobiological effects of ionizing radiation on DNA, considering the physical, chemical, and biological stages of the interactions. Geant4 has also been coupled to the CompuCell3D cell biology simulation platform via the RADCELL module, enabling tumor geometries to be ported to the transport code. The ion stopping powers in various materials are key inputs for these codes. Such stopping powers were discussed in detail in a separate dedicated session at WANDA 2022.

2.4.3. Spacecraft Design

The design of a spacecraft must carefully fold together details of the mission objective, payload instruments and plan, and the subsystems to support the payload including power, propulsion, structure, communications, data handling, and more. Because many of the requirements of different subsystems will conflict, optimization plays a critical role in the overall design. Nuclear physics and spacecraft design overlaps in the area of radiation protection. As noted above, the shielding to reduce the GCR flux is also a target that influences the flux of secondaries, with thicker shielding also impacting the structure and propulsion design.

Two of the major uncertainties in shielding design are the space radiation environment and incomplete information for radiation transport calculations. The space environment changes over the duration of a mission, while realistic radiation transport requires the best transport codes, along with accurate inputs of the radiation environment, all available relevant nuclear data for all particle interactions, and information on stopping powers to better assess damage to electronic systems and astronauts caused by deposited energy. Gaps in our knowledge, especially related to nuclear data, were discussed above for most of these issues – cross sections, nuclear reaction models, transport codes, experimental measurements for code benchmarking, and energy deposition studies. The challenge to the spacecraft designer is to balance conflicting requirements to arrive at an optimal configuration.

Recently, work has focused on improving radiation transport modeling, both by more refined codes and, especially, by improving the nuclear physics input. The previous section detailed the motivations for enhancing the spatial resolution of transport models to simulate the effects of GCR impact on electronics and astronauts: the need to study higher density circuit elements with spatially smaller features and the desire to model sub-cellular tissue damage. Other critical areas of investigation in this field are sensitivity studies and uncertainty quantification; these are described in the following subsection.

Finally, significant advances are being made in the development of surrogate models and in dimensional reduction within a machine learning (ML) framework for optimizing model predictions across enormous parameter spaces. The application of such approaches, especially if combined with GPU acceleration and the use of HPC resources, could advance the design of safer spacecraft.

2.4.4. Sensitivity Studies and Uncertainty Quantification

Understanding the sensitivities of models for space applications to the nuclear physics inputs is necessary to identify the most critical nuclear data gaps in space research. Sensitivity studies of the generation of GCR secondaries have, for example, shown the importance of cross sections for p, n, and alpha particle production under bombardment by particular (*e.g.*, O, Mg, Si, Fe) ions. More such studies need to be done to cover the full range of the physics input to models of GCR damage.

The decades of experience with sensitivity studies in the nuclear data community suggest that critical advances can be made in space science through collaborative, cross-disciplinary efforts. Some of the existing sensitivity tools in the nuclear data community include: TSUNAMI, TSAR, SEN3, and SAMPLER (ORNL); Whisper and Crater (LANL); Nuclear Data Sensitivity Tool (NDaST) (OECD NEA); SUSD3D (JAEA); NUSS-RF (PSI); FICST (McMaster Univ.); RMC (Tsinghua Univ.); and GPT-free in OpenMC (MIT/Purdue/VCU). While many of these tools were built specifically to determine the sensitivities of input nuclear cross sections on nuclear reactor performance (*e.g.*, k_{eff}) or for nuclear criticality safety studies, some are more general and could potentially be adopted to address sensitivities critical for space research.

Sensitivity studies can be used to translate the uncertainties of the inputs to a model into uncertainties in the model predictions. While uncertainty quantification (UQ) approaches in general have been a high priority in the nuclear data community, they are not widely adopted in the space research community. The combination of Bayesian approaches with ML tools have recently begun to set the standard for assigning uncertainties to model predictions in the nuclear science community. Collaborative efforts between the two communities could, for example, enable nuclear cross section uncertainties to be propagated through transport model to uncertainties in the characteristics of the flux of secondaries, and subsequently propagated through specialized codes to assess uncertainties in electronics and tissue damage.

Combining such UQ approaches with sensitivity studies can then guide future work in measurements, nuclear reaction theory, transport models, and stopping power codes. EUCLID (LANL) is the first of a new generation of tools in the nuclear community that uses this combined approach for reactors or critical systems. By combining sensitivity studies, uncertainty quantification, nuclear data set adjustment, and ML-driven design of experimental measurements, this tool will be able to identify which new measurements would provide the tightest constraint on predictions for an end-user application. A EUCLID-like tool for the space research community could assign uncertainties to model predictions, identify critical data and theory gaps, and recommend approaches to best fill those gaps.

3. Discussion

Simulations of the flux of GCR secondaries in spacecraft depends on nuclear reaction cross section measurements and theoretical models, as well as on transport codes and spacecraft materials. The harmful effects of these secondaries subsequently depend on their composition, energy, angles of incidence, and stopping powers in a wide range of electronic devices and human tissue. To make space exploration missions viable and safe, spacecraft designers must optimize shielding configurations that minimize these harmful effects over the duration of a mission with its changing radiation environment and this optimization must handle conflicting constraints imposed by the other major subsystems of the vessel.

An “ideal” inventory of the tools and data needed for such space studies could include the following items:

(a) a complete set of reaction cross sections with uncertainties for the generation of light-ion secondaries (with high-fidelity energy and angle information) from light- and heavy-ion bombardment, at energies up to ~50 GeV;

(b) a radiation transport code with high spatial resolution that can handle complex shielding material configurations and that can generate uncertainties in secondary energies and angles from input nuclear data uncertainties;

(c) simulations that determine the harmful energy deposition of secondaries, along with uncertainties propagated from input uncertainties, in electronic devices (human tissue) at the sub-micron (sub-cellular) level;

(d) codes that can perform the simulations described above in a time-dependent radiation field, and can optimize spacecraft subsystem design within propagated uncertainties;

(e) codes that can utilize sensitivity analysis techniques at each of the above steps to identify the most critical nuclear data and recommend measurement approaches.

Many of these suggestions will require significant efforts, especially the measurements at higher energy and uncertainty propagation through the wide variety of simulations. However, given the expertise of the nuclear data community in these areas, some progress towards these “ideals” can be made by the following collaborative cross-disciplinary research efforts.

(a) Performing measurements at the STAR detector at RHIC to provide some unique data at higher energies than currently available; coordinating beam time requests at accelerators; coordinating plans to effectively re-use dormant accelerators; borrowing approaches from the nuclear data community for the compilation, dissemination, archiving, and data management of accelerator measurements for space research; modifying nuclear reaction models developed in the RHIC community to significantly advance predictions of unmeasured reactions at high energies;

(b) Utilizing HPC resources for MC-based transport codes to enable transport simulations with complex shielding material configurations;

(c) Porting transport codes to GPUs and utilizing HPC resources to enable the higher spatial fidelity simulations needed for modern electronic devices and sub-cellular damage assessments;

(d) Utilizing ML approaches like surrogate models for the optimization in spacecraft design;

(e) Developing a EUCLID-type ML-driven code for space science to automate sensitivity studies, identify nuclear data outliers, and recommend new experiments.

4. Recommendations

The discussions here highlight the many overlaps between space science and nuclear science that can be expanded upon to study the effects of the broad range of GCR energies and species on electronics and humans. By effectively exploiting these overlaps, progress can be made in improving vessel design to make space exploration safer and more viable for humans.

Some of the most fertile topics for collaborative work include: making additional cross section measurements with high energy ions, especially the STAR detector at RHIC; coordinating accelerator beam time requests; borrowing approaches from the nuclear data community for the compilation, dissemination, archiving, and management of nuclear data; utilizing advances in nuclear reaction theory by the RHIC community for modeling reactions important for GCR secondaries; and adopting UQ, sensitivity analyses, ML approaches, and HPC resources to better model highly complex space systems with proper uncertainty propagation.

Through these cross-disciplinary, collaborative research projects, the state-of-the-art in space research could be significantly advanced, resulting in safer space exploration.

APPENDIX B. NEUTRONS AS SECONDARY PARTICLES AND THEIR INTERACTION WITH MATTER

I. Introduction

The primary radiation field in space is composed of galactic cosmic rays (GCR), solar energetic particles (SEP), and when in the magnetic fields that surround particular planets in the solar system, trapped belt radiation [1], [2], [3]. Because the lifetime of a free neutron is short (approximately 880 seconds), there are no neutrons in the galactic cosmic ray spectrum, and an insignificant number in the energetic particle spectrum emitted from the sun. However, as GCR, SEP and trapped belt radiation interact with matter in space, the secondary neutron field created by those interactions can comprise a significant fraction of the radiation environment.

Due to their high penetrability and large biological radiation weighting factors, neutrons pose a risk of radiation induced effects such as cancer, leukemia, heart conditions, neurological malfunction, cataracts, and others. Neutrons also pose a risk to electronics where their interactions in sensitive components can create high-LET (Linear Energy Transfer) recoils leading to detrimental effects. On the other hand, because of their high penetrability and significant nuclear interaction cross sections, secondary neutrons can provide a benefit for planetary geologists looking to determine the elemental composition in extra-terrestrial bodies through detection of neutron-induced radionuclide signatures.

No matter the application, understanding the effects from secondary neutron production in space requires an accurate data base of nuclear cross sections and benchmark measurements. These data will help improve transport model calculations and resolve discrepancies observed with previous measurements, which in turn aid in the development of shielding strategies for manned and unmanned missions. This session on secondary neutrons presented an overview of the current issues and data needs related to secondary neutrons in space relevant to shielding and planetary spectroscopy. Along with the “Nuclear Data for High Energy Ion Interactions and Secondary Particle Production” and ”Stopping Powers, Energy Deposition and Dose” sessions, a comprehensive examination of nuclear data for space applications was presented.

II. Space Radiation Protection

Secondary neutrons are produced by interactions of galactic cosmic rays, solar energetic particles, and trapped belt radiation. The range of particle energies, species and materials included in those interactions is vast. GCR ions span energies ranging from keV per nucleon up to several tens of TeV per nucleon and, span the naturally occurring isotopes in the periodic table [1], [2]. Protons comprise approximately 89-90 percent of the GCR flux, He comprises 8-9 percent, and the remaining 1-2% are ions heavier than He, although the flux drops dramatically after Fe and Ni. SEP are created by solar activity such as coronal mass ejections and are primarily protons, with a small fraction from helium. The flux is dominated by proton energies below 50 MeV, but the energy spectra can go up to several hundred MeV in some events [1], [2]. Trapped belt radiation around Earth contains energetic protons and electrons. The trapped inner belt proton differential spectrum peaks around 20 MeV and drops exponentially out to several hundred MeV [2]. Trapped outer belt electrons range from 10’s of keV up to 10 MeV [2]. The list of materials in which interactions take place also span the stable elements in the periodic table. and materials composed of elements that also span the periodic table [4].

Protecting crew and electronics from the secondary radiation field created by GCR, SEP and trapped radiation is achieved primarily by shielding which limits both the production of neutrons and attenuates the neutron flux once it has been created. Because of the complexity of the space radiation environment, ground-based testing of shielding designs under full GCR/SEP/trapped-belt conditions is impractical. Instead, radiation transport models are used to investigate shielding materials and designs under a multitude of mission scenarios. Those models require an extensive data base of nuclear interaction cross sections and thick target yields to verify the accuracy of their calculations.

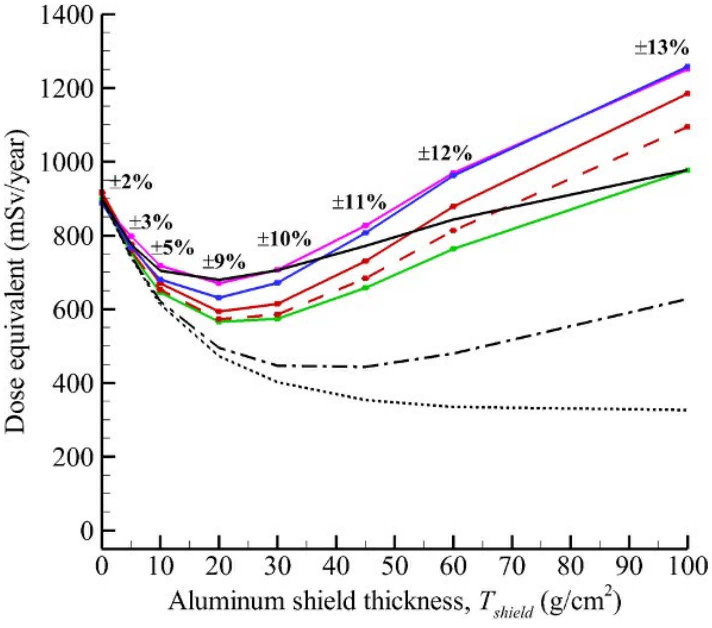

Figure 1: *Predicted dose equivalent rates from neutrons and ions behind varying thicknesses of aluminum using several transport models [5].*

A comparison of the predictions of dose, dose equivalent and effective dose from several transport models was detailed in Ref. [5]. Separate calculations were run for aluminum shielding and polyethylene shielding, with aluminum being a commonly used material for missions in space, and polyethylene being used because of its excellent shielding properties for GCR [6], despite its unfavorable structural properties. **Figure 1** from Ref. [5] shows the dose equivalent as a function of aluminum shielding thickness, with thickness in units of g/cm^2. The increase in dose equivalent beyond 20-30 g/cm^2 is found in Ref. [5] to be due to the buildup of secondary light ions (p, d, t, ^{3}He, ^{4}He) and neutrons, with protons comprising approximately 70% of the buildup. Calculations with polyethylene show similar results, although the dose equivalent doesn't increase beyond 20-30 g/cm^2, but instead remains constant. In either case, the results indicate that there is an optimal shielding thickness for reasonable and cost-effective shielding around 20-30 g/cm^2, and that there is a minimum dose equivalent rate that cannot be lowered with additional passive shielding out to 100 g/cm^2.

The contribution from secondary neutrons to the overall radiation environment is significant to both crew and electronics. The accuracy of transport model predictions of the neutron fluence depends both on the inherent physics models used in those codes as well as the neutron cross section data base. Determination of the accuracy of those predictions ultimately depends on comparisons either with neutron measurements made in situ, or with secondary neutron production cross sections and thick-target yields made at particle accelerators. Whereas measurements made in-situ take advantage of the full boundary conditions for GCR flux and shielding configurations, the instruments used are limited in the dynamic range of neutron energies they can measure. In addition, precise information on shielding thicknesses and external environments can carry significant systematic uncertainties to those measurements. Ground-based measurements at accelerator facilities have the advantage of well-understood experimental systematics and advanced detection systems with a broad dynamic range, but suffer from only being able to test a limited set of GCR ions and energies one at a time. Ultimately, the improvement of transport codes' accuracy in calculated neutron fluences relies both on the data base of in-situ and ground-based measurements to refine the physics models used in those codes.

The secondary neutron energy spectrum and dose has been measured in several space environments, including Low Earth Orbit LEO [7], lunar orbit [8], [9], on the lunar surface [10], and on the surface of Mars [11], for example. Measured neutron energies have been limited to energies up to 10-15 MeV, although the Mars Science Laboratory Radiation Assessment Detector (MSL RAD) has published neutron spectra up to hundreds of MeV. Secondary neutron measurements from the Lunar Prospector [12] were designed primarily to look for water on the Moon but are typical of the dynamic range available for most neutron instrumentation flown in space. **Figure 2** is from Ref. [12] and shows the comparison between measured data (red points) and Geant4 calculations (blue dashed line) of the entire neutron energy spectrum. Agreement between the measured data and code predictions is quite good but is over a very limited range of the calculated neutron energies.

Although the predicted flux of neutrons in Fig. 2 above 10 MeV drops exponentially, the neutrons above 10 MeV make a signification contribution the effective dose to crew members. **Figure 3** is from Ref. [12] and shows the contribution to the neutron effective dose as function of neutron energy, as calculated by GEANT4. The area under the curve is proportional to the lunar neutron effective dose rate. A large fraction of the effective dose is predicted to come from neutrons above 10 MeV, but there us no in-situ lunar data to verify that prediction.

Table I shows the contribution to the effective dose from neutrons determined by two measurements in orbit around the Moon. One measurement is from the Chandrayaan-1 RADOM instrument [13] and the other is from the Lunar Prospector instrument [12]. Shown in **Table II** are two separate measurements of the contribution from neutrons to the total absorbed dose, with one measurement made with the CRaTER instrument in orbit aboard the Lunar Reconnaissance Orbiter [14], and the other measurement made on the lunar surface aboard the Chang’E-4 rover [10].

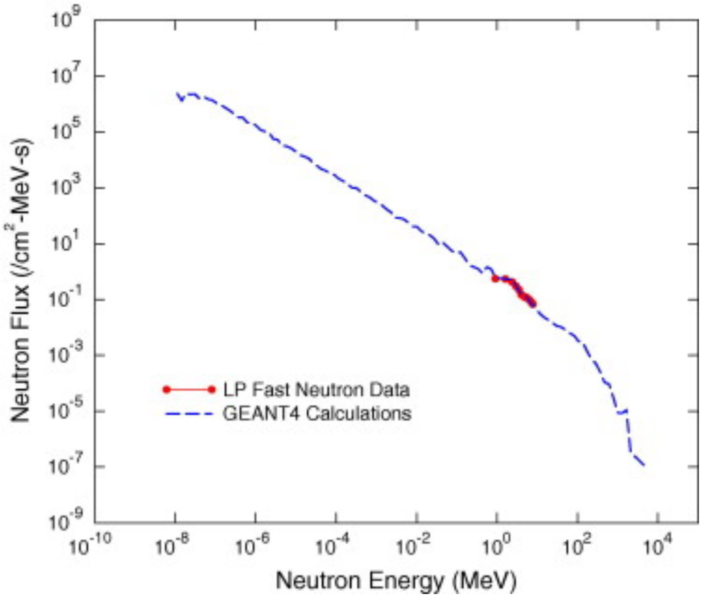

Figure 2: *Measured neutron albedo spectrum from the Lunar Prospector (red points) and GEANT4 calculations [12].*

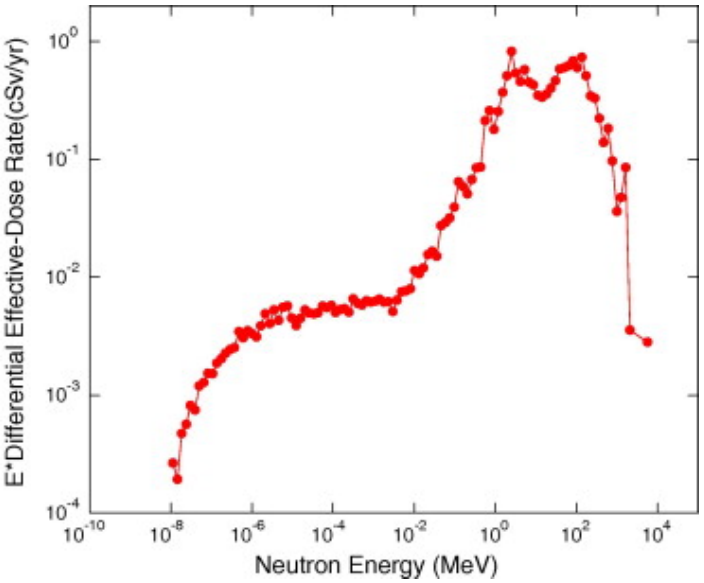

Figure 3: GEANT4 prediction of the differential lunar neutron effective dose rate multiplied by the neutron energy [12].

Table I. *Percent contribution to the total effective dose from neutrons determined from the indicated measurements in orbit around the Moon.*

Measurement	Percent contribution to the total effective dose
RADOM	2 – 20%
Lunar Prospector	16-18 %

***Table II.** Percent contribution to the total absorbed dose from neutrons determined from the indicated measurements in orbit around the Moon.*

Measurement	Percent contribution to the total absorbed dose
CRaTER (LRO)	< 1%
Chang'E-4	~ 23%

The determinations of effective dose by RADOM and Lunar Prospector are in agreement with each other, although the Lunar Prospector measurement reports a large range in its value. Effective dose requires a determination of the neutron energy spectrum to enable a conversion from dose to effective dose, and in the case for both RADOM and Lunar Prospector, required transport calculations to determine the neutron energy spectrum from their measurements. A more direct determination of the contribution from neutrons is the measurement of absorbed dose. There is an appreciable difference between the values of absorbed dose by CRaTER and Chang'E-4 in Table II, indicating the need for additional measurements. The measurement of neutron absorbed dose requires the capability to distinguish the contribution from charged particles from the neutron component, and differences in analysis techniques may be partially responsible for the differences noted in Table II.

***Table III.** Details of secondary neutron production cross sections from heavy ion interactions relevant to GCR transport. See text for explanation of each column. From [15].*

Beam ion and energy (MeV/nucleon)	Targets	Measured spectra	θ (deg)	Emin (MeV)	Facility
He (135)	C, Al, Cu, Pb	ddx n/dΩ total	0, 15, 30, 50, 80, 110	10 (all angles)	RIKEN
He (230)	Al, Cu	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	5.5, 5, 4, 3.5, 3.5, 3	HIMAC (PH2)
C (135)	C, Al, Cu, Pb	ddx n/dΩ total	0, 15, 30, 50, 80, 110	10 (all angles)	RIKEN
C (290)	C, Cu, Pb, marsbar	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	10, 3, 3, 7, 4, 3, 3	HIMAC (SB3)
C (400)	Li, C, CH_2, Al, Cu, Pb	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	8.5, 5, 3.5, 3, 3, 3	HIMAC (PH2 and SB3)
N (400)	C, Cu	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	6, 6, 5, 5.5, 5.5, 5	HIMAC (PH2)
Ne (135)	C, Al, Cu, Pb	ddx n/dΩ total	0, 15, 30, 50, 80, 110	10 (all angles)	RIKEN
Ne (337)	C, Al, Cu, U	ddx total	30, 45, 60, 90	12 (all angles)	LBL Bevalac
Ne (400)	C, Cu, Pb, ISS wall	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	9,6, 3.5, 3.5, 3, 3	HIMAC (SB3)
Ne (600)	Li, C, CH_2, Al, Cu, Pb, marsbar	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	6, 5.5, 4, 3, 3, 3	HIMAC (PH2 and SB3)
Ar (95)	C, Al, Cu, Pb	ddx n/dΩ total	0, 30, 50, 80, 110	10 (all angles)	RIKEN
Ar (400)	C, Cu, Pb	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	10, 7, 3.5, 3.5, 3, 3	HIMAC (PH2 and SB3)
Ar (560)	C, Cu, Pb, marsbar	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	10, 7, 3.5, 3.5, 3, 3	HIMAC (PH2)
Fe (500)	Li, CH_2, Al	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	12, 11, 7, 4, 3, 3	HIMAC (PH2)
Kr (400)	Li, C, CH_2, Al, Cu, Pb	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	20 (all angles)	HIMAC (PH2)
Xe (400)	C, CH_2, Al, Cu, Pb	ddx n/dΩ total	5, 10, 20, 30, 40, 60, 80	10, 6, 5, 3.5, 3.5, 3.5	HIMAC (PH2 and SB3)

Measurements of secondary neutron production cross sections and thick target yields at accelerator facilities have also provided data for validation and verification of the codes' abilities to predict the neutron environment created by GCR and SEP interactions. **Table III** shows a list of secondary neutron cross sections produced from heavy-ion interactions at energies relevant to GCR transport in various targets [15]. Beam energies are in units of MeV/nucleon. Targets include elemental targets, polyethylene, and the composite marsbar target composed of 85% simulated Martian regolith and 15% polyethylene. Where indicated, double-differential cross sections ("ddx"), differential angular spectra (n/dΩ) and total cross sections were measured. The fourth column indicates the laboratory angles where data was measured, and E_{min} indicates the lower threshold neutron energy at the corresponding angle. The accelerator facility is indicated in the last column.

The range of projectile masses covers much of the range of GCR ions. Given that over half of the GCR flux is above 1 GeV/nucleon, however, there is a lack of data at those energies. Most of the existing measurements were taken at forward angles (≤ 90°), and all measurements had energy thresholds no lower than 3 MeV. Neutrons created at angles greater than 90° and at energies lower than 3 MeV are significant contributors to the neutron albedo created by GCR interactions in planetary atmospheres and surfaces.

In addition to secondary neutron production cross section measurements, there have been several “thick-target” measurements, where the targets are thick enough that there is appreciable neutron production via interactions of secondary particles created by primary beam interactions, as well as appreciable interactions of the neutrons as they transport through the target. In most cases, the targets are thick enough to stop the primary beam. These data are typically used as benchmarks for comparisons with transport model calculations, providing an overall test of the codes’ abilities to handle primary and secondary interactions. **Table IV** provides a compilation of secondary neutron yields from thick-target measurements [15].

Table IV. *Thick target measurements of secondary neutrons produced from the indicated beams and targets. Double differential (TTY), angular and energy differential, and total yields were measured as indicated. Spectra were measured at the given angles and energy thresholds. From Ref. [15].*

Beam ion & energy *(MeV/nucleon)*	Targets *(cm)*	Measured spectra	Θ *(deg)*	Emin *(MeV)*
He (100)	C (5.0) Al (4.0) Cu (1.5) Pb (1.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	5.5, 5, 4, 3.5, 3.5, 3
He (155)	Al (8.26)	TTY n/dΩ total	10, 30, 45, 60, 90, 125, 160	10, 3, 3, 7, 4, 3, 3
He (160)	Pb (3.937)	TTY Total	0, 45, 90, 120, 150	10, 3, 13, 13, 13
He (177.5)	C (14.73) H_2O (22.86) Steel (4.445) Pb (3.937)	TTY Total	0, 6, 15, 30, 45, 60, 90, 120, 135, 150	3, 10, 11, 11, 3, 10, 3, 13, 3, 13
He (180)	C (16.0) Al (12.0) Cu (4.5) Pb (5.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	17, 11, 5.5, 6.5, 3.5, 3.5
C (100)	C (2.0) Al (1.0) Cu (0.5) Pb (0.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	4, 4, 3.5, 3.5, 3, 3
C (155)	Al (8.26)	TTY n/dΩ total	10, 30, 45, 60, 90, 125, 160	10, 3, 3, 7, 4, 3, 3
C (180)	C (6.0) Al (4.0) Cu (1.5) Pb (1.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	5.5, 5.5, 3.5, 2.5, 3, 2.5
C (400)	C (20.0) Al (15.0) Cu (5.0) Pb (5.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	8.5, 5, 3.5, 3, 3, 3
Ne (100)	C (1.0) Al (1.0) Cu (0.5) Pb (0.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	6, 6, 5, 5.5, 5.5, 5
Ne (180)	C (4.0) Al (3.0) Cu (1.0) Pb (1.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	9,6, 3.5, 3.5, 3, 3

Beam ion & energy *(MeV/nucleon)*	Targets *(cm)*	Measured spectra	Θ *(deg)*	Emin *(MeV)*
Ne (400)	C (11.0) Al (9.0) Cu (3.0) Pb (3.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	6, 5.5, 4, 3, 3, 3
Si (800)	C (23.0) Cu (6.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	11, 8, 8, 4, 3.5, 3.5
Ar (400)	C (7.0) Al (5.5) Cu (2.0) Pb (2.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	10, 7, 3.5, 3.5, 3, 3
Fe (400)	C (6.0) Al (4.0) Cu (1.5) Pb (1.5)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	12, 11, 7, 4, 3, 3
Nb (272)	Nb (1.0) Al (1.27)	TTY n/dΩ n/dE total	3, 6, 9, 12, 16, 20, 24, 28, 32, 36, 40, 48, 56, 64, 72, 80	20 (all angles)
Nb (435)	Nb (0.51)	TTY n/dΩ n/dE total	3, 6, 9, 12, 16, 20, 24, 28, 32, 36, 40, 48, 56, 64, 72, 80	20 (all angles)
Xe (400)	C (3.0) Al (2.0) Cu (1.0) Pb (1.0)	TTY n/dΩ total	0, 7.5, 15, 30, 60, 90	10, 6, 5, 3.5, 3.5, 3.5

The target thicknesses are given in units of cm in Table IV. All targets were composed of their natural ratio of isotopes. In contrast to the cross-section measurements, some of the thick target experiments included measurements beyond 90 degrees in the lab. The beam energies ranged between 100 and 800 MeV/nucleon, and the minimum neutron energies were between 3 and 20 MeV. Notably lacking in both the cross section and thick target measurements are experiments conducted for He projectiles above 200 MeV. He ions are the second-most abundant species in the GCR spectrum, and model predictions indicate that He interactions account for 25% - 30% of the neutron yield behind Al and polyethylene shielding [16].

The list of proton-induced neutron production cross sections and thick-target yields relevant to GCR transport is extensive (see, for example Refs. [17], [18], [19] and [20] and references therein). A moving-source parameterization of proton-induced cross-sections up to 3 GeV is also available [21].

In general, both the heavy-ion induced neutron production cross sections and thick target yields lack data above several hundred MeV per nucleon, with no He-induced data above ~250 MeV per nucleon. There is a lack of cross section measurements beyond 90 degrees in the laboratory system, and data for neutron below a few MeV is lacking. Nevertheless, the data have been useful for comparisons with transport model calculations [22].

3. Planetary Nuclear Spectroscopy

A. Background

Elemental and molecular composition of planets, moons and asteroids in the solar system through the measurements of neutrons and gamma-rays produced by interactions of GCR ions and their secondary particles in

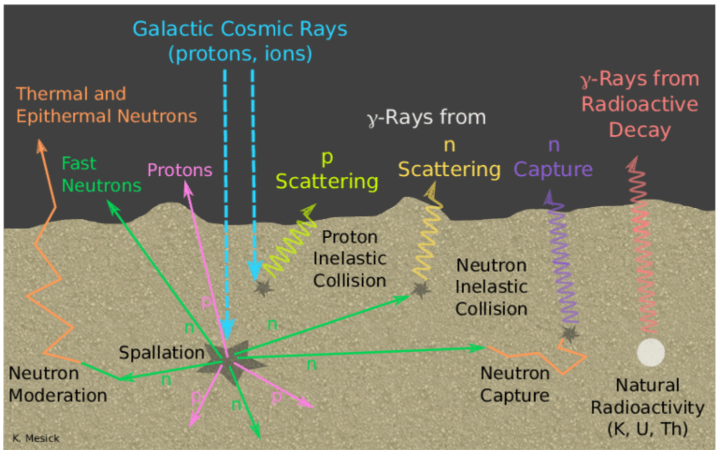

Figure 4: Schematic of cosmic ray interactions with planetary surfaces [29].

the surface of those bodies relies heavily on accurate nuclear data. In the case of secondary neutrons created by GCR interactions, spectroscopic analysis is not only accomplished by the direct measurement of neutrons (such as the studies in orbit around or on the Moon [23-26] and Mars [27-28]), but also through the activation of elements via activation by secondary neutron radiative capture and inelastic scattering. **Figure 4** shows a schematic developed by Mesick [29] that describes the processes leading to neutron production and activation via GCR interactions in local regolith.

Direct measurements of secondary neutrons have led to the findings of hydrogen (most likely water) on the Moon [24] and Mars [27]. The interactions producing those secondary neutrons are the same that lead to the neutron component of the radiation field behind shielding discussed in section II, and the nuclear data needs have been discussed there. Further interactions of those secondary neutrons in regolith, in particular inelastic scattering (n,n'γ) and radiative capture (n,γ), allow planetary spectroscopists to further analyze elemental composition via characterization of the gamma-ray spectra emitted from activated nuclei. The analyses of data involve the use of Monte Carlo radiation transport codes, meaning that the analyses are dependent upon the accuracy of the data libraries used by those codes.

For (n,n'γ) reactions, the neutron energy range of interest is from ~0.1 MeV to 50 MeV (depending on reaction threshold), and the range of interest for (n,γ) is from threshold to several MeV. The accuracy of the results from those studies rely on accurate (n,n´γ) cross section libraries.

B. Benchmarking (n,n'γ) Cross Sections

Recent experiments by Peplowski [30] show discrepancies between measured gamma rays from neutron activation and existing data libraries. Further results presented at WANDA 2022 provide additional evidence of issues between measured data and data libraries. Elements chosen for the experiments were required to have at least a 0.1% abundance in regolith, with O, Na, Mg, Al, Si, S, Cl, Ca, Ti, Fe, Co, and Ni chosen for the studies. The data libraries commonly used in Monte Carlo transport codes were chosen for comparison, including G4NDL 4.5 and 4.6, ENDF VI, VII and VIII, JENDL 3.3, CENDL 3.1, and BROND 3.1. Neutron sources used were a Cf source and DT generator. The gamma-ray channels selected were generally high-energy channels given the need for penetration of activation gamma rays through the surrounding regolith. For example, Si (1779 keV), O (6129 keV), and Fe (846, 1238 and 1408 keV) were chosen because of their relative abundance and high energy gamma ray emissions from (n,n'γ) interactions.

Ratio of model to measured cross sections varied as a function of the data library used in the model calculation. Comparison varied between libraries, and although one library may yield a better comparison for one cross section, another library would show a better comparison with a different cross section. No library was clearly better than any other across the entire set of measurements. If needed, one could select the best library for a particular interaction, or develop a hybrid library that used the best cross section for each interaction. However, that would involve a continual re-evaluation of comparisons between model and individual library and an update of the hybrid library as individual libraries are updated. To assure that comparisons had no dependence on the choice of Monte Carlo code, both Geant4 and MCNP6 calculations were run with the same libraries, and no differences were seen with those results.

Even with the development of a hybrid library, however, none of the data libraries would be able to be used for H, O, Na, Mg, and S (n,n’γ) interactions, where the model and data disagreed by at least 20%.

C. Nuclear Data Needs

As stated in Ref [31], nuclear (n,n’γ) data are the most critical need for planetary nuclear spectroscopy, over a side range of element (H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni), from threshold (0.1 to 1 MeV) to 50 MeV, preferable with less than 5% uncertainty. Also, large discrepancies (>20%) are seen for H, O, Na, Mg, and S targets. In addition to experimental data, continued evaluation of (n,n’γ) data libraries will improve comparisons between models and experimental data.

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APPENDIX C. PHOTON REACTIONS AND TRANSPORT

Background and Introduction:

An understanding of energetic photon transport and reactions are required for a variety of applications including active interrogation, space applicationsfission and fusion reactors. Current data for modeling and simulation are found in the nuclear data libraries maintained by the National Nuclear Data Center. This session discussed facilities and instruments for gamma-ray production, applications using incident photons, and data library production (including theoretical methods).

Facilities and Measurements: The two main accelerator-driven processes used to produce ɣ-ray beams for nuclear-physics research and applications are: Bremsstrahlung (including untagged and tagged sources) and Compton-scattering. The features of the beams produced by these two mechanisms enable complementary research opportunities. The broad energy spectrum of Bremsstrahlung sources enables measurements that survey the responses of nuclei over a wide excitation energy range. The narrow energy resolution of Compton sources gives an enhanced signal-to-background ratio relative to measurements performed using a Bremsstrahlung beam, and therefore provides heightened sensitivity enabling measurements of weaker nuclear excitations. In addition, the availability of linearly-polarized beams at Compton sources enables unambiguous determination of the spin and parity of excited nuclear states. Examples of each type of ɣ-ray beam source were presented in the session: the High Intensity Gamma-ray Source (HIGS), which is a Compton source operated by the Triangle Universities Nuclear Laboratory, and the Darmstadt High Intensity Photon Setup (DHIPS), a Bremsstrahlung source at the S-DALINAC at the Technical University at Darmstadt (TU-Darmstadt). A synopsis of the HIGS beam capabilities and research program is provided by Weller *et al.* [1], and Howell *et al*. [2] summarizes Compton ɣ-ray sources. A general overview of ɣ-ray sources is given in the recent review paper by Zilges *et al.* [3].

Security Applications: Non-intrusive inspection (NII) systems are deployed to generate images of conveyances using x-ray screening and help operators search for threats without opening cargo containers. The term "x-ray" here implies photons whether from atomic (x-ray) or nuclear (gamma-ray) processes. In addition to cargo screening, x-ray systems are used for nonproliferation and safeguards applications of non-destructive assay in material accountancy and object characterization. Photoatomic interactions are important for understanding image analysis and determining the atomic number of screened items, and photofission products are of particular interest for uniquely identifying and characterizing special nuclear material (SNM). Due to the complexity of an NII system, simulations and modeling are vital for system development. However, the complexity of the system and wide range of test cases required for many systems make simulations difficult and time consuming.

Medical isotope production: In nuclear medicine, radioisotopes are used for diagnostic and therapeutic purposes. Radioisotopes are attached to a bioconjugate molecule, such as a peptide, which selectively attaches to cancerous cells.

There is special interest in developing production methods for pairs of radioisotopes of the same element (or chemically similar elements) for which one has characteristics suitable for diagnostics and the other for therapeutics, and for which both can be produced in sufficient quantities and purities.

Photon-induced reactions offer another pathway for producing medical radioisotopes, and in some cases could provide radioisotopes with higher specific activity and/or more economically than current methods.

Photon data: The IAEA released the most recent and updated photonuclear data library in 2019, which is a product of the international research project coordinated by IAEA. The library includes 219 isotopes, and the photon energy was extended to 200 MeV. The evaluations were produced by nuclear reaction model calculations that were tuned to available experimental data. Although the IAEA library is the most complete set of the photonuclear data evaluations, there is room for improvement in both the reaction theories and the evaluated data.

State of the art summary:

Facilities and Measurements: The HIGS at Triangle Universities Nuclear Laboratory provides photon beams to experiments in the energy range from 1 to 120 MeV with an energy spread as low as 2% FWHM. The beam at HIGS has either linear or circular polarization. Measurements performed at HIGS are motivated by questions in nuclear structure, nuclear astrophysics, low-energy QCD, and applications in nuclear and homeland security, medical isotope production and ɣ-ray detector development, e.g., detectors used in space missions. Measurements performed at HIGS include: (ɣ,ɣ’) nuclear resonance fluorescence (NRF) cross sections with linearly polarized beams to unambiguously determine spin and parity of excited states; cross sections of (ɣ,x) reactions using real-time particle detection and activation techniques; photon-induced fission differential prompt and delayed neutron emission and fission product yields (FPY) - independent FPY via real-time detection of fission fragments and cumulative FPY via activation methods; photodisintegration of light nuclei; and Compton scattering from light and heavy nuclei.

The photon bremsstrahlung beam at the S-DALINAC accelerator facility at the TU-Darmstadt is produced by stopping the electron beam from the injector in a copper disk. The injector delivers electron beam currents up to 60 mA with a maximum beam energy of 10 MeV. The broad energy beams at these facilities enable research programs in photonuclear physics that overlap with and complement the program at HIGS below 15 MeV. The major research themes at the S-DALINAC facility at the TU-Darmstadt include: measurements of ɣ-ray strength functions using NRF for nuclear astrophysics applications, total photonuclear cross-section measurements for nuclear structure studies (e.g., shell effects of pygmy dipole resonance), and relative photoabsorption NRF measurements with precision sufficient to test chiral effective field theory calculations of light nuclei.

Security Applications: Current photon-based inspection systems focus on imaging used to search for the presence of special nuclear materials (SNM). Many available radiography systems use a radioactive source (e.g., ^{60}Co) or low-energy x-ray tubes for backscatter imaging. More advanced systems use an accelerator source to eliminate the need for radioactive material and provide better material penetration. The best material discrimination is achieved with a dual-energy source, which can estimate the effective nuclear charge (Z_{eff}) of materials using the differential attenuation of two photon energies. Advances have also been made recently in dual-species radiography, which combines information from both photon and neutron radiography.

Photofission products are currently the most telling and detectable signature of SNM, and interrogation systems should emit photons > 8 MeV (the higher energy in a dual–energy system) to effectively induce photofission. However, current federal and international regulations limit the maximum photon energy to 10 MeV. Efforts are underway in this energy range to measure actinide photonuclear and photofission cross sections, double-differential prompt emission profiles in energy and angle, and delayed emission energy spectra. These measurements will validate or highlight issues with currently available photonuclear data.

Medical isotope production: Simulations (using transport codes like GEANT4) are a cost-effective approach for designing systems for radioisotope production via photon-induced reactions. The reliability of such simulations depends on having libraries of accurate photonuclear reaction data at photon energies across the GDR (Giant Dipole Resonance) region where most of the photoabsorption strength exists. Cross-section measurements are needed to improve the accuracy and fill gaps in the database for photonuclear reactions relevant to producing radioisotopes important for medical treatment and diagnostics. The most straightforward way to measure photonuclear reaction cross-sections is to use quasimonoenergetic ɣ-ray beams produced by Laser Compton Scattering sources. ɣ-ray beams with a few percent energy resolution can map out the cross-section of all relevant photonuclear reactions in the GDR.

Incident Photon Theory and Data: The statistical Hauser-Feshbach codes, such as EMPIRE, TALYS, CCONE, MEND-G, GLUNF, CoH3, and YAHFC, are the central tools for producing the evaluated photonuclear data files. Since these model calculations have been significantly applied to neutron-induced reactions, some confidence in the photonuclear data evaluation can be gained by employing these model parameter inputs. However, efforts on theoretical development are still needed in a few areas including the photon entrance channel, the high-energy photon interaction above the GDR, and characteristics of photofission.

Traditionally, evaluated photonuclear and photoatomic data have been stored in the ENDF-6 format [ENDF6] and this format is currently the most common evaluated format in use. The NJOY [NJOY] processing code from LANL reads ENDF-6 formatted evaluated data and can process the data into the multi-group format GENDF for deterministic transport and the continuous energy format ACE for Monte Carlo transport. Many Monte Carlo transport codes can read the ACE format including the code MCNP [MCNP] from LANL. LANL has publicly released photonuclear and photoatomic ACE libraries which are available at https://nucleardata.lanl.gov. Several years ago, the photonuclear ENDF-6 library IAEA-2019 [IAEA-2019] was released that contains valid ENDF-6 formatted data that NJOY and MCNP did not support. LANL updated NJOY (version 2016.66) and MCNP (version 6.3), and both codes can now handle the IAEA-2019 data. LANL continues to update NJOY and MCNP to improve their support of photonuclear and photoatomic data. Recently, the Generalized Nuclear Database Structure (GNDS) [GNDS] for storing evaluated nuclear and atomic reaction data was developed by an international collaboration to overcome limitations in the ENDF-6 format. GNDS not only replaces the ENDF-6 format for evaluated data but can also replace processed multi-group and continuous energy formats like GENDF and ACE. The python code FUDGE (For Updating Data and Generating an Evaluation) from LLNL is capable of reading, processing and writing GNDS data. LLNL has also developed a C++ API dubbed GIDI+ (General Interaction Data Interface, plus) for reading GNDS files which LLNL uses in its transport codes. In addition, GIDI+ can sample GNDS data as needed by Monte Carlo transport codes. LLNL makes FUDGE and GIDI+ freely available at https://github.com/LLNL/fudge and https://github.com/LLNL/gidiplus, respectively.

The most popular transport codes to simulate photonuclear and photoatomic interactions are the Monte Carlo codes MCNP [MCNP] and GEANT4 [GEANT4]. Both codes can use data up to about 150 MeV incident photon energy. They both also have physics models that can be used in place of data or for higher incident energies. Both codes have been used in a myriad of simulation types including: medical studies, space science, detectors, accelerator studies and nuclear physics. Because of the lack of evaluated photonuclear data, by default MCNP has photonuclear turned off (i.e., users have to 'opt-in' to run with photonuclear interactions).

Discussion:

Security Applications: Beyond currently applied techniques, better understanding of photon interactions in SNM, structural materials and common cargo materials could lead to improved techniques for identification and characterization. In order of increasing maturity, these interactions include nuclear reactions from photons with orbital angular momentum (OAM), nuclear resonance fluorescence, and elastic photon scattering. Better understanding these phenomena may result in detectable signatures by using advanced sources, by making previously impractical measurements possible, or by improving the precision and accuracy of established techniques.

Medical isotope production: The production cross-section of the radioisotopes ^{47}Sc, ^{67}Cu and ^{195m}Pt was measured at the HIGS facility, via all possible photonuclear reaction pathways in targets of ^{nat}Ti, ^{nat}Cu and ^{nat}Pt, respectively. The measured production cross-sections of these radionuclides were a factor of 2-5 times higher than those in the TENDL calculated nuclear data library. These results illustrate the need for improved photonuclear data for reactions that produce medical radioisotopes.

Incident Photon Theory and Data: The photo-absorption cross section is a unique and important quantity in contrast to neutron-induced reaction cases, and the accuracy of the cross section directly propagates to the final evaluation. This issue is crucial for the evaluation of light elements, where the absorption cross section cannot be represented by simple Lorentzians. Predictions by microscopic theories may help, although the quality of the calculated results still does not meet the demand of technology applications. The pre-equilibrium decay in the photonuclear reaction should be revisited, as the current evaluations often mimic neutron-induced reactions. There are some inconsistencies in the pre-equilibrium modeling among the available Hauser-Feshbach codes, which may cause a large uncertainty in the evaluations at high energies. The photofission reaction needs more work, both theory development and experimental data, especially for the prompt and delayed neutrons and ɣ rays. The current evaluations for the major actinides do not contain the ɣ-rays produced by fission fragments, which requires new fission product yield (FPY) evaluations of photofission.

Recommendations:

Security Applications: Photonuclear data are essential for simulating systems that seek to detect photofission signatures, and the accuracy of these data for photon energies less than 10 MeV should be validated for actinides and other common materials. Established imaging techniques would also benefit from improved photon scattering physics in transport codes. Advanced techniques could be better understood and explored with data available for photons with OAM and improved data for NRF, including temperature dependence. Deficiencies have also been noted in the abilities of GEANT4 to simulate photonuclear reactions and produce accurate yields for photon energies less than 100 MeV. Efforts to improve tabular data in this range and implement accurate physics should be supported.

Medical isotope production: Photonuclear reaction production cross-sections of isotopes useful for nuclear medicine diagnostics and therapeutics should be measured, including reactions such as (ɣ,n), (ɣ,p), (ɣ,2n) and (ɣ,pn) at ɣ-ray energies in the GDR region (~1-40 MeV). An emphasis should be placed on isotopes which could be produced with a higher specific activity and/or more economically using photonuclear reactions as an alternative to neutron- or charged particle-induced reactions. The following represents an incomplete selection of isotopes which have been identified as meeting such requirements: ^{47}Sc, ^{44}Ti, ^{51}Cr, ^{64}Cu, ^{67}Cu, ^{99}Mo, ^{103}Pd, ^{117m}Sn, ^{169}Er, ^{195m}Pt and ^{225}Ac. In addition, photonuclear production of radioisotopes already effectively produced via neutron- and charged particle-induced reactions should be investigated as alternative pathways for producing these isotopes.

Facilities and Measurements: Experimental capabilities need to be developed to address multi-neutron emission cross sections at energies beyond the GDR. Exclusive cross-section measurements are also needed to describe individual nuclear reactions, where all of the secondary particles (products, residual nucleus) can be measured using activation techniques with monoenergetic photon beams. For example, (γ,2n), (γ,p), (γ,np) each indicate particular reactions where the particles in the incident and outgoing channels are all identified and known. At this medium energy region, where quasi-deuteron photodisintegration takes place, the pre-equilibrium process starts to dominate. These measurements would help to address the treatment of the pre-equilibrium photon-induced reactions.

Correlation measurements between prompt fission neutrons or photons, and fission fragments properties, in particular yield and total kinetic energy (TKE) as function of incident photon energy, will be very useful to constrain the free parameters used in the fission simulations codes. These data help develop model codes aimed at simulating prompt fission and ɣ-ray emission.

Incident Photon Theory and Data: Photonuclear reaction theories need to be developed in three areas, (i) the photo-absorption cross section, to which microscopic theories may be applied, (ii) the pre-equilibrium photonuclear reaction, and (iii) photofission properties. Photofission data include not only the photonuclear cross sections but also prompt and delayed neutrons and ɣ rays, which will require new FPY evaluations.

The need to transport photons in simulations is growing. Because of this, a more complete evaluated photonuclear library is requested. For example, while ENDF/B-VIII.0 has 557 isotopes with neutrons as a projectile, it has only 163 isotopes in the photonuclear library. Some libraries have many more isotopes in their photonuclear library (e.g., TENDL-2021 [TENDL-2021] has over 2000 isotopes and JENDL-5 [JENDL-5] has 1588 isotopes) but these data are not necessarily tuned to experimental data (i.e., they are not evaluated but model calculated). Several speakers lamented the need for more integral benchmarks to validate photonuclear data and model physics used in transport codes. The need for integral benchmarks is akin to the critical assemblies, reaction ratios or pulsed spheres used to validate neutron projectile data and transport codes. In addition, current photonuclear libraries do not have covariance data and several participants would like to see covariance data added to the libraries. Finally, since many Monte Carlo codes use the ACE format to access data, the specifications of the photonuclear and photoatomic ACE format should be completed and released.

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APPENDIX D. STOPPING POWER, ENERGY DEPOSITION, AND DOSE

Introduction:

Heavy-ions and beta-particles from nuclear reactions induced by the Galactic Cosmic Ray background and Coronal Mass Ejections lead to large local energy deposition (e.g., dose), particularly in the vicinity of the Bragg Peak. However, significant uncertainties exist in charged-particle stopping powers, introducing difficulties in the design of spacecraft shielding, fission fragment detectors, isotope production and ion-beam therapy. This session began with two presentations on the current state of computational codes and what their applicability is (Griffin, Montanari), followed by presentations that identified the shortcomings of some of the codes (Hecht) as well as additional improvements to databases that would be of use for safeguard applications (Croft). Stopping powers and the closely associated linear-energy transfer (LET) is important for NASA and the space community because it impacts the survivability of electronic components in harsh radiation environments. Presentations by Osherhoff, Turflinger, and Johnson, highlighted recent work that has been done on quantifying disruptive events in electronic components. The high-energy density (HED) physics community has recently been able to measure stopping powers of light-ions in hot and dense plasmas (Adrian) - which provides useful benchmark data for computational codes used in the design of HED experiments. Lastly, we also included two presentations on the needs of the ion-beam therapy community (Keppel, Obcemea). This session illustrated the breadth of applications of various stopping power data and its importance across many disciplines.

Computational codes and their applicability:

For stopping powers, computational approaches, such as those incorporated into the SRIM code, provide empirically calibrated stopping powers that can support a first analysis for most application. High fidelity first-principles calculations are also available in other codes and a comparison of these calculations with the empirically-calibrated models shed light on some of the community's needs – with respect to improved modeling and to expanded experimental measurements. Much more work needs to be done to address the stopping power in compounds where there is no pre-existing experimental data and to better understand the uncertainty in using today's approximations, i.e., the Bragg rule for compounds.

Patrick Griffin defined some of the underlying terminology and addressed how the nuclear data needs for stopping power are tightly related to the specifics of the application/mission space, i.e., the mission dictates the particle/type, energy, and material of concern. The application sets the cost/benefit perspective for investments in improving our nuclear data. Our application needs go beyond stopping power itself and most damage assessments focus on the partition of the stopping power into the electronic and nuclear partitions of the damage. While stopping powers are a microscopic metric differential quantity, many of our damage metrics address the integral metric related to the integrated electronic/nuclear damage along the ion track. Both our measurements and modeling of stopping power require a careful treatment of the associated uncertainty. Furthermore, we need to understand the energy-dependent covariance so that we can map these uncertainties into the integrated damage metrics along the ion track. We also need to understand the track structure and the defect evolution if we are to relate the stopping power to the relevant damage metrics. The second presentation by Claudia Montanari addressed the state-of-the-art for calculating stopping power and the status of the available experimental data. The state-of-the-art is captured at the IAEA website, https://www-nds.iaea.org/stopping/, a site that Dr. Montanari maintains for the community. While experimental data is critical, the community supports a range of models that cover different particles and the wide energy ranges (e.g., binary theory, PCA/UCA, TCS-EFSR, SLPA, MELF-GOS, CDW-EIS, etc.). Open areas that need attention include heavy projectiles (Li to U) and complex molecules (plastics and oxides). Significant differences exist between state-of-the-art models and experiment data for some cases, e.g., fission fragments on Mylar, oxygen on silicon nitrate, and gold on ^{238}U. New work in the area is addressing the role of machine language (ML) and deep neural nets in estimating the stopping power for compounds where there is no pre-existing experimental data.

Stopping power needs in the safeguard's community:

The stopping power of heavy ions produced from a fission source such as ^{252}Cf(s.f.) is required to interpret the fission product mass yield measurements. The interpretation of data is typically done using simulation codes such as the commonly used SRIM and MCNP codes. Measurements done at the University of New Mexico by Adam Hecht and his team show that the measured energy loss of a light product through a carbon foil of varying thickness agrees with SRIM and MCNP. However, this is not the case for a heavy product in which experimental measurements are bracketed by the two codes which differ by about 50% from each other in the predicted energy loss. Furthermore, when SiN is used as the target foil the energy loss measurements disagree with both codes for heavy *and* light fission products. MCNP and SRIM both use the Bethe-Bloch formulation of the stopping power but use different models for what the average charge state is of the ion (Z*). In MCNP6.2, Z* is given by the method of Bichsel, whereas in SRIM, the Brandt-Kitagawa method is used. Differences in the charge-state models lead to different predictions of the energy-loss for fission products in various target foils. An additional consequence of these differences is that predictions for the range of a particle is variable, depending on the computational code that is used, making it difficult to interpret experimental data. Improving theoretical models of the charge state distribution of an ion as it travels through a foil is difficult challenge - as was pointed about by Montanari. A potential path forward is to include the atomic physics community in discussions about improving the charge-state distribution models used in the codes. Such a collaboration was already suggested in the WANDA 2019 report.

The presentation by Croft and Favalli focused on the role of (α,n) reactions in nuclear safeguard applications, specifically the role of α stopping powers. (α,n) reactions is a ubiquitous source term in the nuclear fuel cycle and in using non-destructive techniques in probing special nuclear material (e.g., PuO_2). A recent example of how uncertainties in ^{19}F(α,n) energy spectrum impact the thick target yield of ^{234}U can be found in the work by Broughton *et al* in NIM A1009(2021)165485. An important observation by Croft was that the relative α –stopping cross sections in the MeV range for compounds are not as well-known as are the thick-target integrated-over-all-angles yield curves which can be measured with an accuracy of1-2%. Historical works have concentrated on the ^{19}F(α,n), and ^{4}He(^{19}F, n) reactions in gas targets as well as on the CaF_2, ZnF_2, SrF_2, LaF_3, and PbF_2 solid targets. But more work is required for materials of special interest such as UF_6, PuF_4, UO_2:2.5H_2O. An example of the uncertainty in the α stopping power in UF_6 and PbF_2 was shown where the NIST-ASTAR and SRIM(2013) predictions were compared, which are different by 1-3% over the 2-5 MeV range. This uncertainty, in-turn, affects the predicted neutron-yields that can be expected in these materials. Croft and co-workers have used a variety of sources for α stopping powers including (but not limited to) ASTAR, SRIM, MCNP, Ziegler, LaRC (a modified form of Ziegler's work), SPAR, and even early work done by Whaling in 1958. Unfortunately, there is much frustration in finding the original source material that is quoted in some of these databases and there is no consensus on what the "best value" is to use. Furthermore, there are no meaningful discussions on uncertainties of α stopping powers in the literature and there is limited guidance provided for compounds. Perhaps surprisingly, given their importance to the stockpile stewardship program, there are no readily-available $\alpha -$stopping power cross sections tables for transuranic elements such as Pu and Am. Limited data on UPu oxide and carbide exists but the quality of the data and use of the fitting functions don't support meaningful comparisons of UO_2 vs PuO_2 or UC vs PuC stopping powers.

NASA and the Space community:

Jason Osherhoff of NASA/GSFC made a presentation on *LET of Recoil Ions in Space Flight Electronics*. This presentation concentrated on proton recoil ions on wide bandgap semiconductors such as Gallium Arsenide (GaAs) or Gallium Nitride (GaN). He demonstrated the significant difference in the possible atomic number of the recoils (and their relative cross-sections) between silicon (Si) and GaN at energies of 50, 200 and 1000 MeV. However, while the recoil linear energy transfer (LET) is less effected by the proton energy in Si, it is impacted in GaN, and the resultant LETs are also much higher. There is wide interest in having better data on proton/neutron cross-sections and the recoil characteristics in many materials, including, but not limited to wide-bandgap semiconductors such as SiC, GaN and Ga_2O_3, as well as other materials such as GaAs, SiGe, and HgCdTe, as well as Cu, Ag, W, Ti, Ta, Sn and Pb. The question was raised if there is the potential for even higher LET particles from proton/neutron reactions on these materials. This leads to similar reasoning for nuclear data needs in the work by Turflinger, where proton-induced fission events are explored.

Capabilities of *The Berkeley Accelerator Space Effects (BASE) Facility* were presented by Mike Johnson of LBNL. This facility supports a variety of unclassified requests from national security sponsors and US space programs that are interested in the effects of radiation on sensitive electronic components. These tests, collectively known as Single-Event-Effects (SEE), help spacecraft survive galactic cosmic rays, solar particles, and planetary magnetic fields. Electron cyclotron resonance (ECR) ion sources such as AECR and VENUS have allowed for multiple beams ("cocktails"), increased the current and energy in the beams, while also improving the reliability of the beam. Improvements to the MARS ion source will eventually surpass the capabilities of VENUS. The *BASE* facility has the unique capability to make use of cocktail beams in which multiple ions can be injected simultaneously into the cyclotron, thus leading to an efficient method to deposit different amounts of energy (i.e., LET) into the sensitive volumes of electronics components used in SEE testing. Multiple beams allow for ions to be switched out on a timescale of minutes as opposed to 4 hours if only a single ion was used at a time.

Thomas Turflinger, from Aerospace Corporation, presented on *The Impact of Proton-Induced Fission Fragments on SEE: Community Need for Nuclear Data*. This work expanded on the two previous talks by looking at the impact of rare, but consequential proton-induced fission events. In this case, the fissions occurred in a gold-plated lid over the device, which was irradiated with 200 MeV protons. The result was unexpected destructive SEE events (DSEE), which appeared to be consistent with heavy ion data from ions with LETs much higher than expected in proton on silicon reactions. The DSEE event that occurred was well known in SEE literature but was not expected to occur with protons. The effect was also dependent on the electrical bias applied, which led to finding a safe operating area (SOA) for the devices. The study indicated that proton-induced fission events from the gold lid was consistent with the observed results, and suggested that the resulting ion fragments can have LET in the range of 20 – 45 MeV-cm^2/mg. Further research suggested that many other metals used in semiconductors and their packaging materials may also cause high LET fission events. A total of 16 metal samples with $28<Z<83$ were gathered, and further tests were performed where the part was used as the detector instead of the test sample. This study suggests that data on much of the desired proton-induced fission cross-sections does not currently exist. The experimental data demonstrated probable fission events in many of the tests. However, palladium (Pd) showed anomalously high SEE events, while bismuth (Bi) demonstrated anomalously low events. Using data systematics, a first order tool was developed to show what LET and range particles (in Si) are expected with various elements. Issues with tungsten (W), palladium (Pd) and lead (Pb) were used to provide more detail on why such data is required to support future SEE work. It was suggested that this work may be a good subject for a future IAEA-sponsored CRP.

Needs from the high-energy-density physics community:

We also had a presentation by graduate student, Patrick Adrian, that addressed recent experimental measurements of ion-electron energy-transfer relevant for high-energy-density physics (HEDP) systems. These experiments are relevant for matter that is subject to pressures greater than 1 Megabar - a pressure which roughly corresponds to materials at a temperature of 1-10^3 eV – which corresponds to a free electron densities of 10^{21}-10^{24}/cm^3. Validation of stopping power models in this regime is important for inertial fusion applications, the structure of shock waves, and laser absorption via inverse bremsstrahlung. Experimental validation of stopping powers in this regime have recently become accessible at user facilities such as the Laboratory for Laser Energetics (LLE) located at the University of Rochester as well as at the National Ignition Facility (NIF) housed at LLNL. HED experiments are designed using computational codes that are based upon theoretical ion-electron cross section models which broadly fall into the category of “classical-” and “quantum-” based models and are parameterized by the Coulomb logarithm, which is approximately equal to the natural logarithm of the plasma parameter, Λ. Using a spherical implosion geometry, energetic lasers drive and compress a capsule filled with deuterium and ^{3}He gas to high temperatures and densities causing DD and D-^{3}He fusion reactions to take place. The fusion products (T and α), and their corresponding energy loss in the plasma, can be measured with charged-particle spectrometers which can be related back to the Coulomb logarithm. By working in the low-velocity limit, i.e., below the Bragg peak, one can relate the stopping power of the plasma to the ion-electron equilibration rate which, in turn, is related to the Coulomb logarithm - provided accurate measurements of the density and temperature of the plasma can be simultaneously performed. The conclusions of this work show that the quantum Lenard-Balescu model are in good agreement with the data whereas the model by Gericke *et al.* is not.

Needs from the NIH and the ion-beam therapy community

In addition to the importance of stopping powers to the design of shielding for space exploration, they play an important role in modeling ion beam therapy for the treatment of solid tumors. Drs. Cynthia Keppel (Thomas Jefferson Laboratory) and Ceferino Obcemea (National Cancer Institute) gave presentations on this application area.

In her talk, Dr. Cynthia Keppel provided an overview of ion beam therapy, describing how data from Positron Emission and Computer Tomography (PET/CT) are used to guide treatment planning. She pointed out that in many cases calculated rather than measured stopping powers are used. Lastly, she pointed out that, in the case of Carbon beam therapy, the production of secondary particles, including most importantly neutrons, are responsible for a significant portion of the dose [1]. The importance of secondary neutrons to beam therapy highlights the interrelationship between topical areas that are a recurring theme in WANDA meetings.

Dr. Obcemea presented a high-level overview of how stopping powers and dose are modeled in multicomponent tissues through Bragg Additivity. He pointed out that, at low energies (in the vicinity of the Bragg Peak), additivity may no longer be valid due to changes in the charge state of the beam and the collective excitations and electron wake effects causing stopping powers to change deviate significantly from that of water [2]. Furthermore, he noted there is a near complete lack of knowledge of the stopping powers of different cellular structures, including DNA, and that recent results suggesting that DNA was an electrical conductor has profound implications for beam-based cancer treatments [3]. It is worth noting that, while Dr. Obcemea's talk was centered on beam therapy, the issues at low energies he pointed out were equally relevant to energy deposition from targeted alpha-therapeutic radiopharmaceuticals such as ^{225}Ac and ^{211}At. Lastly, he suggested that, at high-fluence, a 60-80% enhancement in stopping powers would take place due to collective excitations [4]. This vicinage [5] effect can be described via the Lindhard formulation and would be particularly important for modeling dose from laser plasma accelerator ion source.

Conclusions:

The needs from various communities regarding stopping powers and associated metrics vary greatly. The computational codes could greatly benefit from more experimental data, especially when it comes to compounds, both to validate assumptions that have been made (e.g., Bragg additivity) as well as to incorporate experimental uncertainties in theoretical predictions of stopping power metrics. The use of machine-learning techniques could aid in supplementing missing experimental data although we caution that such ideas have not yet been rigorously tested. The interpretation of fission product yields and their masses relies on simulation codes such as SRIM and MCNP which, in turn, use theoretical or semi-empirical models of stopping powers. It should be noted that the CEM03.03 code used in fission calculations in MCNP, sets all fission products to zero at Z<66 due to lack of statistically validated models [6]. It was shown that that both the mean ionization charge-state (Z*) and the corresponding charge-state distribution function can have an impact on quantities such as the calculated range of a projectile in a given material. Turning to help from the atomic- or solid-state physics community might provide guidance on improved models of charge state distributions. The safeguards community could greatly benefit from $\alpha-$stopping power cross sections tables for transuranic elements, such as Pu and Am, given their importance to the stockpile stewardship program. Furthermore, additional experimental data on oxides, such as UO_2 and PuO_2, are also desired. The space community is very interested in testing the survivability of electronic components that are made from wide-bandgap semiconductor materials such as GaN, SiC and Ga_2O_3, as well as other materials. It is, thus, of great importance to measure the LET of these materials to accurately assess SEE of these components. Work done by NASA/GFC and the LBNL BASE facility is helping to address this need, although user-requests far exceed the available time on BASE. The HED community has recently been able to measure the stopping power of light-ions in hot and dense plasmas. This work serves to validate the theoretical models that are used in computational design codes that are used to plan future HED experiments. Studying nuclear reactions and associated quantities in hot/dense plasmas is a relatively nascent field and much more work can be done in the future. Finally, the use of nuclear data in medical applications such as ion-beam therapy continues to play an important role. Further engagement with the NIH and NCI is encouraged to address the needs from the medical community.

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APPENDIX E. NUCLEAR DATA ADJUSTMENTS AND IMPACT ON APPLICATIONS

Background and Introduction

Introduction: Adjustement is a key step for ND users. Through this process they gain optimized nuclear data (ND) libraries; they encompass knowledge from basic nuclear physics through the input general-purpose library augmented with validation experiments tailored to represent the user's target application. Adjustment reliably reduces the application's economic and safety margins, and provides a library that can be used with confidence in limited situations.

A user needs the following in order to compute adjusted ND libraries:

1. Tools and databases that enable adjustment and provide needed data (ND mean values and covariances, sensitivities, integral responses, etc.),
2. Integral experiments representing applications,
3. A general-purpose library encompassing all knowledge from basic nuclear physics.

Example of adjustment: A variety of historical integral data are available that can be used to demonstrate the impact of adjustment. Here, we chose one particularly comprehensive set of data: the spectral indices–or actinide fission cross section ratios–measured in the core of several critical assemblies [ICS22]. Information on the assembly neutron spectrum can be inferred by considering actinides of differing fission thresholds and shapes. Additionally, the ratio magnitudes can impact the major actinide fission cross sections through adjustment, as both experimental and evaluated data are reported to have 1-2% uncertainty. Adjustment to seven critical assembly neutron multiplication, k_{eff}, values and the ENDF/B-VIII.0 spectral indices validation data significantly impacts ^{235}U(n,f) and ^{239}Pu(n,n') cross sections and uncertainties [Cas22] in **Figure 1.**

Users that would benefit from adjustment: The use of adjustment in the Nuclear Energy and Nuclear Criticality Safety communities was discussed throughout the session, but a number of other projects would benefit from adjustment as well. These include, but are not limited to, Stockpile Stewardship, Nuclear Forensics, Incident Response, and Nuclear Threat Reduction–all of which were represented in

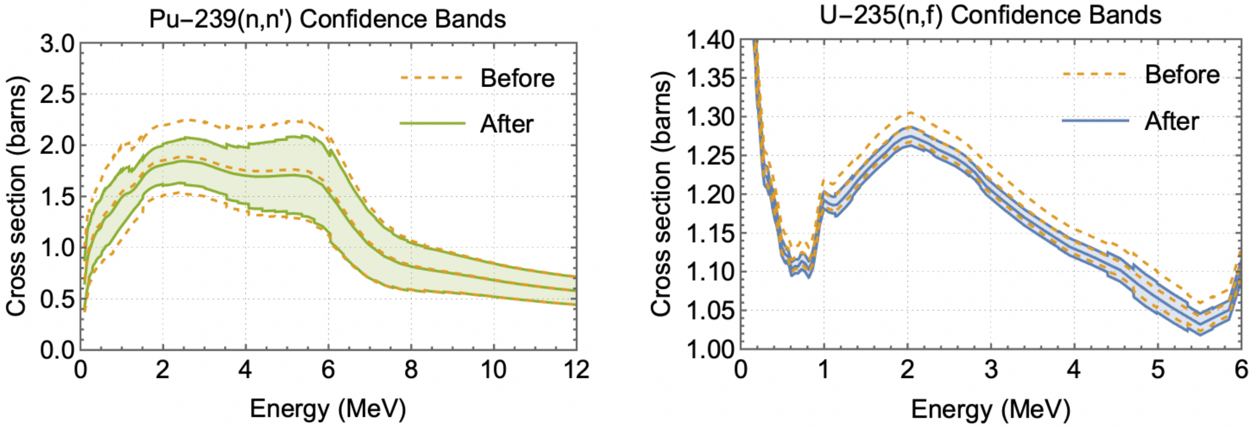

Figure 1: *Impact of adjustment using experimental keff and spectral indices of seven critical assemblies.*

the WANDA 2022 plenary session. Some have adjustment tools developed in-house but without cross-checks to other application areas, while others lack the capability. As was shown in the above example, major actinides can be significantly changed by adjustment, impacting many programs. The benefit of adjustment emerges from integral data having lower variability than the nuclear data they are sensitive to; this means, from a statistical perspective, adjustment filters out some samples to be propagated through an applied model. For programs with unacceptably large uncertainties on quantities of interest, adjusting with carefully chosen integral data can lead to dramatic reduction in those uncertainties.

The role of CSEWG[1] for adjustment: CSEWG provides general-purpose libraries, i.e., the input for adjustment. CSEWG will not provide adjusted libraries for ENDF/B-VIII.1 [Neu22] and leaves this step to the user. However, the same integral responses some users might employ for adjustment are used by CSEWG to validate their libraries (e.g., the effective neutron multiplication factor of selected ICSBEP critical assemblies [ICS22]). Few evaluated ND mean values, usually the average prompt fission neutron multiplicity of major actinides, are tuned within differential data to better predict the chosen integral experiments; ND covariances remain unchanged. This by-hand tuning can introduce compensating errors in a library but unchanged ND covariances should represent this unconstrained physics space.

Summary of state of the art

In the second part of the session, four speakers [Cab22, Drz22, Ris22, Hut22] highlighted that adjustment is already successfully performed to answer needs of application areas ranging from Nuclear Energy, Nuclear Reactor Regulation of novel design, and Nuclear Criticality Safety.

Oscar Cabellos showed that several OECD-NEA-WPEC SGs [SG] are using adjustment to define (a) target accuracies for nuclear data that need to be reached in support of innovative reactor design, (b) find issues and (c) compensating errors in ND libraries. For Nuclear Reactor Regulation, the adjusted libraries are essential for accurately determining the shutdown margin [Drz22]. The NRC performs safety reviews of reactor designs that include biases and uncertainties on several quantities of interest. The reviews of Gen-IV reactor designs have uncovered issues with large uncertainties on ND [Bos21]. They also pointed to a lack of experimental benchmarks that cover the Gen-IV reactor design phase space, with several design reviews relying entirely on computational benchmarks. Adjustment is also used by the Nuclear Criticality Safety program to support criticality safety and reactor analysis/ design [Ris22]. The upper subcritical limit, including a margin for ND uncertainties, is defined for Nuclear Criticality Safety by adjustment to benchmarks selected to resemble the application using the tool Whisper [Whi15]. The SCALE approach can be used for adjustment for reactor analysis but currently misses sensitivities for spectra and covariances for angular distributions. The TSURFER package also allows adjustment and highlights erroneous experimental data [Wia22, Mar22]. The LDRD-DR project EUCLID [Hut22] uses adjustment and associated input data to (1) find issues in nuclear data libraries

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[1] CSEWG (Cross Section Evaluation Working Group) is a cooperative effort of the national laboratories, industry, and universities in the United States and Canada; it produces, validates and disseminates the U.S. Evaluated Nuclear Data File, ENDF/B.

[Neu20], identify unconstrained physics spaces where compensating errors could hide [Neu21], and to design experiments optimized to better constrain ND or a specific application [Mic20]. D. Siefman pointed out during the discussion that adjustment was applied to depletion problems with post irradiation examination data [Sie20]. The authors used randomly sampling to overcome the need for sensitivities and account for non-linear effects in burnup and fission yields.

Discussions on stumbling blocks to adjustment

Integral data: The discussion highlighted that one key cornerstone of adjustment is to have well-characterized, and stringently reviewed evaluated integral data at our disposal. Identification of poor benchmarks or missing correlation constitutes thus a key step in order to obtain reliable adjusted results, and while work on algorithms to identify the former exist, see e.g., Ref. [Sie21], reviewing past experimental data remains one key task for the future. It was mentioned several times [Cab22,Huch22,Hil22] that we need to explore the benefit of including various integral responses, such as, e.g., reactivity effects measurements, count data, and fission gas release [Hil22] that are rarely used for adjustment and validation. Traditionally, neutron-multiplication factors, k_{eff}, of ICSBEP critical assemblies [ICS22] have been used for these purposes; these data are subjected to a stringent quality review and keep being improved [Per22]. However, they do not cover the phase space for all applications and are known to result in compensating errors in ND libraries due to their integral nature [CIE18]. Experimental integral responses beyond k_{eff} help mitigate these issues. However, work would be needed to assemble many of these data in easily-accessible databases and stringently quantify their reported values and uncertainties. The ICSBEP handbook and current improvement work can serve as a model for how this evaluation and documentation should be done.

It is equally important for ND producers and users to work together on creating, characterizing, and using integral data of benchmark-quality to perform application-specific adjustment as well as validation for CSEWG. Reaching benchmark quality is important because inaccurate data or models can introduce bias into the adjusted libraries [Mar22]. The TSURFER code filters automatically such biased data out by a chi-square analysis. Another problem is that correlations between benchmark results are often missing. Due to that, researchers often have to reduce the number of benchmarks to the independent ones.

Differential data: Well-characterized mean values and covariances, reflecting the basic nuclear physics knowledge on each observable, are the foundation for adjustment. Both, under- or overestimated, covariances can bias adjusted data: ND observables without uncertainties are implicitly assumed to be known perfectly, and are not adjusted in most fitting codes; if uncertainties are unrealistically large, adjusted mean values might assume unreasonable values, which can negatively impact the predictive quality of the resulting adjusted library [Mar22]. It is therefore important to enforce a minimum standard on all ND covariances. Work is ongoing as part of CSEWG to more stringently test covariances before their release [WAN20], partially by automatic codes [Wia22, Neu21] and by re-implementation of a peer-review system of the ENDF library [Bro21]. Also, the SCALE code has a procedure for rectifying the covariances that are mathematically incorrect [Wia22]. However, work on the evaluation side is still needed to improve the quality of covariance matrices across the ENDF library as automatic procedures cannot correct for unrealistic covariances. Also, covariances data and formats are missing for several important observables including thermal-scattering law, gamma production, and fission yields.

Formats: New formats are needed to store all correlations arising between adjusted observables. For instance, no format exists to store correlations between PFNS and the neutron-induced fission cross section which are typically introduced by adjustment to k_{eff}.

Cross-validation: Adjustment methods do not generally provide unique solutions [Mar22] but result in adjusted libraries that are safe to be used for a specific application domain. Hence, the limit of applicability and predictive quality of resulting libraries need to be assessed by cross-validation. This step ensures that the resulting libraries can be used for applications such as regulations and licensing. Also, the applicability of application-specific adjusted libraries needs to be clearly communicated and documented.

Outreach: We discussed in detail the issues and stumbling blocks in adjustment, which led to questions about how ND users can participate in the adjustment process. Applications that do not currently use data adjustment may not know how to use their own integral measurements. These integral measurements may be of benchmark quality (or could be with minor characterization and documentation efforts), but cannot be made public in some instances. ND producers and users should support such applications by defining requirements on the quality of integral data for adjustment and provide information on how to create benchmark-quality integral measurements. If these benchmarks can be made public, easily-accessible databases for integral benchmark storage should be made available to capture many integral responses. In the case that the measurements cannot be made public, the adjustment itself would need to be done by the application users. ND producers and users can support these, and all, applications by creating and providing tools for performing the adjustment. Such tools would ensure that the adjustment method is performed consistently and optimally across different applications, and would improve the applicability of the adjusted libraries by including private relevant benchmarks in the creation of the application-specific adjusted libraries.

Recommendations

We encountered two types of user groups in the discussion: these who perform adjustment regularly, while others would be interested in undertaking this but lack tools and guidance to do so. The recommendations listed below capture needs of both user groups.

Tools and Databases

A set of cross-cutting tools are needed to enable adjustment across broad user groups:

- Obviously, a tool to perform the actual adjustment is needed. This tool should be designed such that it can be easily adopted by multiple institutions and programs and enables cross-validation of adjusted libraries.
- Tools are needed to process all pertinent covariances.
- Tools are also needed to compute sensitivities for various integral responses with respect to all pertinent ND observables.
- Users would also benefit from a tool that helps them select an experimental database for adjustment such that the experimental data best represent their application.
- Users would also benefit from a tool that helps them design an experiment optimized for their specific application.

While users new to adjustment might benefit the most from such cross-cutting tools, a sub-set of these tools are novel to regular users of adjustment and thus benefit both user groups.

Both user groups also have the same database needs:

- They need easily accessible databases for storing experimental and simulated integral data of various responses and representing various user groups. These databases should also come along with a detailed characterization for each benchmark.
- Similarly, an easily-accessible database for sensitivities of various integral responses with respect to all pertinent ND observables is needed.

A format needs to be established for storing all correlations between ND arising due to adjustment.

Integral experiments representing applications

Integral experiments, historical or new, are impactful for applications that have similar nuclear data sensitivities. A number of needs were identified regarding uncertainties and the selection of experiments:

- The quality of relevant integral responses of many user groups should be rigorously assessed along with uncertainties and correlations.
  - ICSBEP is a good model for documenting and evaluating validation experiments.
  - Templates of expected measurement uncertainties developed [Neu:te] for differential data or uncertainty standards developed within ICSBEP [ICS:UQ] could also be applied to a wide variety of integral experiments.
- Historical data has been shown to be impactful. An effort is needed to identify historical experiments that can also shed light on underlying basic nuclear physics and might inform more than one use-case and re-evaluate them.
- Tools should be provided to assess the target accuracy needed of new integral experiments such that they impact adjustment.
- We need to gain an understanding of whether small sets of experiments can provide similar value as a full set of benchmarks.
- Methods need to be developed for identification and exclusion of erroneous experiments.

A common thread through the session was that experiments that go beyond k_{eff} are needed.

General-purpose library

One recurring request was that complete and reliable covariances should be provided by CSEWG for all ND observables pertinent to a broad user group. To that end, ND producers should tackle the following:

- Covariances must be consistently checked to ensure that they satisfy all mathematical properties of a covariance matrix and are realistic in size before their release.
- Only low-fidelity covariances are available in ENDF/B libraries for some ND observables. These should be replaced with higher-quality covariances for those deemed highly relevant to several applications.

Covariance data and/ or formats are needed for thermal-scattering law ND, double-differential scattering ND, fission product yields and gamma production ND.

Apart from that, it should be explored how adjustment can inform general purpose libraries.

Outreach needs

First of all, the ND producers should guide users new to the field of ND such that they understand their ND needs to support adjustment. That might entail informing users on what ND need to be taken into account for adjustment, or what tools are available. Also, CSEWG needs to communicate in various forums to users that ENDF/B libraries are of general purpose but are validated and tweaked with respect to a selection of benchmarks, mostly from the ICSBEP handbook.

On the other hand, other ND users may also have integral measurements that could become benchmarks and used to create application-specific adjusted libraries. ND producers should reach out to these users and use their benchmarks for validation if they can be made public. An example of the benefit of such a close connection between ND users and producers is, for instance, the adoption of benchmarks from the ICSBEP handbook and WPNCS SG8 work for validation within CSEWG.

A mini-workshop should be held to create a forum for ND producers and users to communicate and learn together on adjustment, but also create the documentation and tools needed for this kind of outreach to different application areas.

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APPENDIX F. REACTIONS ON UNSTABLE NUCLEI

Subsession I: Direct methods to study reactions on unstable nuclei

Jo Ressler from the Lawrence Livermore National Laboratory presented an overview talk titled "Applications and Reactions on Unstable Nuclei". There is a need for nuclear reaction data on unstable isotopes, but this data is difficult to measure. Due to the difficulty in making measurements, there is a lack of nuclear data to benchmark models, therefore experimental measurements are needed to both provide direct data as well as provide guidance for models. For studies on radioactive isotopes, a significant amount of the isotope of interest must be produced to ensure a signal from the reaction product is detectable. Typically, high particle fluxes are needed to produce sufficient activity and, depending on the half-life, measurements must be conducted immediately at the same facility (second order reaction). The measurement of such data is vital for many areas of nuclear science. In particular, isotopes in nuclear reactors undergo multiple nuclear reactions which can affect isotope production (for medical applications) as well as fuel burn-up (which can affect the reactor itself). Understanding the role of reactions in radioactive species can also help for nuclear safeguards as some of these reactions vary with the neutron flux, providing valuable details about the reactor operation. This is particularly important as a new generation of reactor technology is being introduced, which will have very different neutron environments that are not as well understood and may vary from existing models. A better understanding of the underlying reactions would allow for better modeling to improve safeguards. The Stockpile Stewardship program also is reliant on models for reactions on radioactive species, which have large uncertainties, which could be improved by the measurement of nuclear data to guide these models. Finally, reactions on radioactive species are vital to nucleosynthesis and measuring these reactions can provide valuable data to improve our understanding of the creation of nuclei in the universe.

Sean Kuvin from the Los Alamos National Laboratory presented a talk titled "First direct measurements on Ni-56 and Ni-59 with fast neutrons at LANSCE". LENZ (Low Energy NZ) collaboration has been providing nuclear data needs in studying radiation damage in structural materials like Fe, Cr, Ni, etc., precision (n,α) measurements, and (n,z) reaction studies on radionuclides. Recently, the radioactive Ni-56 and Ni-59 isotopes were developed by Isotope Program Facility for studying (n,z) reactions at the Weapons Neutron Research facility. The directly measured ^{59}Ni(n,p) and ^{59}Ni(n,α) cross sections showed discrepancies compared with the surrogate method measurement and the present nuclear data evaluations. This calls into question the reliability of that application of the surrogate ratio method and highlights the need for direct measurements on unstable nuclei, when feasible. Preliminary cross sections for reactions on radioactive ^{56}Ni and ^{56}Co have been obtained to provide experimentally determined reaction rates to constrain the importance of ^{56}Ni(n,p) in the nu-p process. In LANSCE, the development of an optimized solenoidal spectrometer for radioactive (n,z) studies has begun to significantly improve the sensitivity and the systematic uncertainty over a traditional approach to charged particle detection. LANL demonstrated the feasibility of direct measurement on nuclear reactions with unstable nuclei and presented the new, optimized detection development in order to meet the uncertainty required for applications' nuclear data needs.

John Despotopulos from the Lawrence Livermore National Laboratory presented a talk titled "Reaction studies on Unstable Nuclei at NIF". The Nuclear and Radiochemistry Group at LLNL has developed the capabilities to add radioactive material to the inner surface of NIF capsules. A microinjection system, Apparatus for NIF Doping Automated Robotic Injection System for Targets (ANDARIST), was developed to manipulate very small volumes that can be injected through the fill hole of a NIF capsule to coat the inner surface. The system can manipulate volumes <1 µL, which allows for rare radionuclides to be doped into NIF capsules. However, due to the microcapillary injection, this system requires incredibly clean samples. Another system for NIF capsule doping is the Vacuum Optimized Radionuclide-to-Capsule Administer for NIF (VORCAN), which was also developed at LLNL and is capable of manipulating volumes as low as 4 µL. VORCAN has the advantage that it does not require samples as clean and is simpler to use. These systems have been used to successfully dope both plastic (CH) and diamond (HDC) NIF capsules with cocktails containing isotopes of interest for reaction cross section measurements relevant to Stockpile Stewardship. The first such cross sections to be measured will be the ^{89}Y(n,2n)^{88}Y and ^{88}Y(n,2n)^{87}Y reactions. The ^{89}Y(n,2n)^{88}Y measurement is planned for FY23 and additional shots will be conducted in this year to determine if rare earth elements fractionate during NIF shots. For these exploratory studies, capsules will be doped with a mixture of radioactive rare earths. The data from these shots will be used to plan the measurements of the ^{88}Y(n,2n)^{87}Y reaction cross section at NIF, which will be performed in the future.

Brad DiGiovine from the Los Alamos National Laboratory presented a talk titled "Enabling direct reaction studies with small, highly radioactive samples". To directly measure (n,z) and (n,tot) reactions with highly radioactive, small-quantity samples, various engineering workflows were developed; thin plating and aqueous solutions with chemical compatibility in sample considerations, remote operations and packaging in hot cells during sample production, holistic approach to design the system using modern metrology, advanced collimation based on MCNP simulations, and high-precision alignment with high repeatability. Based on recent successes in LANSCE measurements, fully integrated multidisciplinary effort includes systems engineering approach to design, integrate, and manage complex systems. It also needs precise coordination of intricate operations across multiple teams and to make sure for this methodology to deliver the required speed and efficiency, since short lived unstable nuclei are involved. In all of these efforts, safety is paramount, however now we are in reach of directly measuring many short-lived radioactive isotopes.

Veronika Mocko from the Los Alamos National Laboratory presented a talk titled "Separation of unstable isotopes from irradiated targets in hot cells and their characterization". The Isotope Production Facility utilizes high current, 100 MeV proton beams at LANSCE to produce radioactive isotopes and transfers those irradiated foils to the Hot Cell facility, which is composed of 13 hot cells and the train mechanism to move samples and supplies between cells. Irradiated samples are processed for chemical separation with remote manipulation via dissolution, filtration, evaporation, distillation, column chromatography, liquid-liquid extraction, dispensing, and electroplating. The Ni-56 sample (~ 10 micro-gram) was separated from 46 gram of Co metal, with the decontamination factor of $> 10^4$. For the Zr-88 sample, the micro-liter solution was dispensed in the 1-mm diameter container with lead encapsulation for seal. Once small quantity, highly radioactive samples are separated, the final product is characterized using mass and pH measurement, γ/β spectroscopy, and Coupled Plasma-Optical Emission Spectroscopy (ICP-OES). All of these endeavors rely on multidisciplinary and collaborative work from physicists, chemists, nuclear engineers, accelerator staff, and more.

Subsession II: Indirect methods to study reactions on unstable nuclei

Hendrik Schatz from the Michigan State University presented a talk titled “Overview on reaction on unstable nuclei for astrophysics at FRIB”. As reactions on rare isotopes are critical for most astrophysical processes and are more important than ever, the upcoming Facility for Rare Isotope Beams (FRIB) will be a game changer by reaching out farther in accessible unstable nuclei for better understanding of nucleosynthesis. Dedicated efforts are needed to evaluate nuclear data for astrophysics community via easy access and timely dissemination. Ongoing astrophysics nuclear libraries such as JINA REACLIB, STARLIB, BRUSLIB, nu-Lib, nucastrodata.org, pynucastro, etc., address important aspects, but need to be greatly expanded. A close collaboration among nuclear physicists, computational astrophysicists, observers, and cosmo-chemists is a key to answer open questions in nuclear astrophysics.

Jutta Escher from the Lawrence Livermore National Laboratory presented a talk titled “Theory for Indirect Reaction Studies”. There are robust reaction theories and data evaluation tools capable of describing a large variety of nuclear reactions. However, the predictive power of reaction calculations is limited as ambiguous model combinations, large parameter uncertainties and multiple reaction channels can lead to large uncertainties in reaction calculations. Furthermore, for reactions far from stability, fewer constraints are known, and minor processes may become significant, which complicates theories further. Direct measurements are vital validate theory but are not always feasible. There is an opportunity to improve models with indirect reaction data. Indirect reaction data can provide new insights into reaction mechanisms and provide constraints for reaction theory, but these measurements must be performed alongside new development of predictive microscopic structure and reaction theories to achieve comprehensive reaction models.

In the Oslo method, compound nuclei are produced via nuclear reactions and the γ strength function and level density are extracted from measured γ decay spectra. There are some difficulties associated with this method, however, as the separation of the strength function and level density is ambiguous and requires outside information. Furthermore, the electric and magnetic strength functions are not distinguished experimentally nor are the effects of spin and parity on the decay of the compound nucleus. Theoretical developments are needed to incorporate spin-parity predictions to improve analysis and better understand the associated uncertainty. The β-Oslo method is an alternative to the Oslo method where the nucleus of interest is produced via β-decay, but the analysis and limitations are otherwise the same as Oslo method, and developments are needed to integrate β-decay theory with γ emission.

The surrogate reaction method combines theory and experiment and provides a route to constrain cross section calculations for compound reactions. Surrogate reactions produce the same reaction product as the reaction of interest, for example, (p,d) and (d,p) transfer reactions can be used to investigate unknown (n,γ) cross sections. With (p,d) reactions, there are some challenges associated with the “hole” created in the nucleus, inelastic excitation and decay radiation interference. Theory developments are needed to leverage the dispersive optical model parameterization to describe hole structure as well as implement a two-step reaction description to incorporate inelastic effects and integrate nuclear decay schemes. With (d,p) reactions, theory is needed to describe the deuteron breakup and propagation as well as neutron absorption with optical model potentials. This must also be extended to deformed systems. Inelastic scattering reactions provide a surrogate pathway to measure unknown (n,n’) and (n,2n) cross sections. This could provide a pathway to obtain multiple desired reaction cross sections simultaneously, however, the multiple intermediate nuclei could also present a challenge. To fully understand these reactions, structure theory needs to be integrated into the description of the surrogate reaction. Surrogate reactions, both inelastic scattering and transfer reactions, can provide insights into the fission process as well. Fission is difficult to describe theoretically as a large amount of data needed to provide constraints, but surrogate reaction studies can provide some of the needed data. The reactions of nuclei far from stability present a significant challenge for models as extrapolations from stable isotopes do not necessarily apply and uncertainty is particularly hard to quantify. To improve the current understanding of these reaction, it is necessary to incorporate information from microscopic theories as well as identify suitable experiments to validate and inform theory.

Sean Liddick from the Michigan State University presented a talk titled “Beta-Oslo measurements for indirect neutron capture measurements”. To better predict r-process abundances, neutron capture rates have been identified as one of largest uncertainties in nuclear input. With the newly developed shape method, the beta-Oslo measurements could be applied to infer neutron capture rates on short-lived neutron-rich nuclei. To further constrain neutron capture predictions, spin-independent gamma strength functions were investigated using isomeric states in Cu-70. The FRIB Decay Station Initiator is an integration of community detectors in a reconfigurable infrastructure and its completion will dramatically increase reach of experimentally accessible isotopes for decay spectroscopy experiments.

Andrew Ratkiewicz from the Lawrence Livermore National Laboratory presented a talk titled “Constraining Neutron-Induced Reactions Through the Surrogate Method”. The surrogate reaction method is used to provide constraints on neutron-induced reactions on radioactive targets where a direct reaction is impossible to measure. The surrogate reaction forms the “same” compound nucleus as the direct reaction of interest allowing observation of the decay. In order to benchmark (d,pγ) as a (n,γ) surrogate, a stable target with well understood nuclear structure is needed. In particular, the (n,γ) reaction as a function of neutron energy needs to be well known. The correct theoretical description of the compound nucleus formation cross section and entry spin distribution are required as well. The ^{95}Mo(d,pγ) reaction was chosen as the benchmarking reaction for the surrogate method and experiments were carried out at Texas A&M Cyclotron Institute. The reaction was measured in regular kinematics using enriched (98.6%) ^{95}Mo targets (0.96 mg/cm^{2}) with 12.4 MeV deuteron beams. The beams had an average intensity of ~0.3 nA. The protons and coincidence γ rays were measured with the Silicon Telescope Array for Reactions with Livermore, Texas A&M, Richmond (STARLITER) apparatus. The surrogate measurement agreed with the direct measurements, but this was only achievable through close collaboration between theory and experiment. The surrogate method can also work on odd-odd and odd-even systems with different mechanisms, and has been used successfully with the same experimental apparatus at Texas A&M for the ^{89}Y(p,d) reaction as a surrogate for ^{87}Y(n, γ) and ^{92}Zr(p,d) for ^{90}Zr(n, γ). Other surrogate measurements include: ^{95}Zr(n, γ) (with ^{96}Zr(p, p’)), ^{93}Sr(n, γ) (with ^{93}Sr(d, pγ)), ^{88}Zr(n,γ) (with ^{90}Zr(p, d)), and ^{168}Tm(n,2n) (with ^{169}Tm(p, pn)). The NeutronSTARS neutron detector, the largest in the NNSA complex, will be used to measure fission neutron multiplicity ($\bar{\upsilon}$), fission neutron distribution, and surrogate (n,n’) and (n,2n) reaction cross sections. With the upcoming commissioning of FRIB and nuCARIBU, numerous surrogate measurements will become possible, but this will require investments in theory and experiment.

Georgios Perdikakis from the Central Michigan University presented a talk titled “Development of new capabilities for the measurement of (p,n) reactions with unstable nuclei at FRIB using ReA and SECAR”. Neutron-induced processes are prominent in understanding of the origin of heavy elements, and the neutrino-p process in proton-rich areas shows impacts in neutron-driven winds core-collapse supernovae. The sensitivity study identified the critical role of the ^{56}Ni(n,p) reaction for constraining the neutrino-p process in final heavy element production. However, there is no experimental data, since ^{56}Ni has only 6 days of a half life. The CMU team developed the indirect measurement of ^{56}Co(p,n) reaction using heavy ion beam on a hydrogen target, to constrain theory and estimate ^{56}Ni(n,p) reaction rate. For the large acceptance and transmission, and better energy separation, the use of the SECAR recoil separator is being developed. This technique is portable to take advantage of ReA6's higher beam energies at Facility for Rare Isotope Beams (FRIB).

Shea Mosby from the Los Alamos National Laboratory presented a talk titled "Measuring impossible reaction rates: turning the tables on neutron-induced reactions". Although direct neutron reaction measurements on radionuclides are desired where feasible, not necessarily every interesting reaction on every interesting nucleus is available today if a half life is shorter than days. In order to dramatically expand the reach of direct measurements, a "neutron target" would enable inverse kinematics measurements by bringing an ion beam and spallation neutron source together. Nuclear reaction products will be detected using relevant detectors while radioactive ions are revolving in the storage ring. This concept is under development at LANL and TRIUMF in Canada. To answer key questions like the neutron flux in the neutron target, the control of neutron field, and the impact of radiation field in storage ring measurements, LANL is pursuing resources to assemble the proof-of-principle measurement.

Discussion to solicit the community input

One of the topics was about the limitations of ENDF for this area. Many important reactions on unstable nuclei have limited or no information available in ENDF. This has caused many applications to develop custom databases with reaction evaluations based entirely on theory. There are some examples where ENDF evaluations contain no experimental measurements, but these are considered untrustworthy by many users and are not used by CSEWG. An alternative to ENSDF is using TENDL, which is based mostly on calculations. The library JEFF incorporates TENDL cross sections when no evaluations based on experimental data exist. Using TENDL calculations is useful if there is no alternative but is not considered adequate by most users.

Model uncertainties/reliability of calculations for theoretical cross sections can be very large when extrapolating global models of reaction/structure information to nuclei where no measurements exist. There is a need for more measurements on radioactive nuclei to help constrain theoretical models. To address this issue, supplemental information could be added to ENDF for suggested cross section measurements. As an example, most neutron induced reactions have measurements at thermal energies and at 14 MeV, but very few measurements at energies in between. Suggestions for potential measurements can help guide experimenters as to what measurements are the most important to make.