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Perspective

Current nuclear data needs for applications

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Accurate nuclear data provide an essential foundation for advances in a wide range of fields, including nuclear energy, nuclear safety and security, safeguards, nuclear medicine, and planetary and space exploration. In these and other critical domains, outdated, imprecise, and incomplete nuclear data can hinder progress, limit precision, and compromise safety. Similar nuclear data needs are shared by many applications, thus prioritizing these needs is especially important and urgently needed. Many levels of analysis are required to prepare nuclear measurements for employment in end-user applications. Because research expertise is typically limited to one level, collaboration across organizations and international borders is essential. This perspective piece provides the latest advances in nuclear data for applications and describes an outlook for both near- and long-term progress in the field.

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I. INTRODUCTION

Nuclear data provide the empirical foundation for studies in nuclear energy, safety, security, safeguards, and many other areas of science. They also, however, enable applications that touch many aspects of everyday life. In homes, food is served that has been irradiated by ^{60}Co and ^{137}Cs to kill bacteria, making it safe for long term storage and distribution. ^{63}Ni is used in camera light sensors and long-life batteries. Smoke detectors utilizing ^{241}Am warn of household fires. Some people have benefited from medical scans using ^{99}Tc, while others from artificial joints that have been wear-tested with ^{7}Be.

Nuclear data enable technologies that helps protect the environment. ^{65}Zn and ^{54}Mn are used to understand the flow of heavy metal contaminants in mining wastewater, ^{3}H is used to study sewage and liquid waste, ^{137}Cs helps track soil erosion and deposition, and neutron radiography is used to

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characterize contaminants in a variety of environmental samples. Nuclear data also help characterize and modify materials for many uses, from ^{60}Co used to probe the suitability and longevity of cement storage casks and reactor walls, to neutron scattering used to probe the unusual magnetic properties of quantum materials, and to selenium ion implantations for semiconductor doping.

Finally, nuclear data also provide insight into understanding the world. These data are critical in Nobel prize-winning discoveries like the Higgs boson, because they determine how particles interact with the detectors. Radioactive dating with ^{14}C provides deeper understanding of history. Heavy ion irradiation is used to understand how computer chips will survive cosmic ray bombardment, thereby enabling safe space travel. And the Voyager deep space exploration crafts have been powered by ^{238}Pu since their launch in 1977.

Nuclear data encompass a wide range of structure and reaction quantities such as scattering and reaction cross sections, generally given as a function of energy and angle; nuclear masses, level properties, and their decay modes and parameters; neutron and photon spectra from reactions; and many others. These are needed for every nuclear isotope and their reactions involving neutrons, protons, deuterons, alphas, and photons. Where measured data do not exist, model predictions are sometimes used as placeholders.

Nuclear data collections, or libraries, incorporate data from multiple sources that have been critically assessed by a nuclear data evaluators who review and combine all available data sets, determine the highest quality data, and decide upon a set of standards. These evaluations are stored in specific evaluated nuclear data files consisting of a combination of tabulated data and parameters that can be reconstructed into data sets using specially designed processing codes.

Because of the complexity and diverse skills required for evaluation work, and because of the importance of nuclear data across both basic and applied fields, numerous organizations have been formed to coordinate activities, increase communication, and launch collaborative efforts between evaluators. For reactions, these include the US National Nuclear Data Center (NNDC) [1], International Network of Nuclear Reaction Data Centers (NRDC) [2] and the International Nuclear Data Evaluator Network [3], under the auspices of the Nuclear Data Service (NDS) of International Atomic Energy Agency (IAEA) [4]; the Cross Section Evaluation Working Group (CSEWG) [5] bringing together the efforts of US and Canadian national laboratories; the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Cooperation (WPEC) [6]; and the Japanese Nuclear Data Committee [7]. These organizations have, for example, helped address differences between nuclear reaction data sets in the US [Evaluated Nuclear Data File (ENDF)] [8], Japan [Japanese Evaluated Nuclear Data Library (JENDL)] [9], Europe (the Joint Evaluated Fission and Fusion File (JEFF) [10], TALYS-based Evaluated Nuclear Data Library (TENDL) [11]), Russia [Russian Evaluated Nuclear Data Library (BROND)] [12], and China [Chinese Evaluated Nuclear Data Library (CENDL)] [13]. Additionally, WPEC subgroups [6] and IAEA Nuclear Data Section Coordinated Research Projects [14] have worked to improve data evaluation techniques, data formats, and general and user-specific evaluated data sets. For nuclear structure, evaluation work is coordinated by the US Nuclear Data Program [15] managed by the US NNDC, the IAEA NDS [4], and the Nuclear Structure and Decay Data (NSDD) Network [16]. Cooperation between organizations leads to better, more reliable international nuclear data evaluations and standards.

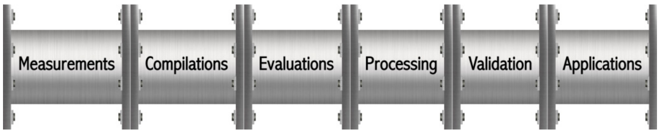

FIG. 1. Schematic example of a linear data pipeline showing how the components of the pipeline contribute to the production of data libraries used by applications. Given the multidisciplinary nature of nuclear data, some activities may involve more than one component.

Evaluated nuclear data sets are critical inputs for predictive modeling and simulations in various applied science and engineering disciplines. Nuclear power and associated fuel cycle operations, national security and nonproliferation applications, shielding studies, materials analysis, medical radioisotope production, diagnosis and radiotherapy, and space applications are only a handful of applications that rely on accurate and precise nuclear data. In many cases, the same nuclear data sets can provide cross-cutting support to a number of different applications.

Extensive experimental campaigns to measure nuclear data were made from the 1950s to the 1990s. Since then, computational modeling and simulations of nuclear systems have undergone a period of rapid expansion. The computational power available for detailed modeling of physical systems has grown by several orders of magnitude. Consequently, the predictive power of many simulations such as radiation transport codes is effectively limited by the fidelity of the input nuclear data. The limits of this predictive power have economic, safety, and security consequences that must be addressed. For example, safeguards and homeland security applications rely on hybrid methods of radiation detection and computational solutions of the inverse radiation transport problem. If modeling of these systems is limited by nuclear data, the ability to detect smuggled nuclear materials, for example, is correspondingly limited.

A. The nuclear data pipeline

The nuclear data pipeline, shown in Fig. 1, is a term used to describe the many interconnected steps required to prepare nuclear measurement results for use in end-user applications. While this pipeline has been described in numerous ways, there are, in general, six essential steps: measurements, compilation, evaluation, processing, validation, and applications. Measurements are made, both for fundamental science and for specific user-related requests. Compilation involves collecting the data from new measurements and historical literature and inserting these data and related information from measurements into both bibliographic databases (such as Nuclear Science Reference (NSR) [17] and Computer Index of Nuclear Reaction Data (CINDA) [18]) and numerical databases (including Experimental Unevaluated Nuclear

Data List (XUNDL) [19] and Experimental Nuclear Reaction Data (EXFOR) [20]). The next step, evaluation, is critical to provide a recommended best value for all pieces of nuclear data by expertly combining new measurements with previous measurements and nuclear model predictions. Evaluated nuclear reaction data is inserted into ENDF [8] and disseminated online by a variety of tools including Sigma [21] from the US NNDC [1] and ZVVIEW [22] from IAEA-NDS [4]. Evaluated nuclear structure and decay data are inserted into the Evaluated Nuclear Structure Data File (ENSDF) [23] and disseminated online via NuDat [24] from the NNDC.

Processing is the fourth step of the pipeline, wherein evaluated data sets are converted to formats required by specific end-user applications. In some cases, these processed data sets are distributed to the community, such as the Nuclear Wallet Cards [25] and the Medical Internal Radiation Dose (MIRD) database [26]. In other cases, evaluated files are processed and stored on local computers and serve as input files for end-user simulations. For example, NJOY [27] and other codes (e.g., NECP-ATLAS [28]) are used to process the ENDF evaluated data file into the ACE format [29] for input to transport codes such as the Monte Carlo N-particle transport code (MCNP) [30]. Validation, the next step in the pipeline for reaction databases, involves quantitative model comparisons [31–35] with independently measured values from benchmark-quality experiments such as for criticality safety [36], employing the newly processed evaluated data as input. Iterative adjustments are made to reaction evaluations on the basis of this validation process. Finally, the processed and validated nuclear data files are disseminated for use in applications. New applications or more stringent requirements for existing applications could require new data, starting the flow of the pipeline again.

The lengthy passage of data through the full pipeline, from new experimental measurements through evaluation, processing, and validation, requires expertise at each step. For nuclear structure data, all nuclides of a particular mass number are often evaluated simultaneously, because their levels are interconnected by beta decays. Such mass chain evaluations can take half a year to two years to complete, containing all properties and decays of $\sim 10^5$ levels, and then up to another year or two for critical peer review and quality assurance checks. Additionally, many nuclides are evaluated individually. The average time between evaluations, currently approximately 7 years, is limited by the available evaluation workforce. Upon completion, evaluations are entered into the ENSDF database in a process of continual updates. For nuclear reaction data, the ENDF database [8] is organized into 15 sublibraries (e.g., "Neutron for neutron-induced reactions), and further subdivided into evaluations of each isotope where *all* reaction channels are simultaneously evaluated. In some cases, individual reaction channels (e.g., partial cross sections) with over $\sim 10^6$ data points require months to years to complete, and a full evaluation for the nuclide in a sub-library can take significantly longer. Some of the processing and validation steps have been recently automated [8], as well as a new release of the full ENDF library, that includes all evaluations completed since the last release, is made approximately every 5 years.

B. Key topical areas in nuclear data

In 2021, six topics were selected collectively by the nuclear data producer and user communities [37] that best reflect deficiencies or opportunities relevant for current and emerging applications with crosscutting themes that enable support of the data pipeline for multiple programs [38–41]. (See Ref. [42] for more information.) In the remainder of this section, each of the six topics are briefly introduced. The following sections will discuss the highlights and outcomes of each topical discussion in more detail, with specific outlooks highlighting the most urgent nuclear data needs in each area.

1. Advanced computing for nuclear data

Computing plays a critical role in applied nuclear data, ranging from execution of high-fidelity physics models that form the backbone of data evaluations and experimental analysis and interpretation, propagating uncertainties through a complex chain of heterogeneous codes, to processing large training datasets through supervised machine learning algorithms. Resources for these activities include hardware from clusters to supercomputers, scalable algorithms, and extensive efforts in coding, applied mathematics, and domain-specific applications. This topic covers recent computing developments and highlights the challenges of adapting complex, legacy, or mission-critical codes to the latest, and next, generation of rapidly evolving architectures. Machine learning methods for emulating computationally expensive physics models, validation, and uncertainty quantification (UQ) are also discussed. Developments needed to realize the potential of quantum computing (QC) for nuclear data, far beyond the bounds of classical computing, were also presented.

2. Predictive codes for isotope production

In situations and energies where well-characterized experimental data on cross sections or isotopic yields are unavailable, the isotope production community, as well as other users of these data, relies upon predictive codes to provide estimates of needed data. Unfortunately, accurate modeling of even moderately high-energy reactions is notoriously difficult. The lack of an acceptable predictive capability in modern reaction codes presents a cross-cutting need for the nuclear data community, as it impacts the casual user of these codes, the data evaluation pipeline, and applications such as isotope production, neutronics, shielding, and detection. With a broad range of applications and an impact on multiple programs, this topic is of great interest. This section focuses on how to improve the predictive capabilities of these codes to benefit the breadth of the data community.

3. Expanded benchmarks and validation for nuclear data

Because much of nuclear science and engineering relies on predictive computational modeling and simulation, many areas of the community would benefit from the development of well-characterized and documented benchmarks for code validation. While critical assembly benchmarks are very useful for validating some aspects of nuclear data, a broader suite of benchmarks are needed to provide more complete validation of nuclear data and physics important for other applications.

There are many different applications that can leverage the framework used by the criticality safety and reactor physics communities to develop benchmarks needed to validate the nuclear data they depend on. New and historical experiments that could be turned into benchmarks to strengthen nuclear data validation in cross-cutting application areas was a major focus of this discussion.

4. Nuclear data for space applications

The space radiation environment is a complex mix of photons, electrons, protons, and heavy ions with energies ranging from several eV to several TeV per nucleon. Characterizing interactions in the environment of space is important in a number of areas critical for space research and exploration due to the secondary radiation fields they create. For example, creating effective shielding for crew and electronics requires fundamental cross section data on high-energy heavy-ion interactions that produce complex secondary radiation fields. Similarly, the secondary neutrons and gamma rays produced by interactions of cosmic rays with the surfaces of planets, moons, and asteroids enable their chemical composition to be characterized through the use of nuclear spectroscopy. Converting measurements to elemental information requires knowledge of relevant neutron inelastic and capture cross sections and gamma-decay intensities. As space agencies around the world prepare for human exploration beyond low-Earth orbit, there is renewed interest in fission power and radioisotope systems. These systems introduce an additional source of radiation that can impact instrument response and crew health. Nuclear data relevant to the performance of man-made radiation environments and their interaction with surrounding materials is necessary to understand their impacts on these missions.

5. Nuclear data for advanced reactors and security applications

Nuclear data impacts design, efficiency and operation of advanced reactors and security applications. With new advanced reactors and micro-reactors being designed using different fuels, coolants, and moderators than the current fleet, there is a potential need for improved nuclear data, including new differential and integral measurements, as well as new evaluations. Security applications are even more diverse, covering a large range of detectors, systems, and interactions. There is also a large overlap in the nuclear data needs of these two areas, especially for microreactors. The essential questions to address in this topical area are where refined nuclear data can increase safety, reliability, and economic viability.

6. The human pipeline for nuclear data

Researchers play a key role along the entire nuclear data pipeline, not only contributing effort to process data through the pipeline, but also to improve links between pipeline components and to advance the underlying fundamental physics. However, the subcritical, aging, homogeneous nuclear data workforce must be transformed to evolve the pipeline to meet the growing international demand for nuclear data, to branch out into new application areas, to embrace new advances in big data, to transfer knowledge to the next generation, to benefit from the available diversity of thought, to attract younger researchers, and to continue to keep the ENDF and ENSDF databases as international standards of nuclear information. Some initial efforts to address these critical issues are described in Sec. VII.

II. ADVANCED COMPUTING FOR NUCLEAR DATA

Computing plays a central role in the nuclear data pipeline, from the analysis of data collected through experiments to the production of evaluated data to the use of these data in applications. The collection and analysis of experimental data strongly leverages computing for data acquisition and to execute mathematical analyses including signal processing techniques, statistical methods, and much more. Evaluations rely on a set of theoretical models, implemented in nuclear physics codes, to simulate the structure, reactions, and decay of atomic nuclei. Nuclear data are then used by application-specific simulation codes, e.g., computer programs simulating the structure of a neutron star, the formation of elements in nucleosynthesis, critical assemblies, or reaction networks for active interrogation. Because of the inherent complexity of nuclear processes and the often multiphysics nature of nuclear data application codes, quantifying and propagating uncertainties of the data throughout the pipeline also plays an essential role in the nuclear data community. Many of the statistical methods used for UQ require significant computing resources.

Thanks to advances in computing and in the understanding of the nuclear many-body problem, nuclear theory has become ever more sophisticated with descriptions of the structure and reactions of light nuclei [43,44], low-lying states in medium-mass nuclei [45,46], the mean-field description of heavy nuclei [47], and improved theories of nuclear fission [48,49]. A broad range of fundamental nuclear theory problems from neutrino physics to fission to neutron reactions that are highly relevant to the nuclear data community were in fact identified as priority research directions requiring the development of exascale computers [50,51]. By integrating some of these theoretical developments into the nuclear data pipeline, there is a unique opportunity to increase the fidelity of evaluations. This approach anchors the calculation of nuclear observables to the best knowledge of nuclear forces and quantum many-body methods, thereby improving the underlying physical foundations of the data. However, such a task requires a long-term vision for code development to keep pace with hardware developments, robust software maintenance plans, and personnel with cross-cutting skills in software engineering and nuclear science. Revising legacy codes to fully exploit new features of the latest hardware architectures, especially GPU-based ones, often requires expert assistance and collaboration with computer scientists.

Similar challenges are encountered in the development of popular transport codes such as, e.g., MCNP [52] or TRIPOLI [53], that are used to simulate many nuclear systems including reactors, nondestructive assays, and isotope production. In contrast to nuclear physics models, the linear Boltzman transport equation is well understood, so the primary computational challenges involve system geometry, numerical precision, or the need to calculate sensitivities to all integral quantities, all of which require susbtantial computational throughput. These observations also apply to computer programs implementing the reaction network simulations relevant for stockpile stewardship or nucleosynthesis, where the simulation uncertainties primarily arise from input nuclear physics uncertainties rather than the underlying thermodynamic conditions. The sensitivity of criticality calculations or astrophysics simulations to nuclear data inputs are examples of grand challenge problems that require leveraging high-performance computing (HPC) techniques and resources.

In addition to nuclear theory, transport codes, and network simulations, artificial intelligence (AI) and machine learning (ML) are driving a significant expansion of the role of computing in nuclear data. AI/ML has already seen applications throughout the sciences in the areas of design, control, augmented simulations, science and math comprehension, generative models, inverse problems, multimodal learning, and decision making [54]. In the nuclear data pipeline, it has been used for knowledge extraction, automation, surrogate models, and uncertainty quantification [55], and its use is anticipated to grow exponentially for a number of reasons. First, AI/ML enables new approaches, often originating in other fields, to address longstanding problems in nuclear data. Second, new open source software libraries are available that facilitate the use of AI/ML algorithms with both CPUs and GPUs. These Python-based software frameworks [56,57] include tools for classification, prediction, ML via deep, recursive, and/or convolutional neural nets, and natural language processing. These libraries are not, however, completely plug-and-play solutions, and collaborations with AI/ML experts and statisticians are often needed to exploit their full potential for nuclear data applications. Third, there is an intense interest of (especially early career) researchers to apply AI/ML approaches to challenging data-intensive problems, providing an exceptional opportunity for AI/ML to serve as a recruiting gateway for the nuclear data field. These last two points are addressed further in Sec. VII.

Finally, simulation of quantum many-body systems, such as nuclear reactions, requires exponentially increasing classical computing resources as the number of particles increases. In theory, universal quantum computers can achieve the same exponential scaling, with the upshot that a quantum computer with thousands of qubits could simulate some nuclear reactions not possible even on future exascale classical supercomputers [58]. Moreover, because quantum computers are unitary, they are ideal for simulating quantum real-time evolution such as in nuclear interactions. Quantum supremacy—performing a calculation on a quantum computer impossible on a classical supercomputer—has been demonstrated, albeit on carefully selected problems that are currently largely uninteresting other than for tractability on current quantum computing hardware [59,60]. It is thus relevant to determine the potential of QC in the particular area of nuclear data.

This section addresses the state-of-the-art of advanced computing in three primary focus areas and the associated opportunities for the nuclear data community. Section II A provides an overview of current and emerging HPC technologies in the context of nuclear data needs and applications. Section II B addresses the ways in which AI/ML may be applied to advance capabilities at all stages of the nuclear data pipeline. Section II C explores the opportunities and limitations to address nuclear data problems.

A. High-fidelity modeling and simulation with high-performance computing

With the increasing sophistication of modeling and simulation approaches and the expanding number and size of available datasets, capabilities to address nuclear data needs and applications are increasingly reliant upon powerful HPC tools for efficient execution. HPC methods may be applied to advance computational nuclear structure and reactions by increasing the performance of existing nuclear physics codes and enabling more elaborate theoretical modeling including previously inaccessible complex multiphysics calculations [61]. In fundamental nuclear theory research, novel methods to perform *ab initio* calculations of nuclei, such as coupled-cluster [62] or in-medium similarity renormalization group [63], have only become possible thanks to progress in HPC. New insights into the structure of neutron stars [64] or the formation of heavy elements in the universe [65–67] rely critically on complex simulations of nuclear properties on supercomputers [68,69]. Multidisciplinary collaborations involving applied mathematicians, computer scientists and domain scientists are often key to enabling such progress [70]. The Scientific discovery through advanced computing (SciDAC) program [71] and the Fission In R-process Elements (FIRE) topical collaboration in nuclear theory [72] are examples of how to organize and support such multidisciplinary collaborations.

HPC can also play important roles in the verification of methods and codes and in validation of commonly used approximations, by testing against more fundamental and predictive theories. Examples include *ab initio* calculations of thermonuclear reactions that can test the correctness of more phenomenological R-matrix fits [73], explanations of β-decay rate quenching with microscopic methods [74], or the quantum-mechanical simulation of quantities that are essential for simulating the deexcitaiton of fission fragments [75]. By providing robust extrapolations where data are not available, establishing useful trends (as a function of Z, A, spin, energy, etc.), or validating empirical laws and systematics, such fundamental simulations play an important role in the nuclear data pipeline.

The scope of HPC tools extends beyond large-scale nuclear physics computations. For example, HPC resources can be leveraged to simulate nuclear reaction processes directly in transport simulations. While such an integrated capability is not always needed (and should be avoided in favor of more rapid approximations when appropriate), the integration of nuclear physics models and transport codes opens the opportunity to implement more realistic physics which is required for some applications (e.g., detector response, unique nuclear signatures). This capability could mitigate the increase in time and reduction in speed incurred by frequently accessing large nuclear datasets and also be used for a baseline against which to estimate corrections when employing more rudimentary models in transport simulations.

Another area where HPC provides a major opportunity for nuclear data is UQ and uncertainty propagation for applications. There is some evidence that Bayesian statistics, for example, provides more flexible and realistic estimates of uncertainties compared with frequentist approaches [76]. However, the application of these methods relies directly on sampling the parameter space of the model. The number of samples can be extremely large for models with many parameters. In such cases, the absolute cost of running the model (in terms of CPU time, memory, I/O access, core-count, etc.) becomes critical. Recent examples from basic nuclear theory [77] show that code optimization capable of leveraging existing HPC resources can be key to generating sufficiently many samples. While the number of samples may not be sufficient to perform a full statistical analysis, they may be sufficient to build a realistic *emulator* of the physics model: a mathematical/computational model whose outputs are numerically equivalent to the ones of the physics models for a well-defined subspace of the parameter space; see Sec. II B. The propagation of nuclear data uncertainties from covariance matrices has been accomplished in some scenarios [78], but more precise simulations enabling the systematic quantification of uncertainties in simulations for both energy and nonenergy applications is desired. The incorporation of cross-reaction and cross-isotope covariances across the nuclear chart would represent a grand challenge in this regard. Finally, one should verify whether mean values and covariance matrices, which implicitly assume linearity, are sufficient to truly describe nuclear data uncertainties.

To fully harness the benefits of HPC technologies to advance the nuclear data pipeline, the nuclear data community must address key aspects and limitations of computational nuclear physics. First, focused efforts to improve the modeling of atomic nuclei are needed across the entire nuclear chart, a capability that is essential to the understanding of nuclear structure and properties. HPC resources can facilitate the execution of computations of atomic nuclei, but dedicated effort is required to enable high-throughput computing in an HPC environment [79]. Second, a cost-benefit analysis of computing architectures is needed, including hybrid architectures, to ensure focused investments in large-scale computing facilities and related technologies for state-of-the-art nuclear data computations. Third, collaborations with the computational community should be prioritized to ensure optimal use of HPC architectures. Success stories in the area of basic nuclear theory suggest that such cooperation has the potential to greatly advance the nuclear data pipeline, in part because physics models and codes are applied in areas that have yet to be experimentally probed.

B. Artificial intelligence and machine learning

As AI/ML approaches become more prevalent and refined, new promising capabilities are emerging relevant at all stages of the nuclear data pipeline with the potential to transform the compilation, evaluation, processing, and validation workflow. These include natural language processing (NLP) to search and assess nuclear science literature, physics-aware ML models to both guide evaluations and learn new parametrizations directly from the observables, and ML capabilities to guide experiment, theory, and evaluation. Some of the latest concepts and developments in these areas are briefly described below.

Container workflow solutions provide the opportunity to connect HPC, AI/ML, and cutting-edge software engineering to enable automatic updates of ENDF [80,81], a reaction library critical for basic and applied research. This approach, which would represent an overhaul of the decades-old workflow of library updates, is based upon the use of containers (lightweight virtualizations akin to virtual machines) that hold experimental results, reference parameter sets, theory codes, benchmark experiments, and evaluations of individual nuclides or reactions. When these containers are properly nested and interlinked, they can be treated as nodes in a Bayesian network. When any nodes in the network are updated (e.g., by the addition of new experimental data), Gaussian process regression can be used to update the network output, automatically yielding a new ENDF library [82].

Physics-aware ML models represent another exciting development for the nuclear data community. One category of such models involves adding a component to the loss function of a neural network that arises from the deviation of a physics model prediction with the data [83]. In this way, the adjustments of the biases and weights of the underlying network are more grounded in physics. A complementary approach is to use ML simulations to "learn" underlying physics, such as predicting ground-state properties and excited state energies by learning the features of a theoretical model [84] or understanding the physics behind high-energy particle collisions [85]. By using ML algorithms to help design experiments that address specific nuclear data gaps (e.g., criticality experiments [86]), ML can become more tightly interwoven into data activities. ML can similarly be interwoven with theory by learning discrepancies from existing models [87–89] or averaging model predictions [90]. ML can also guide evaluations in numerous ways such as taking detailed experimental conditions into account (as in an evaluation of the ^{239}Pu(n,f) reaction [91]) or by identifying data outliers (such as the problematic ^{19}F neutron inelastic cross section in ENDF validation studies [92]). These uses of physics-aware approaches will continue to grow, banishing the stigma of ML as a physics-free, uninterpretable methodology.

ML also has tremendous potential to emulate the input-to-output mapping done by computationally expensive application models like transport simulations. ML-based emulators or surrogate models can enable studies that would otherwise be computationally prohibitive. In particular, surrogate models are now starting to facilitate large-scale UQ studies whereby nuclear data uncertainties are propagated via ML methods (e.g., for advanced nuclear reactor studies [93]). Such utilizations are expected to significantly expand in the future, to the level where ML-enhanced UQ at the nuclear chart scale becomes accessible, benefiting research in both basic nuclear science, including astrophysics and radioactive ion beam facilities, as well as in applications such as nuclear forensics.

AI/ML is also being applied to extract knowledge from published literature. Convolutional neural nets have been used with edge detection techniques to automate the extraction of data (tables, plots, numbers) from papers, reports, and other documents [94]. ML-enhanced textual analytics or NLP is widely used to process text. Such a capability can greatly enhance the US Nuclear Data Program databases; for example, through extracting keywords from documents as needed for the Nuclear Science References bibliographic database [17]. Emerging NLP algorithms go beyond entity and phrase recognition to automate the extraction of meaning from documents, including distinguishing between synonyms and homonyms through semantic awareness. Such analyses enable automated generation of natural language answers to queries of published literature [95] as well as possible outlooks of theoretical and experimental investigations based on latent knowledge in the literature [96].

While ML approaches are now an enabling technology for a wide range of nuclear data activities, their full potential cannot be realized until nuclear data formats are modernized and fully machine-readable. Examples include utilizing the Generalised Nuclear Database Structure (GNDS) format [97] for the ENDF library and replacing text-based comments in the ENSDF library with modern equivalents that provide suitable extraction of "metadata"; see for example the work by the WPEC Subgroup 50 of the Nuclear Energy Agency [98].

Finally, ML algorithms development cannot be carried out in a vacuum but should be embedded with both theoretical developments and experimental measurements. This means that theorists must strive not only to provide estimates of the uncertainties of their calculations, but possibly functional relationships between the inputs and outputs of said calculations. Such relationships can be encoded in generic assumptions such as linearity, or encoded in a neural network, but they must be available for uncertainty propagation. A similar effort should be required from experimentalists: uncertainties on measurements are, of course, essential, as are estimates of the correlations between these uncertainties. These data form the backbone of many ML efforts.

C. Quantum computing

The long-term potential impact of QC on nuclear data could be significant. Universal quantum computers exploit the entanglement between qubits to achieve the exponential state-space scaling that limits classical computers. In fact, "the simulation of highly entangled quantum matter is the natural arena where quantum computers seem to have a clear advantage over classical ones" [99]. Opportunities for impactful nuclear physics simulations on near-future, so-called noisy intermediate-scale quantum (NISQ) [99] computers are currently limited. Aside from short coherence times and high error rates, these systems have limited numbers of qubits with limited connectivity. The small maximum number of entangled qubits in particular generally limits the scale of computations to proof-of-principle demonstrations otherwise better solved on classical computers.

Two areas of short-term research investment with potential for high impact are identified. The first is to design and optimize the quantum circuits necessary to encode nuclear system Hamiltonians to perform nuclear physics simulations. Calculations run on current and near-future hardware must be optimized for resiliency to typical error sources. For example, because two-qubit gates are a dominant source of error in current systems, reducing several multiqubit universal gates to a single custom operation can dramatically improve accuracy and enable more calculational steps, as was recently demonstrated in a calculation of the time propagation of two interacting neutrons [100]. This technique and others that reduce the circuit depth, i.e., the minimum calculation time, also increase robustness against limited coherence times [101]. The current state of these efforts is closely tied to specific quantum computing hardware, both in identifying error sources and designing appropriate robust circuits. To achieve widespread benefits from these techniques, hardware-independent generalizations must be developed, analogous to compiler optimization of high-level programming languages as opposed to assembly code. Looking forward, there is opportunity to co-design future QC capabilities, such as by standardizing hardware-independent implementations of custom gates commonly arising in nuclear physics calculations.

The point where QC transitions from a topic of research to a tool enabling new science is not well defined. To prioritize community research efforts, a series of grand challenge problems relevant to nuclear data should be identified. These challenges should be intractable on even exascale classical computers, and representative of or enabling a broad field of related research. In the near future of noisy quantum computers, it is essential that the result of these calculations be verifiable. For example, Shor's algorithm allows prime factoring of large numbers impossible on a classical computer, with trivially verifiable results. In the context of nuclear data, verification likely means comparison to empirical measurements. Posing grand challenge questions which could identify areas where more high-quality measurements (or data) are required for verification.

III. PREDICTIVE CODES FOR ISOTOPE PRODUCTION

Radioisotopes, with unique nuclear properties and decay signatures, are broadly used in medicine, industry, and research. Large-scale production of radioisotopes in the 20th century was a monumental achievement, leading to life-altering therapeutic and diagnostic medicines, materials interrogation and characterization techniques, long-lived carbon-free power sources, and the discovery of new elements to push the understanding of the structure, properties, and behavior of atomic nuclei. Radioisotopes are produced through bombardment of a target material with a flux of particles or gamma rays to induce nuclear transmutations. Effective calculations of the reaction rates and isotope yields resulting from an irradiation are essential to experimental design, both to optimize the radioisotope production and to maintain the safety and radiological inventory of the target. The calculation of reaction rates and isotopic yields is performed through a combination of modeling and simulation, coupled with experimental validation and benchmarking.

There are extensive nuclear data needs for this work, in all portions of the nuclear data pipeline. Priorities include improving data for isotopes with established applications, developing energy-dependent cross sections for isotopes of emerging importance, and ensuring that gaps in available data and predictive capabilities are addressed. Of particular importance are high-energy (i.e., $E_n \gtrapprox 5$ MeV) neutron-induced reaction cross sections in ENDF [102] including certain (n, p)

reactions, as well as photonuclear reactions and proton- and deuteron-induced reactions up to 200 MeV.

The need for a robust predictive capability in modern reaction codes presents a cross-cutting need for the nuclear data community, as it impacts both the casual user of these codes, the data evaluation pipeline, and application spaces such as isotope production, neutronics, shielding, and detection. The intent of this section is to spark collaborations between code developers and users to explore the modeling and simulation tools available for prediction of interaction rates and isotope yields, the data needed for effective use of these codes, and the needs for further validation. Addressing the identified gaps from this discussion will improve the predictive capabilities of these codes and benefit both the field of isotope production as well as the breadth of the data and applications communities.

A. Prediction of isotopic yields

Predicting isotopic yields by modeling and simulation relies upon a wide range of computational tools, and may be categorized by a three-part process, each with its own set of predictive codes. First, estimating nuclear data for reaction channels involves evaluating experimental and theoretical models of reaction channels to produce an energy-dependent cross section for each reaction channel, as well as associated secondary-particle spectra. Second, modeling particle transport to determine reaction rates requires simulating transport of particle or gamma-ray flux through the materials in the experiment to determine the effective interaction rates for each reaction channel. Third, simulating irradiation to calculate the activation and depletion of materials over the duration of the experiment and beyond. If the interaction rate changes over the timeline of the experiment, due to transmutation of the material, calculating the yields requires an iterative process between the second and third steps, with different modeling and simulation tools employed in each stage. However, one open problem related to all three of these categories is that, while current predictive tools may generally be able to reproduce nuclear data and observables for known isotopic reactions and routine production activities, they often lack a reasonable predictive capability when applied to emerging isotope production pathways. While experimental data and measurements are always considered the gold standard, this lack of a predictive power has created a situation where time, funding, and experimental capabilities are necessary to consider when exploring any new production pathway. Without reliable predictive tools, new production pathways must be explored experimentally, requiring significant effort even to show that one proposed pathway is inferior to another. To improve this situation, the following sections describe the current state of the art, the available codes used in each stage of the predictive process, and identify current gaps in knowledge and capabilities.

B. Summary of current predictive capabilities and needs

1. Determination of nuclear data for reaction channels

Because such data are used by the nuclear energy industry, nuclear data for neutron interactions near the regions of stability are generally quite robust. The standard format for these data is that used in the ENDF library, which includes evaluations of neutron cross sections and distributions, photon production from neutron reactions, a limited amount of charged-particle production from neutron reactions, photoatomic interaction data, thermal neutron scattering data, and radionuclide production and decay data, including fission products [102]. As reaction data beyond neutron-induced reactions are quite sparse in ENDF, further evaluated data for charged-particle and photon-induced reactions may be found in a number of application-specific databases coordinated by Nuclear data section of the IAEA. However, due to both the time involved in nuclear data evaluation, as well as the inherently application-specific nature of many of these databases, on-demand access to unevaluated experimental nuclear data is needed by users. This information is compiled in the EXFOR database [103], which contains cross sections, differential data, particle spectra, and other nuclear reaction quantities induced by neutron, charged-particle and photon beams. There are nearly 24 000 experimental works which have been compiled in EXFOR, where approximately 46% are (n, x) reactions (approximately 95% of which are for $E_n < 14$ MeV), 20% (p, x), 9% (d, x), and 6% (γ, x). While the data compiled in EXFOR represent a far broader swath of experimental nuclear data than the evaluated data contained in ENDF, there are still a wide number of reaction channels and residual products with limited or no available data. This is especially the case for the production of a number of radionuclides that are of critical importance to nuclear medicine and other communities. In situations and energies where well-characterized cross section data are unavailable, the isotope production community, as well as other application users, relies upon predictive codes to provide estimates. Unfortunately, accurate modeling of even moderately high-energy reactions is challenging. The current suite of predictive reaction-modeling codes is only accurate to within approximately 20% for (p, x) and (n, x) reaction channels where a large body of experimental measurements currently exist. In cases where few data exist, these codes often exhibit discrepancies anywhere within a factor of 2–50.

Four codes—TALYS, EMPIRE, COH$_3$, and ALICE—fall into the first category of codes capable of predicting nuclear physics cross sections. The calculation of energy-dependent cross sections for residual nuclei is generally accomplished by employing various nuclear statistical models. The two most common approaches are the Weisskopf-Ewing formalism [104], which accounts for conservation of energy, charge, and mass, and the Hauser-Feshbach formalism [105], which additionally accounts for angular momentum and parity.

The TALYS code, using the Hauser-Feshbach statistical model, is employed for both fundamental nuclear physics research and other applications. It is streamlined so that all important nuclear reactions are incorporated into one code scheme [34,35,106]. It currently covers incident neutrons, light ions (up to α particles), and photons, with energies up to 200 MeV (and, in some cases, up to 1 GeV). TALYS is used, along with a number of companion codes, to produce the TENDL reaction library [35], which includes (for incident neutrons) cross sections for total, elastic, nonelastic, capture, single- and multiparticle production, inelastic transitions to discrete levels and the continuum, fission, residual production, isomers, total particle production, angular distributions, double differential emission spectra, gamma production, and (critical for isotopes) particle production yields. TALYS has many adjustable parameters, which are optimized for the TENDL library using an extensive validation process. The predictive power of TALYS is numerically established for incident neutrons (above several keV), with charged-particle reactions to follow. Efficient access to all experimental data is essential to improve this code. Validation data for tuning multiple pre-equilibrium and level density models are needed to improve predictive power: specifically, a nuclide-by-nuclide TALYS parameter adjustment. Quality experimental data are essential for making these adjustments.

The EMPIRE-3.2 code, which also uses the Hauser-Feshbach statistical model, provides predictions for incident energies up to 150 MeV and projectiles up to alpha particles in addition to neutrons, photons, and heavy ions [31]. It provides reaction cross sections, residual production cross sections, angular distributions, spectra, and angle-energy distributions of reaction products. Nuclear data needed to improve the predictive capability of EMPIRE include data for tuning level density models, information on pre-equilibrium emission at energies greater than 30 MeV, and reliable theoretical models for going off the line of stability and experimental data to calibrate phenomenological input parameters.

COH$_3$, the coupled-channel and Hauser-Feshbach code, employs a statistical model for compound nuclear reactions. This code can calculate nuclear reactions for incident neutrons of greater than 1 keV and targets of masses $A > 20$ [33,107–109]. This code provides complete information on nuclear reactions, including reaction cross sections as well as energy and angular distributions of secondary particles. The nuclear data needs of this code include information on pre-equilibrium particle emission because, though exciton models work when phenomenological parameters are well-tuned, crude approximations are always involved. Ongoing development of quantum mechanical models have the potential for large improvements in this area. Another identified need is information on nuclear level densities, as this is the most important quantity for predicting unknown isotope production cross sections and could have large uncertainties on high-energy reactions. Specifically, experimental data on nuclides with masses close to target reactions of interest is essential.

ALICE is a Monte Carlo code using the Weisskopf-Ewing evaporation and geometry-dependent hybrid pre-compound decay models [110,111]. Required inputs include the mass and charge of the target and projectile as well as the projectile energy. In order to improve the predictive capability of this (more simplistic) code, benchmarking of the nuclear level density models near shell closure would be valuable for recommending best choices as a function of shell proximity and to indicate areas where more data may be needed. It is also recommended that recent codes based on the Hauser-Feshbach formulation be used both due to their improved physics, and because these newer codes are actively maintained.

2. *Modeling particle transport to determine reaction rates*

MCNP, LISE++, and FLUKA are three codes that fall into the second category of predictive tools: transport codes with some predictive physics models employing imported data libraries.

MCNP6 is a continuous-energy Monte Carlo radiation transport code that can be used for neutron, proton, photon, electron, or coupled neutron/proton/photon/electron transport [112,113]. It has internal activation and depletion capabilities for some applications and can be coupled externally to provide this capability for other applications. The internal physics models of MCNP are optimized for reactions at MeV energies. Improvements currently being implemented or planned for future work revolve around the modularization of the code components, as this will facilitate improved testing and correctness of the code, easier maintainability, and future ease of feature development and integration. The event record, currently in the form of a history file, will be deprecated in favor of a particle tracking (PTRAC)-based capability. There are currently ongoing developments, specifically code improvements related to charged-particle transport, with data and physics model updates as necessary. To improve the predictive capabilities of MCNP6, validation is needed in the form of benchmark experiments and models that integrate collision physics data and models as well as residual nuclide and production/depletion calculations.

LISE++ is a code that predicts intensities and purities of rare isotope beams for the planning of future experiments with in-flight separators [114,115]. This capability is essential for tuning rare isotope beams where results can be quickly compared with online data. This code is applicable for low, medium, and high-energy facilities including fragment- and recoil-separators with electrostatic and/or magnetic selection. This code has a strong reliance on databases for ionization energies, experimental production cross sections, compound materials, and fission barriers. The LISE++ internal physics models are optimized for reactions at MeV energies. In order to improve its predictive capabilities, a wide range of nuclear data on exotic isotopes is needed, especially an isomeric state database, production cross sections, and information on fission barriers and fragment momentum distributions. Additionally, detailed information on the excitation energy of fissile nuclei after abrasion is needed.

FLUKA is a general-purpose tool for calculation of particle transport and interactions with matter [116]. It is capable of computing excitation functions from thermal energies to multi-GeV energies. It also has a built-in capability for evolution and buildup of induced activity, with up to five different decay channels per isotope. The internal physics models of FLUKA are optimized for reactions at GeV energies. In order to improve the predictive capability of this code, reliable experimental data in the form of low-energy neutron transport, charged-particle reactions, and nuclear reactions are needed. In addition, nuclear structure data are essential, particularly when populating residual nuclei near drip lines where mass, levels, spin, parity, and decay data for exotic isotopes are important.

3. Simulation of irradiation to calculate the activation and depletion of materials

Four codes are in the third category, activation and depletion codes: FISPIN, ORIGEN (as used in HFIRCON), CINDER, which was tangentially covered in the MCNP6 discussion, and ISOTOPIA.

FISPIN is a standard code used in the UK over the last 60 years to calculate the composition and evolution of irradiated nuclear fuel and related waste streams [117]. FISPIN11 has been in development for approximately four years and was a complete rewrite of the FISPIN solution method to include nuclear reaction data for accelerators. This code makes several assumptions, including thin targets and neutron-only sources. It is being pursued as a means of handling accelerator-based neutron energy spectra. Quality nuclear data are essential to improve the predictive capability of this code, as models are no longer limited by computational capabilities, but by the uncertainties and covariances in nuclear data. Decay data and neutron transmutation cross sections are of specific interest.

ORIGEN is a generalized activation and depletion code packaged as part of the SCALE code suite [118]. ORIGEN solves the system of ordinary differential equations that describe nuclide generation, depletion, and decay of all nuclides in the system, as well as computing the alpha, beta, neutron, and gamma emission spectra during decay. HFIRCON is a multicycle neutronics and depletion analysis toolkit to automate many irradiation calculations at the High-Flux Isotope Reactor (HFIR). It is used for materials testing, isotope production, and target and core design [119]. HFIRCON couples an enhanced version of MCNP5 to ORIGEN with ADVANTAG variance reduction [120–123]. MCNP5 transport utilizes ENDF/B-VII.0 and ENDF/B- VII.1 cross sections supplemented with gamma production data from JEFF3.1.2 [124,125], JENDL4.0u [126], CENDL3.1 [127], and TENDL-2013 [35]. Depletion calculations use SCALE-ORIGEN data. In order to improve its predictive capability, reaction cross sections for isotopes which are not currently in the ENDF or JEFF libraries are needed, for example ^{187}W and ^{188}W. A full evaluation with scattering and secondary particle production is not needed for ORIGEN in this application space. Gamma production data are also extremely vital for these calculations, as predicted local heat generation rates are often significantly misestimated.

CINDER is an activation and depletion code that can be used for both neutrons and protons [128]. Discussion of planned MCNP6 development indicated that CINDER will be made a callable library for use in coupled calculations in MCNP6 and other codes. The current version of MCNP6 does include an embedded version of CINDER90 that can be used for k-eigenvalue calculations only. Currently, MCNP6 can be coupled to CINDER as well as ORIGEN and FISPACT.

ISOTOPIA [129] is a code that predicts medical isotope production with charged-particle accelerators. The computational engine behind the IAEA Medical Isotope Browser [130], this code uses cross sections from the IAEA medical isotopes library [131] for 150 reactions combined with TENDL-2017 for all other reactions. Once the parameters for a production run are entered in the web browser, the buildup and depletion curves for the isotopes of interest (or all products) are plotted. As with all activation and depletion codes, the reliability of the predictions depends strongly on the input reaction cross sections. Thus improved cross sections, as well as more reaction channels, will be of significant benefit for this easy-to-use package. Extensions of ISOTOPIA are in progress for reactor and photonuclear production of medical isotopes.

IV. EXPANDED BENCHMARKS AND VALIDATION FOR NUCLEAR DATA

Nuclear applications that use computational models built on underlying nuclear data would benefit from the development of well-characterized and documented experimental benchmarks, both critical assemblies (configurations of nuclear material measured at the point of a self-sustaining nuclear chain reaction) and other classes of integral experiments (experiments that test multiple nuclear data types at once). While critical assembly benchmarks are very useful for validating nuclear data, a broader suite of benchmarks are needed to provide more complete validation of nuclear data and physics important for a broad range applications. Critical assembly benchmarks provide a measure of system criticality known as the effective multiplication factor k_{eff}, which is the ratio of the number of neutrons in one generation to the number of neutrons in the previous generation. There are many different applications that can leverage the framework used by the criticality safety and reactor physics communities to develop the additional benchmarks needed to validate the nuclear data they depend on. This section explores new and historical experiments that could be turned into benchmarks to strengthen nuclear data validation in cross-cutting application areas.

A. Importance of benchmark models

Benchmarks are models of well-characterized experiments for which experimental uncertainties and the biases and uncertainties of any geometry and material simplifications have been assessed. In order to improve their accessibility to users, they should be well documented and provide sample input and calculation results. Benchmarks are then used to validate that the analytical methods used to model a particular application adequately represent reality. Ideally, they should provide an integral test of the evaluated nuclear data, data processing codes, and transport codes used to model the application. They can be designed to either test multiple data (isotopes, reactions, energies) at once or, in some cases, designed to be particularly sensitive to one piece of data (for example, a thermal neutron scattering law). When used properly, benchmarks are an essential part of the validation process for evaluated nuclear data and provide the applications feedback needed to improve the data. Examples of benchmarks used in nuclear data validation can be found within documentation for ENDF; one specific example is shown in Fig. 2, which shows the χ^2 improvement in calculated k_{eff} for critical benchmarks for the ENDF/B-VIII.0 [8] nuclear data library compared to ENDF/B-VII.1 [132].

Validation is often understood to come at the end of the nuclear data pipeline, but it is actually fundamental to ensuring the proper functioning of all parts of the pipeline and providing confidence in the predictive power of application

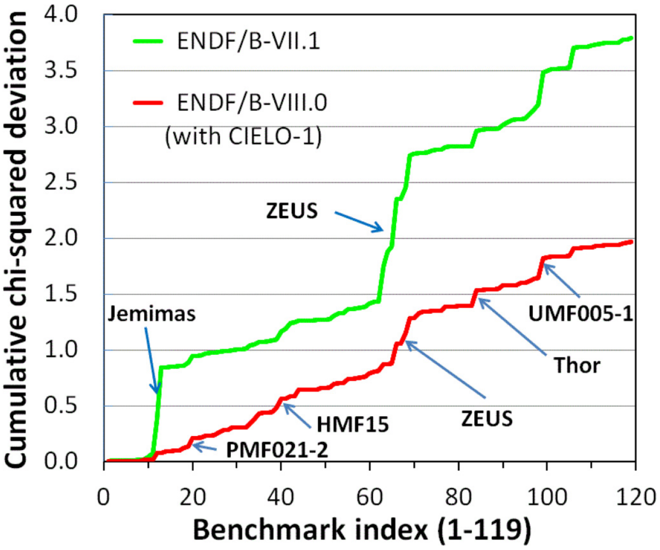

FIG. 2. An example from the Collaborative International Evaluation Library Organization (CIELO) project which shows validation using ICSBEP criticality benchmarks. This shows that, overall, ENDF/B-VIII.0 nuclear data performs better than ENDF/B-VII.1 for ICSBEP benchmarks. (From Ref. [133].)

models. Validation benchmarks specific to an application area can provide a way to systematically prioritize nuclear data needs and determine where funding is needed along the nuclear data pipeline.

The US Department of Energy Nuclear Criticality Safety Program (NCSP) funds research and technology relevant to Nuclear Criticality Safety (NCS) and can be considered a model of holistic nuclear data investment driven by validation data. An early focus of the NCSP was ensuring an adequate suite of integral benchmarks were available for nuclear data and code validation, and NCSP has been the main US contributor to the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook [36] for thirty years. Validation testing against real experiments highlighted problems in underlying nuclear data, data processing, and codes. Therefore NCSP actively funds the nuclear data pipeline to ensure the subcritical predictions are correct, and uses validation needs as a driver and prioritization tool. NCSP directly funds improvements to multiple radiation transport codes–important for code-to-code validation. The program is among the main sources of funding of US nuclear data evaluators (particularly resonance and thermal scattering evaluators), provides funding to the US NNDC at Brookhaven National Laboratory, and maintains its own Nuclear Data Advisory Group to prioritize funding of NCS data needs. NCSP funds and directs integral experiment research at National Criticality Experiments Research Center (NCERC) and Sandia National Laboratories and produces validation benchmarks for nuclear data and NCS, including critical and subcritical benchmarks. The NCSP can serve as a model for other programs who rely on code predictions to accomplish their missions.

As a direct result of the benchmarking efforts of the NCSP and international criticality safety community, critical experiments have come to dominate the current nuclear data validation scheme for all applications. Data analysis of the output of criticality benchmarks is also simple, as it is one number, k_{eff}, but that one number is subject to a fortuitous cancellation of errors in the underlying nuclear data. Calculations of sensitivities to this one parameter are also straightforward compared to sensitivities for other types of experiments, and many codes exist to calculate these sensitivities. The critical assembly benchmarks do not adequately test data for all applications, including gamma emission, scattering data, and time history of fission. Validation using other types of integral or semi-integral experimental measurements could be used to provide a wider test of nuclear data and code predictions. The goal of an adequate validation should be to have overlapping coverage from multiple different kinds of benchmarks, analogous to sensor fusion for a self-driving car. Cameras, LIght Detection and Ranging (LIDAR), and RAdio Detection And Ranging (RADAR) signals combine such that the car can be safely driven in all scenarios. Similarly, it is important to test all the ways codes can employ nuclear data with multiple types of experiments, which will ultimately constrain the potential solutions and eliminate the hidden problem of fortuitous cancellation of errors.

B. Past and present benchmarking efforts for nuclear data validation

The most well known compilations of integral experiment benchmarks are international efforts coordinated and maintained by NEA of OECD. The ICSBEP [36] is the oldest and most trusted NEA compilation, and contains criticality, shielding, fundamental physics, and subcritical benchmarks, although the majority of the included benchmarks are critical experiments. The other three NEA-managed compilations are the International Reactor Physics Experiment Project (IRPhEP) [134], the Shielding Integral Benchmark Archive and Database (SINBAD) [135], and Spent Fuel Composition (SFCOMPO) [136] databases.

A few suggested improvements for these benchmark compilations for nuclear data testing are to address the lack of experimental correlations in the ICSBEP Handbook (only approximately 2% of benchmarks have documented experimental correlations), improving usability, uncertainty analysis, and trust of other experimental data resources (SINBAD, SFCOMPO), and to incorporate legacy experiments that underpinned past validation campaigns (e.g., STEK [137]). Additionally, the expectations for benchmark quality (such as uncertainty analysis and acceptance of modeling simplifications have evolved over time and it would be appropriate to reevaluate some of the earlier benchmarks and bring them up to modern standards.

Other sources of historical integral data include the CSEWG Benchmark Book [138], last updated in 1991, a research reactor database compiled by the IAEA [139], as well as a selection of electronic citations from the US Office of Scientific and Technical Information (OSTI) [140–142]. While there are many existing experiments in these resources that could be useful for validation in other application areas, they are currently underutilized for validation. One of the main reasons is that these experiments are not necessarily evaluated as benchmarks and might have no uncertainty analysis at all beyond the experimentally reported uncertainty. Additionally, models of the experiments with modern codes may not exist, few tools exist to easily use these results for validation, and few tools exist to assess cross section sensitivities in the measured parameters. These compilations could provide an excellent starting point to find experiments that could be evaluated as validation benchmarks which would be useful for multiple application areas.

C. Experimental measurements that could become benchmarks

In addition to historical experiments, there are many experimental measurements that, if adequately vetted and documented, could become benchmarks, including quasi-integral experiments (experiments that are highly sensitive to a particular reaction, but might provide data as a function of time, energy, angle, etc.). This work uses the terms semi-integral, quasi-differential, and quasi-integral interchangeably. The following section describes examples of these types of experiments, but is in no way an exhaustive list.

1. Quasi-integral experiments

Neutron-induced neutron emission experiments are highly sensitive to neutron scattering and can be used to capture angular dependence information. In these experiments, a well-collimated pulsed neutron beam hits a thick sample of interest and detectors surrounding the sample detect neutrons which have undergone scatter or result from fission (for the case of fissionable materials). These experiments are usually conducted using neutron beams in time-of-flight facilities and the neutrons are detected as a function of their time-of-flight. Rensselaer Polytechnic Institute (RPI) has conducted these experiments using incident neutron energies from 1 keV to 20 MeV with a carbon sample as a reference to assist with data interpretation for many different materials [143–149]. A picture of the RPI experimental set-up is shown in Fig. 3. The ^{238}U experiment was used to inform the physics and the ENDF/B-VIII.0 evaluation of ^{238}U [150,151]. Comparing the experimental results with detailed time dependent simulations of the experiments can provide information for nuclear data evaluations, but a detailed model of the experimental setup could be completed to provide integral validation, as well.

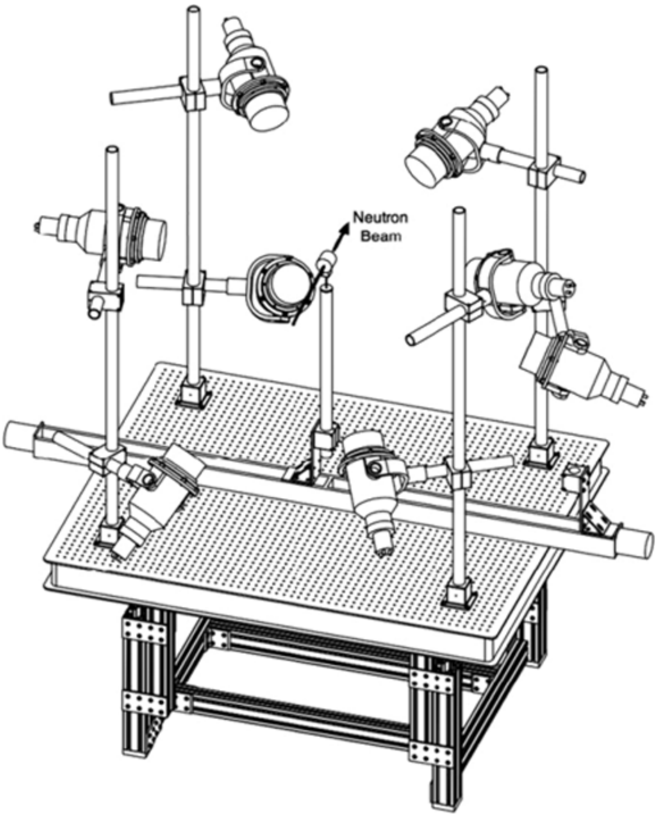

FIG. 3. Example setup of a time-of-flight neutron scattering experiment using organic scintillators at the RPI LINAC. (From Ref. [148].)

A slightly different set of neutron-induced neutron emission experiments that could provide excellent integral data are pulsed-neutron die-Aaway (PNDA) experiments. PNDA measurement techniques were used to characterize thermal neutron diffusion properties in water in a study by Nassar and Murphy [152]. As shown in Fig. 4, a deuterium/tritium neutron generator was used to provide a pulsed source of 14 MeV neutrons incident upon spherical Pyrex flasks of water of various radii at room temperature. Large-radius spheres have low geometric buckling and are relatively insensitive to thermal scattering, allowing validation of the absorption cross sections employed. Small-radius spheres have high geometric buckling and are very sensitive to the integral and differential thermal neutron scattering cross sections employed. After establishing thermal and spatial equilibrium, the neutron flux was measured over time with a BF_3 detector immersed in the water. The apparatus was surrounded by a cadmium-shielded box to minimize room return. Fundamental-mode time-decay eigenvalues were calculated from the recorded count history. The Nassar and Murphy experiment could be evaluated as an ICSBEP Fundamental Physics Experiment, with the experimental set-up modeled in a radiation transport code and predicting the neutron die-away, and additional experiments

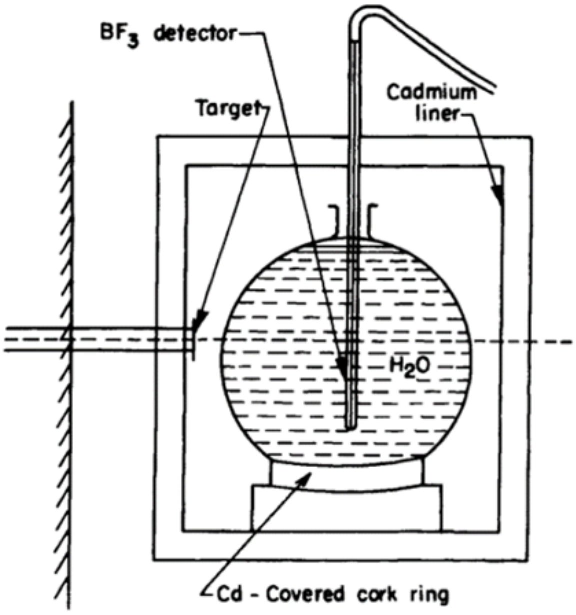

FIG. 4. Example setup of a PNDA experiment. (From Ref. [152].)

of this type would provide needed tests for thermal scattering laws. An example of this is the use of PNDA experiments to validate the ENDF/B-VIII.0 hexagonal ice TSL evaluation [153].

Instead of detecting neutrons reacting with a target, a similar type of quasi-integral experiment that could become a benchmark measures gammas from inelastic scattering reactions. An example of these types of measurements are documented in the Baghdad Atlas, a database of flux-averaged inelastic scattering gamma intensities measured at the Al Tuwaitha research facility outside of Baghdad in the 1970s [154] that has since been digitized and updated to reflect the current ENSDF [23] structure values [155]. The database contains gammas from 105 different samples, of which 76 are natural abundance and 29 are isotopically enriched. Each gamma is presented as a flux-weighted intensity, relative to the ^{56}Fe 847 keV gamma, allowing for the conversion to flux-weighted cross sections. This database is unusual in its broad coverage of elements across the periodic table, including many isotopes that do not have many differential measurements. The measurements were done consistently, with the same flux, detector, and experimental setup. The detector used was a single Ge(Li) detector placed 90 degrees from the beamline. Unfortunately, the flux was not well-characterized and the uncertainties on many data points are quite high compared to conventional benchmarks uncertainties. However, as many samples measured as part of the Baghdad Atlas have no other differential data measurements, these measurements can indicate where large discrepancies exist in evaluated inelastic scattering cross sections. More benchmark experiments should be performed that are similar to the Baghdad Atlas in purpose, but that have improved technology and characterization and that have fluxes similar to the application flux.

The study of neutron and gamma ray emissions from fission fragments applies to several application areas. These emissions are signatures for the detection and characterization of nuclear materials. To perform experiments in this area, University of Michigan recently developed Fission Sphere (FS-3), an array of forty organic stilbene detectors operated in time-coincidence [156,157]. The FS-3 is used to measure the prompt emissions of neutrons and gamma rays from ^{252}Cf spontaneous fission. These new data will be used to validate physics-based prediction codes, including CGMF [158] and FREYA [159], and will be useful in future ENDF and ENSDF evaluations. The first experiments using FS-3 and a ^{252}Cf spontaneous fission source recently took place. These measurements provide useful information on the correlations among energy, multiplicity, and angles of emitted particles.

2. Subcritical experiments

Neutron multiplicity counting (NMC) is important for several application areas, including nonproliferation, criticality safety, and in-core reactor monitoring. NMC accumulates the frequency distribution of observing coincident neutron counts during a coincidence gate that is typically several hundred microseconds to a few milliseconds wide, depending on the neutron lifetime of the subcritical system and the time constant of the neutron multiplicity counter. For multiplying systems (i.e., those containing fissile or fissionable materials), the measured NMC distribution is broader than a Poisson distribution with the same mean because the bursts of coincident neutrons measured by the multiplicity counter are correlated across multiple generations of fission chain reactions sustained in the system. In general, as neutron multiplication increases (i.e., as fission chain reactions grow longer), the NMC distribution broadens further. Furthermore, the higher moments (e.g., the variance, skewness, kurtosis, etc.) of the NMC distribution are more sensitive than the first moment (i.e., the mean neutron count rate) to changes in nuclear cross sections (fission, capture, and scattering) and other parameters (probability of the number of neutrons emitted during fission, etc.). A great deal of NMC and other neutron noise research has been performed in recent years due to improved hardware and simulation capabilities [160–170].

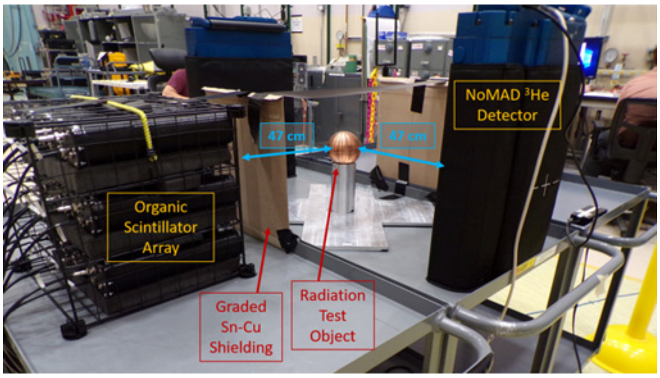

FIG. 5. An example of subcritical neutron noise measurements utilizing both ^{3}He and organic scintillator detectors measuring a sphere of Pu. (Modified from Ref. [176].)

NMC measurements have not previously been used for nuclear data evaluation because there was no computationally efficient method to estimate the sensitivity of the higher moments to energy-dependent cross sections and other transport parameters. Recently, North Carolina State University developed a new adjoint-based first-order sensitivity analysis for higher order NMC moments [171,172].

Other neutron noise methods can also be useful for nuclear data validation. A system based on stilbene organic scintillators (Oscar) has been developed by the University of Michigan. Oscar, shown in Fig. 5, is capable of pulse-shape-discrimination and digital acquisition and has been shown to yield accurate estimates of k_{eff} for several subcritical special nuclear material configurations [173–177].

D. Validation needs from application areas

Not all application areas use the same specific nuclear data for computational predictions. A nuclear reaction data library contains hundreds or thousands of individual isotopes, each with multiple reaction cross sections and related data over many decades of energy. Ideally, the specific data used to predict an application observable should be identified and tested against an experimental benchmark measurement, which will help highlight data areas for improvement. The following section will describe integral needs for several application areas to allow adequate testing of relevant data.

1. Capture gamma benchmarks needed for multiple application areas

Despite being relevant to many application areas, the production of secondary gammas due to neutron capture is often overlooked. This type of data is needed for shielding design and analysis, but it is also important for reactor simulations to correctly model energy deposition due to gamma production (gamma heating) [178]. Additionally, gamma emission from active neutron interrogation provides a physical mechanism for unambiguously assessing the isotopic composition of an object (*i.e.*, material identification), invaluable for nonproliferation studies. An additional example of nuclear data issues involving secondary gammas has been previously illustrated for oil exploration applications [179].

As an example of validation demonstrating a shortfall in data, researchers at the European Spallation Source (ESS) found some important high-energy gammas produced by neutron capture in nickel were missing from ENDF/B-VIII.0, although they were present in ENDF/B-VII.1. The application the ESS is interested in is shielding around a neutron scattering instrument that uses a neutron supermirror primarily comprised of layers of nickel and titanium at the end of a cold neutron beamline. The shielding design around this beamline and the scattering instrument can be dominated by gammas produced by neutron capture, especially in the layers of the neutron supermirror. The important capture gammas [180] missing have energies of 7.819 and 8.998 MeV.

The US National Nuclear Security Administration Office of Defense Nuclear Nonproliferation funded a study that produced a prioritized list of elements relevant to nonproliferation applications that require improved reaction cross sections. The major driving interest is related to secondary gamma emission from active neutron interrogation. This prioritized list comprises elements that make up structural and shielding materials, controlled or dangerous substances, and detector materials. While not all isotopes of elements on this list have known issues with reaction data in ENDF-B/VIII.0, there is a need to review identified existing gamma production cross section data for validity, assess any unvalidated existing data for acceptability to correct existing data, or fill in missing cross section data. Additionally, there should be a concerted effort to reconcile discrete gamma-ray energies, multipolarities, branching ratios, and primary/secondary gamma-ray spectral data between the ENDF/B-VIII.0 and ENSDF libraries.

Benchmark experiments that primarily test radiative capture (n, γ) and inelastic scattering $(n, n\gamma)$ reaction data would be the most useful for these varied applications. An additional consideration should be given to the usability of the resulting benchmarks, as benchmarks that measure integral quantities like dose can take more computational time to run and do not provide specific information about gamma emission as a function of energy. Measurements of gamma spectra would be ideal.

2. Benchmarking needs for advanced reactors

The wide variety of advanced nuclear reactor concepts being considered also have additional nuclear data needs. Some of these nuclear data needs include fission product yield and decay data to more accurately predict isotopic inventories. More precise data needed to predict source terms and shielding requirements are also needed, including prompt neutrons and gammas from fission, gamma emissions from fission products, material activation and decay, and neutron and gamma attenuation. Improvements to thermal neutron scattering laws for many moderators (YH_x, FLiBe, reactor-grade graphite, etc.) would also be desirable. HALEU (High-Assay Low Enriched Uranium) integral experiments are needed for validation. It would also be highly desirable for material damage cross sections to be evaluated and disseminated in the manner of ENDF. Critical experiments performed to support the design and development of these advanced nuclear reactor concepts should be benchmarked to drive improvements in the nuclear data relevant to these applications.

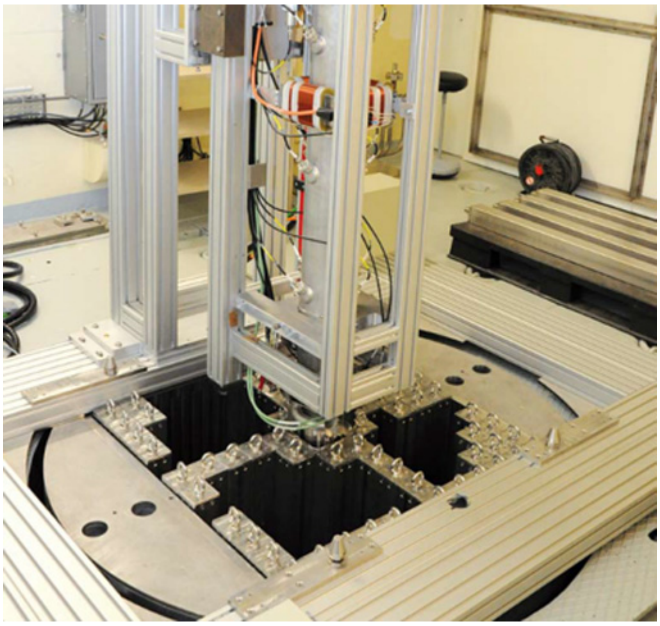

FIG. 6. The VENUS-F Zero Power Reactor, which was used to generate benchmark data for the design of the MYRRHA accelerator-driven system. (From Ref. [181].)

Engineering mock-up critical experiments have historically been used to support the validation of nuclear reactor designs. One recent example is the use of the VENUS-F zero-power reactor [181] to support the reactor physics design of the multipurpose hYbrid Research Reactor for High-tech Applications (MYRRHA) facility being designed at the Belgian Nuclear Research Centre in Mol, Belgium [182]. MYRRHA has been conceived to operate in subcritical or critical mode, as an Accelerator Driven System (ADS) or as a fast reactor cooled by lead-bismuth eutectic, respectively.

To validate the nuclear data and codes for the MYRRHA design, several core configurations with four different compositions of fuel assemblies were studied in VENUS-F, shown in Fig. 6. This core combines metallic uranium fuel (30 wt.% enrichment) with aluminum oxide (for simulating oxide fuel) and includes lead and bismuth as coolant simulators. Global parameters (k_{eff}, β_{eff}, and Λ_{eff}) and local parameters (spectral indices, axial and radial fission rate distributions or differential control rod worth) were measured. These experiments could provide valuable data to support Pb-Bi cooled fast reactor, ADS, and shielding applications if they were turned into accessible benchmarks. Similar benchmarking efforts for other advanced reactor concepts would provide the necessary data to check computational models, nuclear data, and assumptions.

E. Sensitivity-based nuclear data validation

Another barrier to wider use of benchmarks to inform nuclear data is that some integral experiments require nontrivial and computationally intensive analysis that can only be analyzed by a select set of experts using specialized software. The utility of these benchmarks could be vastly improved by using sensitivity coefficients (response functions) to provide near instantaneous nuclear data feedback. With energy and reaction-dependent sensitivity profiles, data evaluators could quickly and easily predict the outcome of a cross section change to benchmark performance. Sensitivity methods to k_{eff} are the most advanced (due to considerable investment from NCSP), but response functions to other benchmark values (calculated spectra, reactor physics observables, burnup, subcritical variables, etc.) would increase the usage of these complicated benchmarks by the nuclear data community and would assist in designing new experiments to have maximum impact on applications. Development of platforms for automated testing, both using traditional calculations and sensitivity feedback, are also important to data feedback. Example efforts in this area include ADVANCE (BNL) [183], NDAST (NEA) [184], as well as the recently developed CRATER [185] (LANL) tool.

Sensitivity methods, especially when coupled with a ML algorithm, can be a powerful tool for finding issues in nuclear data. LANL recently used ML [186] to find issues in nuclear data using the LLNL pulsed sphere experiments [187–189]. Pulsed spheres exist for many distinct materials containing, by careful choice, only few isotopes. This allows one to draw specific conclusions on how well nuclear data of specific isotopes perform when simulating pulsed-sphere neutron leakage spectra. The pulsed spheres have distinctly different sensitivities to nuclear data than critical assemblies. For instance, they are distinctly more sensitive to angular distributions than critical assemblies. In addition, ratios of sensitivities to fission-source term observables differ compared to critical assemblies. These differences allow for disentanglement of the effect of spectra, fission cross sections, and multiplicities when both critical assemblies and pulsed-sphere neutron-leakage spectra are used for nuclear data validation with ML algorithms [92,186].

V. NUCLEAR DATA FOR SPACE APPLICATIONS

As humanity works to extend its technological reach deeper and more resolutely into space, the sophistication of the missions and equipment being launched has also been accelerating. In turn, the engineering and scientific needs to support those missions have continued to grow and nuclear data are no exception. From anticipating effects due to the vast collection of cosmic rays that moves freely in the vacuum of space to humans sending sources of radiation into space to support their missions, utilizing nuclear data and models—generated mostly for terrestrial uses—for space applications is becoming more widespread. This section details existing and anticipated nuclear data needs for space technology. These topics included protection/shielding from space radiation, planetary nuclear spectroscopy, space reactors, planetary defense, and detecting nuclear detonations in space.

As the impact of nuclear data to applications is recognized by a growing number of programs, it is important to examine the many cross-cutting nuclear data needs for the space mission. Enhancing outreach to relevant programs will enable more comprehensive discussions and collaboration among interagency partners. Future discussions related to space needs should: seek to build awareness of space applications in the nuclear data community; carve out a permanent place in the nuclear data community for discussing their needs; document critical data gaps, especially those affecting multiple applications; and suggest steps to meet those data needs. Though only a starting point, the remainder of this section includes a brief introduction to each space-based research topic, the pertinent nuclear data, and what improvements would be most useful for that aspect of the field.

A. Space radiation protection

The radiation environment in space poses unique risks to humans and electronics, necessitating an understanding of the interactions of galactic cosmic rays (GCR), solar energetic particles (SEP), and trapped Van Allen belt radiation. The range of particle energies, species and materials included in those interactions is vast, spanning energies ranging from keV per nucleon to up to several tens of TeV per nucleon; ion species that span the naturally occurring isotopes in the periodic table; and materials composed of elements that also span the periodic table [190–192]. The effort to understand those interactions includes measurements in space [193–199], measurements at particle accelerators [200], and modeling [201].

The free-space radiation environment is generally well understood [190]. Except for cases where instruments and electronics are exposed to the free-space environment, the radiation environment for most operations in space will be composed of the particles and energies present after the primary radiation field has passed through varying thicknesses of materials that make up spacecraft and habitats. In shielded environments, the radiation environment is composed of primary, free-space ions that have slowed down due to electromagnetic interactions (stopping power), and a secondary radiation field created by nuclear interactions of primary ions with shielding materials. The secondary radiation field is complex and also includes particles not present in the free-space environment, such as neutrons. The calculated yields of secondary light ions (p, ^{2}H, ^{3}H, ^{3}He, ^{4}He, and n) have been predicted to contribute 50% of the dose equivalent behind 5 g/cm^{2} of Al and 80% of the dose equivalent behind 30 g/cm^{2} of Al [202]. The calculated secondary light ion yields are also responsible for most of the differences seen between the various codes [203] behind shielding

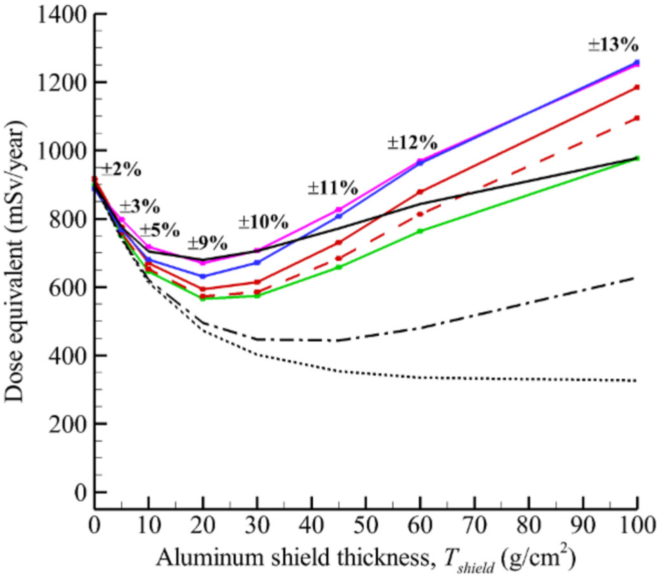

FIG. 7. Predicted dose equivalent rates from neutrons and ions behind varying thicknesses of aluminum using several transport models: FLUKA (green), GEANT4-QMD (dashed red), GEANT4-INCLXX (red), MCNP6 (pink), PHITS (blue), and 3DHZETRN with $N = 1$, 3, and 34 (black). The percentage presented corresponds to relative variations in the model results. (From Ref. [203].)

thicknesses greater than 5–10 g/cm^2 and are the largest source of uncertainty in those calculations (see Fig. 7). As such, the secondary radiation field created by nuclear interactions within spacecraft, habitat, and other materials requires an accurate quantification of the electrons, protons, heavy charged particles, and neutrons that make up that field.

Radiation transport models, both Monte Carlo and deterministic, are the primary tools used for mission design and prediction of crew doses and electronic effects in space. Experimental nuclear data are needed for verification of code predictions, improvements in the physics models used in those codes, and reduction of the uncertainties in their predictions. A review of the double-differential and total reaction cross sections important to the understanding of GCR and SEP transport was conducted [200,204], and key gaps in the experimental data have been identified. For GCR transport, He-induced inclusive double differential light ion (p, ^{2}H, ^{3}H, ^{3}He, ^{4}He, n) cross sections at beam energies from 0.1 up to several GeV per nucleon and on targets of H, C, O, Al, and Fe have been identified as a critical need, as well as total reaction cross sections for most GCR ion species and targets at beam energies above 1.5 GeV per nucleon. In some cases, such as Fe + O, no total reaction cross section data exists. Secondary particle production includes hadronic and electromagnetic particle showers which spread dose geometrically as well as impact the depth of particle penetration through some material thickness. Angular dependence in production cross sections is a critical need for understanding showers. These data needs of the planetary spectroscopy community are similar to the needs of the isotope production and medical physics communities.

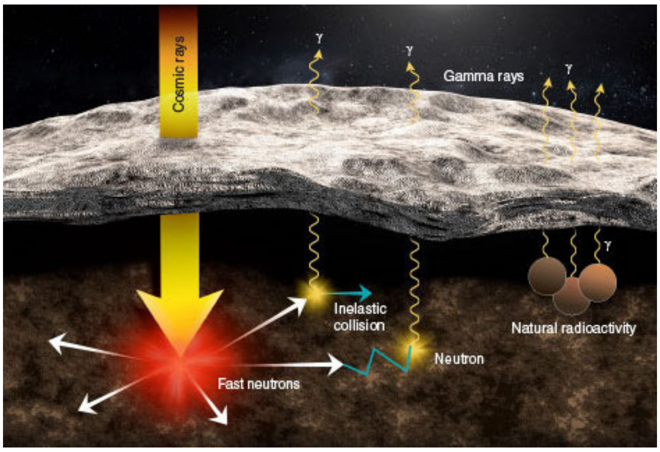

FIG. 8. Schematic of cosmic ray interactions with planetary surfaces. (Rendering by Veronica Chen [225].)

B. Planetary nuclear spectroscopy

1. Background

Planetary nuclear spectroscopy is an established subfield of planetary science where measurements of gamma-ray and neutron emissions from planetary surfaces are used to characterize the chemical composition of the surface. First proposed as a means of characterizing the hydrogen [205] and major-element composition [206] of the Moon, the technique has now been applied to a wide variety of planetary objects. To date, nuclear spectroscopy experiments have been carried out from orbit around the Moon [207–210], Mars [211,212], Mercury [213–215], and the asteroids 433 Eros [216], 4 Vesta [217], and 1 Ceres [218]. Although less common, in situ experiments by landed spacecraft have also been carried out on Venus [219], asteroid 433 Eros [220], and Mars [221]. Missions are currently planned for asteroids 16 Psyche [222], Phobos, a moon of Mars [223], and Titan, a moon of Saturn [224].

Most planetary nuclear spectroscopy experiments rely on galactic cosmic rays to stimulate neutron and gamma-ray emissions from planetary surfaces, as shown in Fig. 8. In this scenario, high-energy primary cosmic-ray particles (>30 MeV), primarily protons, initiate nuclear spallation reactions to depths of a few meters in the surface. Spallation neutrons can escape the surface and the energy-dependent shape of the neutron spectrum provides constraints on the bulk composition and hydrogen content of the surface. Moreover, the neutrons interact with subsurface materials and stimulate gamma-ray emission via inelastic scattering and neutron radiative capture reactions. The resulting gamma-rays provide element-diagnostic measurements of the surface composition to depths of tens of centimeters. NASAs upcoming Dragonfly mission to Titan will use a $^2\mathrm{H}+{}^3\mathrm{H}$ neutron generator to stimulate gamma-ray emission from the surface. However, the underlying nuclear reactions of interest are neutron inelastic scattering and radiative capture.

2. Current status of nuclear data

Although a number of benchmark experiments have been conducted [226,227], the wide variety of processes that are important for nuclear spectroscopy experiments means that data analysis efforts require intensive radiation transport simulations that rely on cross section libraries to provide the knowledge of the physics processes of interest. Relevant processes include spallation; neutron elastic scattering and inelastic scattering; and neutron radiative capture. More specially, spallation cross sections for protons and alpha particles are needed over a wide variety of materials, from energies of a few tens of MeV to hundreds of GeV. Neutron elastic scattering cross sections are required for energies of ~50 MeV down to thermal (~0.2 eV). Neutron inelastic scattering cross sections for $(n;n'\gamma)$ should be studied in major elements, with concentrations of 0.1 wt% (percentage by weight) or higher, over energies of ~50 MeV down to threshold (typically ~0.1 to ~1 MeV). Neutron radiative capture, $(n;\gamma)$, cross sections are also needed for elements with concentrations of 0.1 wt% or higher. In the cases of inelastic scattering or capture, both primary, (e.g., $n;\gamma$), and secondary cross sections for γ-ray production are relevant as both contribute to the final measured γ-ray environment. For known planetary materials, this can include H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni. Currently, uncertainties on the neutron interaction cross sections are the dominant source of systematic uncertainty. Planetary geochemists require measurements with less than 1% uncertainty while 5%–25% uncertainties are currently the best that can be achieved.

3. Nuclear data needs

The highest priority nuclear data need for planetary nuclear spectroscopy is $(n,n'\gamma)$ for H, C, O, N, Na, Mg, Al, Si, P, S, Cl, Ca, Ti, Cr, Mn, Fe, Co, and Ni, from threshold (~0.1 to ~1 MeV) to ~50 MeV, with less than 5% uncertainty. This overlaps with data needs from safeguards and stewardship applications, where neutrons are used for nondestructive characterization of nuclear waste materials and homeland security applications. The data must be provided to the community via cross section libraries, e.g., ENDF and JENDL, that are compatible with the GEANT4 [228] and MCNP6 [229] transport codes, which are widely used by the planetary nuclear spectroscopy community. Comparisons of laboratory-measured gamma-ray production via neutron inelastic scattering to predictions based on ENDF/B-V to ENDF/B-VII, and ENDF/B-VIII reveal a significant degradation in the accuracy of the secondary gamma-ray energy distributions since the release of ENDF/B-VI [179]. Additionally, cross sections for secondary gamma-generation are also affected.

Nuclear spectroscopic investigations also require knowledge of spallation cross sections from energies of a few tens of MeV to hundreds of GeV in typical rock-forming elements. The number of neutrons released in a spallation reaction is particularly important. Because of the wide variety of elements and energies in question, benchmarking experiments are particularly valuable [230] for guiding the decision of physics simulations for GEANT4 and MCNP6. These data needs overlap with the needs of the radiation shielding and isotope production communities.

Another important data need is (n,γ) cross sections. While these are generally known with better precision than the prior two examples [231], unexpectedly high cross sections are currently being identified [232] and high-capture cross section elements can be relevant for planetary nuclear spectroscopy measurements, even if the element is present at ~ppm concentrations and thus not directly detectable via nuclear spectroscopy measurements [233].

C. Space reactors

With the US returning to the Moon this decade (Fig. 9), along with crewed missions to Mars later this century, NASA has resumed looking at nuclear options for propulsion, surface, and on-board power. Past efforts in nuclear thermal propulsion (Project Rover), nuclear electric propulsion (Project Prometheus), and surface power (Kilopower [234], KRUSTY [235]) have been conducted and form the basis of current research efforts. In addition to the existing reactor designs from those projects, new reactor designs (gas, liquid, and solid) and fuels are being explored for space applications. One critical aspect of reactors that will be used in space is the need for autonomous control, a need that places additional emphasis on uncertainty quantification of the nuclear data used in the design of these systems. The data needs for many of the advanced reactor concepts for terrestrial use are very similar to the needs for space reactor development. These needs include: fission product inventories, with accurate data for individual and cumulative yields; secondary radiation generation and deposition; cross sections needed for the assessment of irradiation damage that are not currently available in the ENDF libraries; reduction of uncertainties on fast neutron reaction cross sections on uranium isotopes.

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

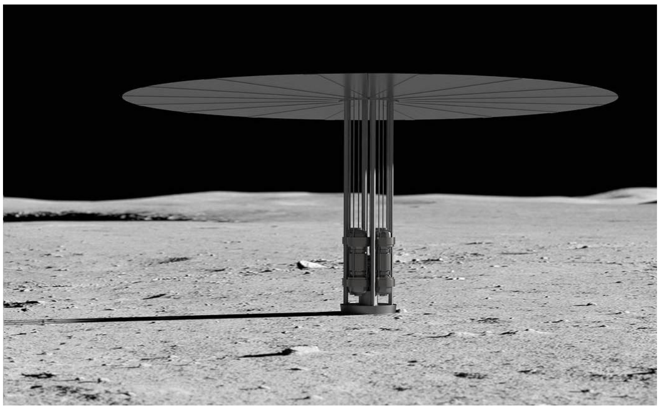

FIG. 9. Illustration of a conceptual fission surface power system on the Moon which may potentially be used for the upcoming Artemis Mission. (From Ref. [236].)

D. Planetary defense

Planetary defense is a field of research devoted solely to the purpose of preparing for a scenario where a near-Earth object, such as an asteroid, could potentially collide with the Earth. Though an asteroid impact similar to what caused the extinction of the dinosaurs is an extremely low-probability event, there are many other smaller asteroids that pose a threat and could cause extensive damage; a recent example is the 20 meter asteroid that exploded over Chelyabinsk, Russia in 2013. It is estimated that there are about 130,000 near-Earth asteroids that are greater than 100 m in diameter and only ~20% have been accounted for and their orbits characterized [237].

In the event that the Earth did need defending from an asteroid impact, the preferred mitigation mission would be a kinetic impactor, which is both the simplest and currently the most developed option in terms of technology [238]. However, in the event that a kinetic impactor would be insufficient to prevent an asteroid impact, either from the asteroid not being in the correct size range or there not being enough time for the orbit of the asteroid to be deflected, sending a spacecraft carrying a nuclear device to intercept the asteroid is an alternate option. A nuclear mitigation mission could be utilized two different ways, depending on the need. Upon detonation, the device would emit mostly x rays and neutrons that would heat up and vaporize the illuminated surface of the asteroid, causing material to expand and be ejected. If the intended mission was to deflect the asteroid, the ejected material would impart a push of momentum to the asteroid in the opposite direction, while keeping the bulk intact and altering the orbit enough to miss the Earth. If the intended mission was to disrupt the asteroid, the x-rays and neutrons would cause a shock wave to penetrate through the entire asteroid, breaking it into many small, fast moving fragments that would miss Earth by a large margin or vaporize in the atmosphere.

1. Simulations with nuclear data and uncertainties

Correctly simulating the energy deposition from the radiation of the device and the subsequent ejecta while designing a mitigation mission would be essential to its success. Such simulations would require accurate cross sections of all interactions and reactions for neutrons at the energies around the output of a nuclear device for the elements that make up asteroids. Though the output neutrons have a variety of energies, the most probable energies are 14.1 (from the $^2\mathrm{H} + {}^3\mathrm{H}$ fusion reaction), 2.45 (from the $^2\mathrm{H} + {}^2\mathrm{H}$ fusion reaction), and ~1 MeV (peak value of the fission spectrum Watt distribution for $^{235}\mathrm{U}$) [239]. Asteroids are roughly composed of various stone-line materials such as silicates, hydrocarbons, metals such as iron or nickel, and potentially some ice, depending on its particular type [240]. Those compounds predominantly include the elements H, C, O, Mg, Si, S, Ca, Fe, and Ni, though others are possible (see Sec. V B). Chondrites and other meteorite samples can be used to provide insight into variations in initial particle (including photon) interactions and energy deposition with such astronomical bodies.

Currently, the most efficient way to simulate the nuclear deflection/disruption of an asteroid is to first generate an energy deposition function from the radiation (such as in Fig. 10), which in the case of neutrons, would utilize Monte Carlo transport codes such as MCNP [229] or MERCURY [242]. The energy deposition function could then be used to initialize a standard hydrodynamics code (which includes damage models) that would calculate the reaction of the asteroid to the energy deposited from the radiation over longer timescales [241,243]. The most recent versions of MCNP and MERCURY get their neutron cross section data from the ENDF/B-VII.1 Library and the Evaluated Nuclear Data Library (ENDL), respectively. An example of the type of nuclear cross sections used to calculate the deposition in Fig. 10 can be seen in Fig. 11.

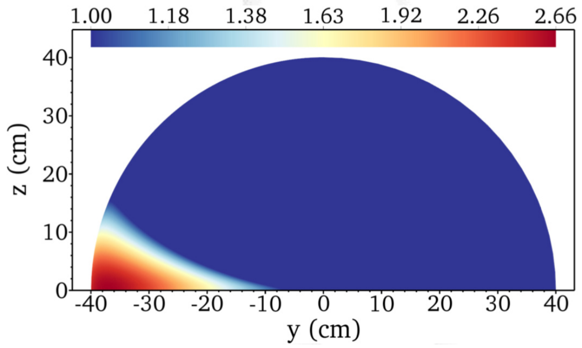

FIG. 10. Energy deposition from a 50 kt yield neutron source visualized in a 80 cm $\mathrm{SiO_2}$ asteroid using MCNP. The color scale corresponds to the number of factors above the melt threshold the asteroid was heated. Dark blue indicates the material was unmelted. (From Ref. [241].)

In part because the choice of a nuclear mitigation mission will likely be made after locating an incoming asteroid with little warning time, the properties of the asteroid itself will contribute the largest uncertainties when formulating the mission. Key characteristics such as the material composition, structure, rotation, and even the mass/size will likely be poorly constrained before a launch if minimal data on the asteroid has been collected. Even if a full reconnaissance mission to the asteroid has been achieved beforehand

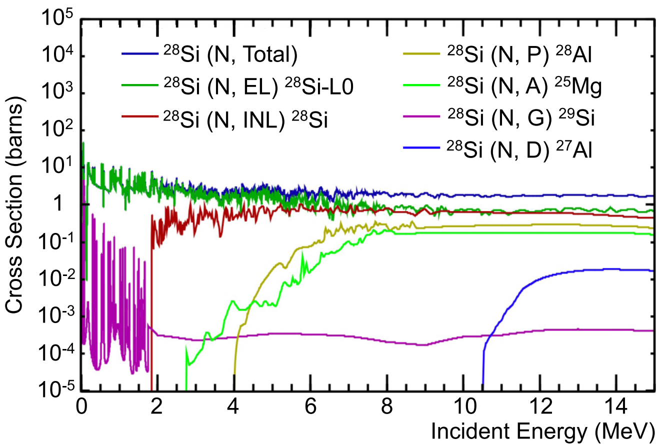

FIG. 11. Neutron cross sections in $^{28}\mathrm{Si}$ for reactions ocurring an energies below 15 MeV. (From Ref. [244].) Curves are taken from Ref. [132].

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

E. Space-based nuclear detonation detection

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

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

The applicable energy and time domains for detecting the gamma rays and neutrons from a detonation via satellite cover a fairly large range. The gamma ray energies are in a range from ∼100 keV to ∼8 MeV. The prompt gammas arrive at early times (100 ns to 1 ms), whereas delayed gammas can arrive at up to 100 s. Neutrons are emitted with energies between ∼1 and ∼20 MeV and arrive roughly within the same time frame as the delayed gamma rays [239].

The early time-delayed gamma rays that arrive within 100 μs to 100 ms and result from short-lived isomeric decays have significant uncertainties associated with their energies and half-lives. In particular, production estimates from ^{235}U, ^{238}U, and ^{239}Pu are important in calculating predicted fluxes of delayed gammas. There are also significant uncertainties on fission product yields (FPYs). There is a need for more incident neutron energies and more precise isotopic decay half-lives that are shorter than ∼0.5 s. Some experiments have been completed and are underway with the hope of eventually measuring FPYs with decay times of order 1 s [245–247]. In the case of a nuclear detonation in air, knowing the neutron cross sections with elements in the air, such as H, O, N, and C, may also be important for understanding the light output of the detonation.

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

VI. NUCLEAR DATA FOR ADVANCED REACTORS AND SECURITY APPLICATIONS

There is a great diversity of advanced reactor designs in neutron spectra (thermal or fast), moderating materials, coolants, fuels, cladding, and structural components. Most importantly, the advanced reactor designs proposed today differ significantly from the majority of nuclear reactors which have been operating for the last half century and thus also differ in their nuclear data needs. Specific reactions and isotopes have been identified for advanced reactors and security applications will be summarized below. It would be advantageous if a centralized database of nuclear data needs for the US nuclear industry could be created, similar to but more specialized than the NEA OECD High Priority Request List (HPRL) [248].

The diverse nuclear data needs and the economically competitive nature of advanced reactor companies make it difficult for national funding agencies to establish a completely prioritized nuclear data needs list in support of advanced reactor development in the US. Challenges include: combining disparate nuclear data needs for different reactor types in an equitable manner; adding considerations of cost-benefit analyses; and weighing the need for missing data such as damage cross sections or thermal scattering uncertainty data against the need to improve existing data.

This section on advanced reactor and security applications first addresses nuclear data needs for advanced reactor development in the US. Next, covariance data and uncertainty quantification are discussed in a broader sense, as common requirement across all applications. Then, improvements of the ENDF/B-VIII.0 nuclear data library for advanced reactors are discussed, in comparison to the preceding ENDF/B-VII.1. Finally, a summary of ideas to address competing nuclear data needs among advanced reactor design, security applications, isotope production, criticality safety, and nuclear physics is presented.

A. Summary of specific advanced reactor nuclear data needs

In the case of advanced reactor design, accurate reaction rate calculations are necessary for many of the materials in the core in order to be able to determine power distributions, the reactivity-worth of control mechanisms, shutdown margins, and the sign and magnitude of different dynamic feedback coefficients, such as Doppler and void reactivity coefficients [249]. These calculations use a substantial fraction of the nuclear data library content, far beyond what is present in criticality benchmark experiments traditionally used to test the evaluated nuclear data libraries. Especially when considering reactor operation, with many advanced reactors achieving high fuel utilization and building up considerable fission product inventories, previous nuclear data library validation efforts may be missing many relevant cases. Therefore individual and cumulative fission product yields may be of increased importance, as they play a central role in many transients, decay heat, and severe accident source terms. Evaluation of reactor kinetics parameters are also necessary to accurately predict the performance of designs under normal and accident conditions.

Secondary radiation generation and deposition is also important for predictive modeling and simulation of advanced reactor performance. These data include prompt neutrons and gammas from fission, gamma emissions from fission product decay, neutron capture and gamma emission data, material activation and decay, neutron and gamma attenuation, and energy deposition in all materials. Secondary radiation generation and deposition data are primarily required for advanced reactors studies, as are irradiation damage cross section information for a wide range of materials. Because damage cross sections are specialized and outside the scope of a general library like ENDF, it would be beneficial to create a dedicated library for them so that reactor designers can assess material lifetimes under actual operating conditions which will most likely not be duplicated in a prototype system.

Thermal scattering law data are also important for reactor designs operating with a thermal spectrum. One of the challenges regarding thermal scattering law nuclear data are the abundance of compounds that can be used in a nuclear reactor. At kinetic energies above 10 eV, neutron-induced reactions can safely be approximated (for reactor applications) as collisions with an unbound nucleus and only "free-atom" nuclide-specific cross sections are needed. However, for neutron energies below 10 eV, the molecular binding forces on the target atom play a significant role in the collision kinematics and can have a measurable effect on the predicted reactor behavior. The thermal scattering law data introduce additional data sets for specific nuclides *in each moderating compound*. This introduces modeling choices and code complexity, such as how to handle the introduction of isotopes without scattering law data during irradiation in moderating compounds or the selection of a "nearest" thermal scatterer when the one that is needed does not exist in the nuclear data library, instead of resorting to the "free-atom" treatment, which is most likely a worse approximation. Yet another challenge that has been brought up by the community of nuclear data users is that certain thermal scattering law evaluations appear to give good predictive performance only when the nuclear data for the other materials in the system come from the same nuclear data library. Combining new thermal scattering law evaluations with nuclear data from older libraries does not provide consistent results. This implies error cancellation within an evaluation or a specific campaign, such as CIELO Pilot Project [133] with continuation of those principles in the International Nuclear Data Evaluation Network [3].

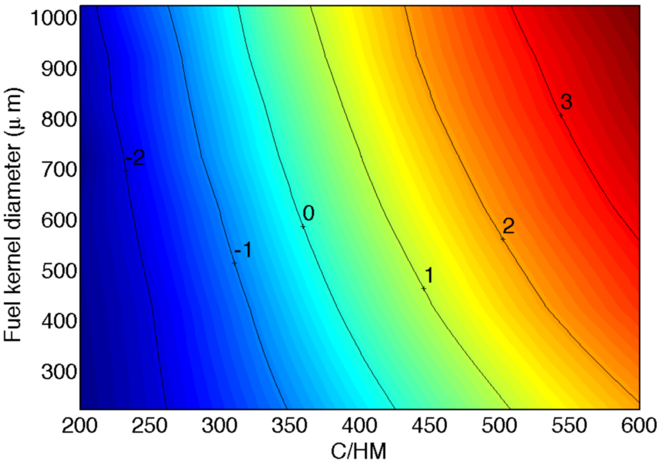

FIG. 12. KP-FHR coolant temperature reactivity coefficient isolines for different C/HM ratios. (From Ref. [253].)

The effective "free-atom" neutron cross section at any temperature can be calculated by Doppler broadening the cross section at 0 K or easily interpolated between effective cross sections at neighboring temperatures. Thermal neutron scattering data, however, do not have this luxury, and they must be generated for each temperature used in the calculation. This presents a particular challenge to thermal nuclear propulsion systems which can operate at temperatures exceeding 3000 K. Determining a reliable method for interpolating and extrapolating thermal scattering law nuclear data in the temperature domain is an open question in the field.

New nuclear data evaluations are needed for advanced moderator and reflector materials which are being proposed for use in combination with HALEU fuel (enrichment between 5% and 20%). Yttrium hydride is of particular interest, highlighting the progressive nuclear data needs of the advanced reactor community in two ways. First, it is a material which has not been widely used in the past and second, nuclear data in a different neutron energy range will be important.

The advanced reactor community needs not only new nuclear data but also their associated uncertainties. Nuclear data sensitivities and uncertainties are actively being used to inform where extra margins may need to be added for design safety [250–252]. As an example, an estimation of Kairos Powers Fluoride-salt cooled High-Temperature Reactor (KP-FHR) coolant temperature reactivity coefficient as a function of design parameters carbon-to-heavy metal ratio (C/HM) and fuel kernel diameter is shown in Fig. 12. Employing the probabilistic collocation method (pcm) to propagate uncertainties in nuclear data, a 1200 pcm one standard deviation uncertainty in system eigenvalue and a 30% one standard deviation uncertainty in the coolant reactivity coefficient due to ^{7}Li(n, γ) was found. Ideally, design parameters would be selected to have a small, negative coolant temperature reactivity. However, Kairos Power does not depend on the nuclear data for a final design. A prototype reactor, HERMES, will be used to inform this aspect and many other aspects of the final design.

In Molten Chloride Fast Reactors (MCFR), nuclear data-induced uncertainties of 900–1700 pcm in k_{eff} have been reported with uncertainties arising from both ^{239}Pu and ^{35}Cl(n, p).

A particularly important uncertainty arises from angular distributions. Currently, the uncertainty on the angular distribution from elastic scattering is reported only for a small number of isotopes in ENDF/B-VIII.0. A concern is that the scattering angular distributions are known to have a significant impact on criticality of small nuclear systems relying on a reflector, such as the MCFR design which utilizes an MgO reflector/moderator. While the reflector material has an known impact on the criticality of that reactor design, there is no uncertainty information in ENDF/B-VIII.0 on the ^{24}Mg elastic scattering angular distribution and thus this effect is unaccounted for in uncertainty studies. Current mechanisms for systematic propagation of nuclear data uncertainties treat missing/unreported uncertainties to have zero uncertainty, exactly the same as quantities which are perfectly known. This is not a conservative approach from the perspective of safety. Furthermore, if an uncertainty is not reported, it usually means that a given quantity has not been investigated thoroughly and a large uncertainty may be possible.

Beyond the need for nuclear data uncertainty, there are also specific needs for integral experiments for nuclear data validation to support advanced reactor development. The ICSBEP contains on the order of 5000 critical and subcritical integral experiments, with a select few benchmarks used for nuclear data validation. Currently, there is a complete lack of criticality benchmarks for nitride fuels in thermal reactors. Nitrogen scattering cross sections for ^{14}N and ^{15}N in the thermal range have little experimental justification. Dedicated experiments may be necessary to provide integral reaction rate measurements in specific advanced reactor neutron spectra and at elevated temperatures.

Computational modeling and simulation of nuclear security around advanced reactor design has its own nuclear data requirements. Nuclear security applications based on antineutrino physics require accurate fission product yields and beta decay chains. Fission product detection in molten salt reactors (MSRs) requires more accurate nuclear data for the following isotopes: ^{95}Nb, ^{103}Ru, ^{106}Rh, ^{106}Ru, ^{125,126,127}Sb, ^{129m,132}Te, ^{131,132,134}I, and ^{138}Xe. Further, improved fission yield data are specifically needed for ^{233}U, ^{232}U, ^{232}Th, and ^{233}Pa for Thorium MSRs. Lastly, gamma ray and x-ray data must generally be improved to support safeguards applications for MSRs. Targeted needs are in gamma ray and x-ray energies, branching fractions, and x-ray line widths, (γ, n) neutron energy spectra, mass attenuation coefficients (for gamma attenuation and neutron self-shielding), and activation product yields. Figure 13 shows the uncertainty contribution for nuclear data alongside other uncertain parameters such as detector statistics and the efficiency model. A recent paper identified uncertainty in branching ratios as a key contributor and performed additional measurements to achieve a factor of 2 to 3 reduction in 5 key branching ratio uncertainties [254].

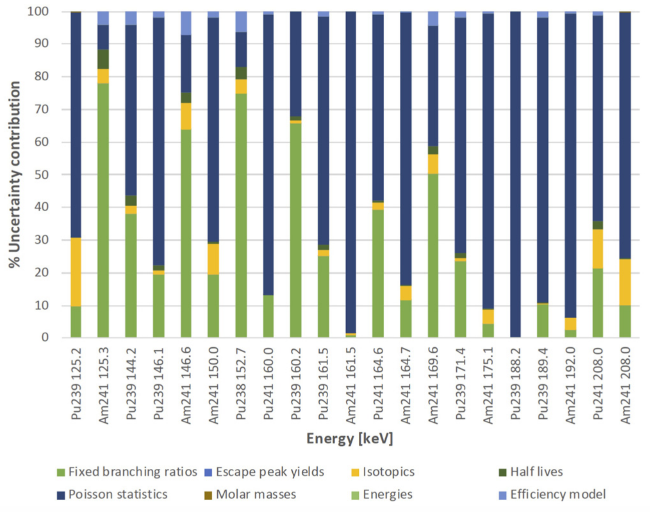

FIG. 13. Uncertainty analysis for signatures used in nondestructive assay of MSRs. (From Ref. [254].)

B. Covariance data and uncertainty quantification

"Covariance data" here refers to all uncertainty data and correlations which has traditionally taken the form of covariance matrices, approximating the joint probability density functions of the entire set of nuclear data as normal distributions. Covariance data are important for predicting the uncertainty in nuclear reactors due to (estimated) errors in the nuclear data at the design stage. During the prototype stage as well as with measurements and system behavior, these data become less important. Nonetheless, sensitivity and uncertainty tools and nuclear data uncertainty propagation are now widely used to understand this possible source of uncertainty, however there is some concern that covariance data are not predictive enough. For example, the biases observed comparing calculations to critical experiments (0.1%–0.5%) are in general much lower than the results of nuclear data uncertainty propagation (0.5%–1.5%).

One of the fundamental challenges of employing covariance data is that the current ENDF/B format cannot represent and store certain types of covariance or correlation information, such as correlations between fission product yields and decay data. The newly developed GNDS format is striving to allow all possible covariance data to be stored. However, work remains to be done to ensure that all potential sources of uncertainty can be represented, stored, read out and used in the new format.

Another challenging area for covariance data evaluation is the difficulty in validation. Since covariance information in evaluated nuclear data represents a degree of certainty in the reported mean values, it is not a physically measurable quantity. Therefore validation of covariance data is not possible in the strict sense of validation. There is a need for robust (ideally open source) covariance verification, checking, and adjustment codes which can be used across all applications.

It is technically possible to generate application-specific covariance matrices which are calibrated to a set of measurements. The clear advantage of this process is the gain in predictive power [255]. The disadvantage is the potential for misuse, such as an application outside the original intention, and the inability for these application-specific "corrections" to feed back into the fundamental data. A further downside is the potential for conflicting adjustments based on different application bases. It is the strong opinion of the community of nuclear data producers and users that it is the responsibility of nuclear data evaluators to declare which integral experiments have been used in the evaluation process and how those experiments were used, either systematically or nonsystematically. Such declarations will help ensure that those experiments are not used in the code validation process.

There are significant gaps in the covariance data library. Missing or unreported covariance data are simply neglected in systematic uncertainty propagation methodologies. Regretfully, this is mathematically equivalent to having perfect knowledge of the quantities as missing covariance data results in zero propagated uncertainty attributed to that source. Missing covariance data and correlations which have the most immediate impact on advanced nuclear reactor modeling are currently missing thermal scattering law covariance data, angular distribution covariance data, and correlations between independent fission yields and decay data. Furthermore, there are gaps in code capabilities to systematically propagate the impact of some currently existing and future covariance data. For example, sensitivity coefficients for thermal scattering law data may not be calculated in MCNP, SERPENT [256], or SCALE [118].

C. Incorporating new nuclear data libraries into advanced reactor analysis

Although the ENDF/B-VIII.0 nuclear data library was released in February 2018, adoption of this evaluation has been slow among some nuclear data users. Differences in light water reactor depletion numerical benchmark results have been observed with reactivity biases that increases as a function of burnup. Thus, while simulations of fresh fuel may match measurement very well, depleted fuel can have a significant bias in reactivity (700 pcm) [257]. In the HTR-10 high-temperature graphite reactor benchmark ENDF/B-VII.1 has a 270 pcm bias compared to experiment and ENDF/B-VIII.0 has a 580 pcm bias using the crystalline graphite TSL evaluation [258]. The nuclear data evaluation community maintains that ENDF/B-VIII.0 performs better than ENDF/B-VII.1 in validation on the set of criticality safety related benchmarks in the ICSBEP when the correct graphite porosity is used. A reactor grade graphite TSL evaluation with 20% porosity is needed to better approximate the graphite used in HTGRs. Additional high-quality reactor and depletion benchmarks would help resolve this issue.

ENDF/B-VIII.0 also includes various thermal scattering law libraries for graphite at different porosities. While this is a large step forward, it also requires knowing the correct graphite porosity in order to properly simulate the results. For example, with HTR-10, simply swapping one porosity for another leads to a 665 pcm difference in reactivity [258]. An unexpected trend with ^{16}O has also been found whereas the energy corresponding to the Average Lethargy of Fission (EALF) increased, reactivity decreased compared to ENDF/B-VII.1. A similar trend was found with plutonium-solution-thermal (PST) benchmarks. The set of PST benchmarks had a positive bias in reactivity as EALF increased, suggesting an issue in the Plutonium evaluation above thermal neutron energies [259].

It is recommended that during the nuclear data evaluation validation process, proposed nuclear data evaluations are compared against a wider subset of benchmarks and benchmark-like data, particularly where there can be large impacts on advanced reactors.

VII. THE HUMAN PIPELINE FOR NUCLEAR DATA

Humans play key roles in every aspect of the nuclear data pipeline from measurements to calculations, evaluations, validation, processing, and dissemination. However, a serious, far-reaching effort is urgently needed to transform the nuclear data workforce to ensure that the pipeline will keep functioning in the future. There are numerous reasons for this. First, as the field of nuclear data grows in breadth and depth, an expansion of the workforce is absolutely essential to capitalize on new areas while simultaneously maintaining the evaluation activities required to keep the core databases up to date. For example, automation, machine learning, and high-performance computing have the potential to revolutionize nuclear data only if researchers with these skills are brought into the program. Additionally, keeping ENSF and ENSDF current is critical, as the US provides the overwhelming majority of the evaluated nuclear data in these databases [260], data that the world downloads each day and relies upon for their basic and applied nuclear research.

Next, the aging demographics in the nuclear data workforce imperils the transfer of knowledge to the next generation, while the overall homogeneous demographics means that the field does not benefit from the available diversity of thought. Unfortunately, it is a challenge to attract younger, more diverse scientists to the field. This is both because the importance and significance of nuclear data to the scientific community are often overlooked, and because the "service" components of the field (e.g., preparing data measured by others for use in applications) can lack the excitement and appeal that pure research offers.

Finally, long-term workforce planning is essential because of the specialized training needed to work at each stage of the pipeline. This is particularly critical to nuclear data, because the skill set of the workforce must evolve to keep pace with the latest developments in big data science (e.g., machine learning, automation, databases) and nuclear science (e.g., Bayesian approaches, covariances, reaction and structure theory).

Below, recent efforts to expand and evolve the workforce to begin to address these critical issues are described.

A. Workforce expansion efforts

1. Outreach

A variety of nuclear science outreach activities exist to engage and educate the general public, students of all age levels, and researchers both within and external to the nuclear science community. These activities are coordinated by universities, national laboratories, and university-national laboratory collaborations, and include, for example public events or displays that expose the general population to nuclear science concepts and provide a general overview of the field. As an example, Michigan State University provides a range of different successful programs to engage members of the public beyond the nuclear science community [261–265]. Opportunities for younger students also exist through university and broader collaborations [266–268]. Teach-the-teacher programs provide school teachers with knowledge and materials for introducing nuclear science at precollege levels [269,270]. Such activities provide an early introduction to nuclear science and may influence a student's selection of undergraduate or graduate-level coursework.

It is critical to note, however, that these outreach activities are focused on nuclear physics rather than on the specialized field of nuclear data. They therefore serve to *indirectly* expand the nuclear data workforce. While there are some nuclear data-specific outreach activities, these need to be significantly expanded to educate the community about the value of nuclear data, as a critical step for enhancing recruitment into the field. Two current outreach activities include a nuclear-data component of the Exotic Beam summer school [271], an annual event for graduate students, and a working group session on nuclear data at the annual Low-energy community meeting [272], organized by the FRIB Working Group on Nuclear Data [273].

2. *Internships and research opportunities*

Another effective way to enhance recruiting is to increase the opportunities for students to engage with nuclear data mentors. While students have a range of opportunities to take part in nuclear physics research, through undergraduate and graduate research and conferences [274,275] as well as educational summer programs (for example, see Refs. [276–281]), the creation of nuclear data-specific internships would be extremely beneficial to enlarging the workforce. A range of scholarships and fellowships from federally sponsored programs (e.g., see Refs. [282–293]) can be used for academic research and connections to the national laboratories and nuclear application areas. The national laboratories have a variety of outreach activities to connect to undergraduate and graduate students, as well as faculty [294–303]. Students and faculty can participate in focused research efforts through internships or ongoing collaborations. Specific awards for in-residence research also exist at each laboratory.

Additionally, university-laboratory collaboration efforts are a natural way to create opportunities to recruit young talent into the field. Two current examples include the DOE NNSA Consortia (NA-22) (e.g., Refs. [304,305]) and Stewardship Science Academic Alliance (NA-11), including Centers of Excellence [306]. These larger groups have a range of concurrent efforts, providing several research opportunities and outreach activities. For example, the Nuclear Science and Security Consortium [304] has a multifaceted research effort including nuclear data. Expanding the number of nuclear data-related projects in these collaborations would benefit the human pipeline in nuclear data. Some USNDP centers have also brought interns into their programs, and a targeted expansion of those efforts is needed.

Furthermore, evolving the nuclear data workforce through increasing diversity and inclusion is now considered a best practice. The DOE Office of Science, which funds the USNDP, makes its commitment to diversity, equity and inclusion (DEI), as well as anti-harassment policy clear on its website [307]. All DOE national laboratories are engaged in DEI initiatives, see Ref. [308]. The National Science Foundation, which funds a number of university nuclear physics groups, has its own Office of Diversity and Inclusion [309]. More broadly, the Inclusion, Diversity and Equity Alliance for the American Physical Society (APS-IDEA) [310] is a new initiative to support DEI at all levels of the physics community. DEI and anti-harassment policies also play a large role in the APS Guidelines on Ethics [311]. By embracing these initiatives, the nuclear data community can further broaden and enlarge the workforce in the future.

B. Evolving the pipeline

Advances in computational tools, containerization, and machine learning algorithms have opened the door to automate significant portions of the nuclear data pipeline. New technologies can eliminate or minimize many rote or tedious activities currently comprising the pipeline, enabling evaluators to focus more on the physics and on their invaluable interpretations. Continuous integration and deployment software now automates portions of the pipeline used to generate revisions of ENDF, serving also to increase the quality of each evaluation [183]. Machine learning techniques have the potential to decisively augment an evaluator's interpretation to find trends in large, complex datasets that are impossible to discern by humans [91,92]. While computational advances have lowered the human workload in processing and verifying the nuclear data libraries, it has also increased the complexity and volume of nuclear data in the libraries.

It is, however, critical to note that these advances to evolve the nuclear data pipeline will only be possible if the skill set of the nuclear data workforce also evolves. While the expertise of evaluators will continue to remain vital to interpreting the results as well as casting existing data in meaningfully interpretable forms for algorithms and improving the physics, a new set of skills will be needed to automate the pipeline. It will be critical for the community to determine which roles can and should be automated in the future, and delineate which new skills are the highest priority. These can then be used to target recruitment efforts that can most effectively automate and transform the pipeline. The community should prepare for, and embrace, these new developments that will provide improved nuclear data, more rapidly, for a wide variety of applications.

VIII. SUMMARY

A brief summary of the needs and outlooks for the topics discussed above is reiterated below. These needs, as identified by close interactions of nuclear data users, producers, and funding managers across multiple programs, provide a clear picture of the cross-cutting nuclear data research priorities in the US.

A. Advanced computing for nuclear data

Nuclear data are fundamentally tied to computation. Accurate nuclear data enables predictive computation for nuclear science and engineering. Computational hardware has been rapidly developing through advanced architectures, including GPU-enabled architectures, presenting a unique opportunity to significantly improve the predictive power of nuclear modeling methods with current nuclear databases by allowing more complex calculations to be carried out.

Porting existing software bases to advanced architectures, including GPU-enabled ones, should be a priority for code developers—whether for nuclear models, applications or production codes. This could upgrade could enable integration of at least some nuclear physics capabilities directly into transport codes. When experimental data are missing or inconsistent, such a capability could help generate data on-the-y by simulating nuclear reaction processes, either with the actual physics model or an emulator of that model built with ML tools. The trading of memory (stored data) for flops (on-the-fly data generation) in application codes may soon be necessary to cope with the future trends of supercomputer architectures. Increased computational capabilities, together with high-fidelity emulators of physics models, would also greatly facilitate the quantification and propagation of uncertainties throughout the nuclear data pipeline, which has been identified as an urgent priority.

Machine learning algorithms could aid the extraction of physics from nuclear data, thereby helping design experiments to address specific nuclear data gaps or identify critical modeling needs that could have the largest impact on evaluations. AI/ML also offers a unique opportunity to automate some tasks currently performed by humans, especially parsing and processing data from literature. One could exploit the application of NLP tools to extract data from tables and perform semantic analyses of research papers. To unleash the full potential of AI/ML for automation, data must be machine-readable throughout the nuclear data pipeline (from EXFOR to validation experiments and uncertainties). This could take the form of well-specified Application Protocol Interfaces (APIs), ideally in a variety of programming languages to maximize portability and interoperability. Such APIs are key to develop fully containerized solutions to nuclear data evaluations.

In the longer term, progress in high-performance computing and increased dissemination ML techniques could pave the way to grand challenge problems such as uncertainty quantification at the scale of the entire chart of isotopes. Such grand challenges are extremely relevant for basic science research in areas such as astrophysics, especially with the ramping up of next-generation radioactive ion beam facilities like the Facility for Rare Isotope Beams (FRIB). Looking even further ahead, classical computing may soon hit its limits: QC may have the potential to revolutionize computing. While QC cannot now be a priority for the nuclear data community, it could be relevant to invest in some small scoping or feasibility studies to ensure that this future technology will be useful.

B. Predictive codes for isotope production

A robust, validated predictive codebase for reaction data is the single highest priority for the isotope production community. This is, in fact, a cross-cutting need for the entire nuclear data community because many other applications rely on the same codes.

All codes require a large body of well-characterized experimental data to help tune and benchmark their capabilities. In particular, GeV-scale predictive codes are lower priority because limited isotope production occurs in this energy region. Although there is an urgent need for validated codes up to 200 MeV, only limited improvements are possible for reaction channels measured in narrower energy ranges. Global fits are needed to enhance the predictive capabilities of all codes, requiring experiments which report all possible measured reaction channels for a given interaction. Improved level density and pre-equilibrium models are needed for global rather than local improvements.

In addition, the community needs a set of integral isotope production benchmarks for validation, similar to those developed by the nuclear criticality community. While required data uncertainties will vary based on the application, accuracies of $\sim 10\%$ have been considered an acceptable target for the isotope community. As part of these global fits, evaluators need reliable calibration points: measurements of competing channels will be valuable for placing calculational constraints, particularly at high energies and when fission barriers come into play.

Several overarching observations related to isotope production are detailed here. First, large-scale reaction data measurement campaigns need to be continued to obtain quality data for model refinements. Although stacked-target experiments provide information about many channels across a wide energy range, this is just one class of experiments needed. Going beyond production cross sections, other reaction observables are needed, including stable isotope production cross sections and secondary particle spectra. Stable isotope production has often been neglected in isotope production measurements. Because these data are measurable, they provide constraints on code performance. However, stable isotope measurements will require techniques beyond decay spectroscopy such as chemical and physical methods (including inductively coupled plasma mass spectroscopy and other chromatographic techniques), as well as prompt gamma spectroscopy, which can provide detailed information on angular momentum and level densities. Secondary particle spectra, while challenging to measure, particularly at higher energies, are useful for modeling. These spectra, measured as a function of angle, can partially constrain both level densities and contributions from compound and pre-equilibrium reaction mechanisms.

Second, the organization of measurement campaigns should be improved. Many past nuclear data measurement campaigns have been designed to determine production rates for particular reaction channels of interest for isotope production. Instead, a combined working group of both theorists and experimentalists could perhaps more efficiently identify viable measurements with the biggest potential improvements to predictive code capabilities.

Next, nuclear structure data are needed to enhance level density and pre-equilibrium models used to calculate yields in production codes. Because the nuclear astrophysics community has established detector arrays and analysis codes for such measurements, collaborative partnerships with that community could efficiently measure these data without establishing an independent capability. Pre-equilibrium models could be improved through quantum mechanical models of pre-equilibrium emission. High-performance computing resources would likely be required for this effort.

Finally, evaluations of charged particle-induced reactions are needed. Currently, the isotope production community uses a combination of modeling codes and EXFOR data when production data are needed. Aside from beam monitor reactions and a selected set of reactions for production of therapeutic or diagnostic isotopes, there is no ongoing effort to evaluate charged-particle production data. Many other production channels also lack proper evaluations. The isotope production community needs an evaluated database for the currently employed production data. Predictive codes are important for these evaluations. A charged-particle evaluation subcommittee should be added to CSEWG in order to maintain a sustained focus on this effort. While charged-particle needs are not unique to isotope evaluations, the high-energy modeling required is unique. Relative to most reaction evaluations, which focus on neutrons below 14 MeV, the reaction mechanisms and pre-equilibrium processes at these higher energies place unique and challenging constraints on models. A charged particle database for isotope production would function, similar to ENDF, as a standardized resource supporting a wide range of codes and applications. With a global improvement of predictive capabilities, fewer specific experimental measurements would be required to address new reactions.

C. Expanded benchmarks and validation for nuclear data

Accurate predictions for nuclear systems require adequate testing of both the codes and underlying nuclear data against real experiments. One of the biggest challenges for validating nuclear data against benchmark experiments is the paucity of benchmarks for certain applications. There are a wide variety of well-documented benchmark experiments covering different aspects of criticality as well as a collection of benchmark experiments for reactor physics. As discussed in Sec. VI, the reactor benchmarks are incomplete, especially considering the wide variety of reactor designs and the quantities impacting them. The documentation of shielding and transmission benchmarks also lags behind criticality benchmarks in quality. There are few benchmarks to support other applications, such as predictive codes for isotope production, discussed extensively in Sec. III.

The existing benchmarks used in the validation component of the nuclear data pipeline are heavily influenced by a subset of criticality benchmarks. The user community should carefully review both current experiments and historical records for benchmark-quality data pertinent for specific applications. Each user community should develop their own set of benchmarks sensitive to the reactions and energy regions of interest for each particular application. These application-specific benchmarks should become part of the validation process to enable general-purpose nuclear data libraries, such as ENDF, to have the greatest utility for the widest range of nuclear data applications.

In addition, sensitivity methods should be developed to benchmark observables beyond $k_{\rm eff}$ for both new and current benchmarks. These methods should be employed to produce and archive sensitivity profiles of calculated cross sections. A library of sensitivity profiles for a wide range of benchmark experiments would permit fast and efficient data testing by nuclear data producers without relying on specific applications.

D. Nuclear data for space applications

The nuclear data needs for space applications have only begun to be addressed by the nuclear data community. However, there are strong overlaps with the needs of isotope production, medical physics, safeguards, stewardship, homeland security and terrestrial-based nuclear reactors. In this perspective, only the nuclear data needs for radiation protection and planetary spectroscopy were highlighted.

Some space-based needs are already being addressed by ongoing work. in support of terrestrial applications. For example, the needs for space reactor development will, in many cases, follow those for terrestrial reactors, see Sec. VI. Similarly, the needs for satellite-based nuclear detonation detection are being addressed by ongoing fission product yield and decay research.

There are a number of specific critical needs for space radiation protection, such as He-induced inclusive double differential light ion (p, ^{2}H, ^{3}H, ^{3}He, ^{4}He, n) cross sections for beams from 0.1 to several GeV per nucleon on H, C, O, Al, and Fe targets. Total reaction cross sections for most galactic cosmic ray ion species on targets at beam energies above 1.5 GeV per nucleon are needed. Such needs overlap with those of the planetary spectroscopy community which requires spallation cross sections for energies from $\sim$10 MeV to hundreds of GeV for elemental components of planetary surfaces.

The planetary spectroscopy community also requires precise $(n, n'\gamma)$ cross sections for rock- forming elements between $\sim$0.1 and $\sim$50 MeV with less than 5% uncertainty. Such cross sections are also of interest for safeguards, homeland security and planetary defense.

E. Nuclear data for advanced reactors and security applications

The nuclear data needs for advanced reactors are driven by material choices for coolants, moderators, control materials, advanced fuels, and cladding materials. Nuclear data needs are driven by the materials chosen for each design and the sensitivity of a wide range of performance and safety characteristics such as include core reactivity, decay heat, power distribution, and source terms. In addition, reducing uncertainties in gamma-ray and x-ray energies, branching fractions, and x-ray line widths for nondestructive isotopic analysis on important isotopic ratios is key to enabling a robust, economic safeguards and security approach to advanced reactors and nuclear fuel cycle facilities to ensure reactor security.

Understanding the characteristics of a diverse set of reactors requires a wide range of nuclear data which has not been rigorously validated previously. Studies utilizing uncertainty propagation of current nuclear data libraries can result in large model uncertainties, forcing nuclear reactor designers to implement additional engineering safety margins. One possible way to prioritize needs is to require accurate predictions of reactor behavior during steady-state and transient operations by employing sensitivity analysis (SA) and UQ for regulatory requirements set by the US Nuclear Regulatory Commission (NRC). The SA/UQ is sensitive to the covariance data used for uncertainty propagation.

Another way to prioritize nuclear data needs for reactors can be based on the timescale over which they are required. Deployment time is critical for advanced reactors and most reactor designers will adjust their margins and continue with system deployment if their data needs cannot be fulfilled over a short timeline. The flow of data through the pipeline from need, experiment, and modeling to evaluation, validation and library release is too long to effectively support advanced reactor deployment over 4–8 years. A plan for long-term impact is important if improvements are needed because long-term, committed effort is necessary to significantly accelerate the nuclear data pipeline. This effort must be balanced with short-term, targeted R&D investments. Detailed feedback from developers is needed for an effective evaluation effort.

Finally, needs could be prioritized by considering only those critical for advanced reactors. Some specific isotopes key to advanced reactor development include elastic scattering of ^{24}Mg for MCRE; thermal scattering data for graphite and FLiBe, and ^{19}F, ^{9}Be, ^{6}Li, and ^{7}Li cross sections for FHR. It is not clear which nuclear data are critical for deployment, i.e., reactors cannot be built without them. Targeted experiments or reactor prototypes can fill many gaps. Adding design margin and lower core lifetime because of gaps in data could potentially significantly increase costs based on design specifics. If the NRC became involved in data needs prioritization based on license applications, increased costs and review lengths could result.

Reducing uncertainties in gamma-ray and x-ray energies, branching fractions, and x-ray line widths for nondestructive isotopic analysis on important isotopic ratios is key to enabling a robust, economic safeguards and security approach to advanced reactors and nuclear fuel cycle facilities.

The top nuclear data priorities to support deployment of advanced reactors in the US and development of nuclear security for advanced reactor applications, are five-fold: address missing data and any artifacts discovered in ENDF/B-VIII.1; improve evaluations with large uncertainties that are relevant for currently considered designs with the expectation that data may come from new experiments and/or reactor prototypes and not new differential measurements; extend evaluated data files to include correlations; improve the verification and validation processes used in the next ENDF/B release to include more cases representative of advanced reactors; and continue to develop and improve methodologies for uncertainty evaluation, not only of nuclear data, but also in the associated costs/benefits of refinement.

F. The human pipeline for nuclear data

To expand, diversify, and retool the nuclear data workforce, a number of efforts have been identified. First, efforts to engage the community about the value of nuclear data, and increase the opportunities for students to engage with mentors in the field, should be increased. Second, collaborative efforts between universities and national laboratories should be expanded to further create opportunities to recruit young talent into the field. Third, a robust community commitment to DEI, in line with the goals of the funding agencies that sponsor nuclear data activities, is essential. Fourth, the community needs to determine which roles can and should be automated in the future with the introduction of artificial intelligence and automation in the nuclear data pipeline. Subsequent recruitment efforts must then be targeted towards researchers with the skill set needed to achieve this pipeline automation. Although there will always be a role for humans in evaluating and interpreting nuclear data, that role will evolve with data activities in the future.

G. Summary of cross-cutting opportunities

Gatherings of the nuclear data community facilitate discussion of the future direction of nuclear data research in the US. There are a number of persistent themes which have been recommended across several of the six topics covered here.

Nuclear data are inextricably tied to computational modeling and simulations. Modeling and simulations need to be both precise *and* accurate to have meaningful impact on the programs they support. Computational accuracy can be improved both by better measurements and by integration of physics models. First, more accurate experimental nuclear measurements are necessary to supply the beginning of the nuclear data pipeline, which after evaluation, processing, and validation will be incorporated into application codes. While measurement needs for specific isotopes and reactions have been discussed for each area above, much of the focus has been on replacing historical, low-fidelity, evaluated nuclear data. Gamma-ray production data, charged particle reaction data, and comprehensive measurements of all reaction channels are emphasized. Second, by fully integrating nuclear physics models in application codes rather than relying on tables or single-valued data, predictive modeling and simulations can achieve increased accuracy. The rapid expansion in computational power is now enabling this exciting possibility.

The precision of predictions from modeling and simulation is also a cross-cutting topic of great importance. The quality of the evaluated uncertainties in the current nuclear data libraries is in general lagging behind the quality of evaluations of the mean quantities. Many of the evaluated quantities are missing covariance data altogether. Furthermore, methodologies for uncertainty propagation are not currently implemented in the computational toolbox in many applications (e.g., nuclear engineering), even though uncertainty quantification is sought out by most nuclear data users.

All predictive modeling and simulation codes in nuclear science and engineering should be validated on benchmark-quality integral experiments. This practice validates the combination of the particular modeling code with the nuclear data inputs. The difficulty lies in developing a wide representation of applications to produce a comprehensive set of benchmark experiments for code and data validation. A further call to action to the entire community is to ensure that all benchmark experiments are considered in the validation and testing of updated nuclear data libraries.

The last recurring theme is automation. The rapid development of AI/ML in recent years has shown great potential for use in the nuclear data pipeline. Natural language processing technology has the potential to automate the early, compilation, stage of the pipeline. Nuclear physics emulators can accelerate on-the-fly computation of nuclear physics models. Machine learning and outlier detection technology can be used in validation. Integration of these technologies presents new challenges and opportunities to the nuclear data pipeline workforce. The opportunity to connect multiple, automated segments of the pipeline is a grand challenge for nuclear data, which can lead to greater reliability and reproducibility. Ultimately, automation has the potential to significantly accelerate the response time of the data community and their databases to the needs of the users.

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