Progress towards the ENDF/B-VIII.1 release

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Abstract. The efficient, safe, and high-performance design and operation of nuclear reactors, and other nuclear systems, rely on complete and accurate nuclear data files. The ENDF/B library is the main nuclear reaction data library in the United States and one of the main ones in the world. It encompasses sub-libraries for neutron, proton, alpha, deuteron, ^{3}He, and gamma projectiles, in addition to thermal neutron scattering law, fission product yields and three atomic sub-libraries. The last release of ENDF/B was ENDF/B-VIII.0 in 2018. Since then, many important and impactful developments have been made for actinides, structural materials and light elements. Some of these contributions are part of the IAEA-coordinated International Nuclear Data Evaluation Network (INDEN). The scale and impact of these changes warrant a new library release, namely ENDF/B-VIII.1, which is scheduled for early 2024. This release is planned to happen in both ENDF-6 and GNDS-2.0 formats. The present work describes the updates expected to be present in ENDF/B-VIII.1, as well as the review process and quality control procedures developed and implemented at the National Nuclear Data Center (NNDC). Preliminary results from the Beta versions already released are also shown.

1 Introduction

Many nuclear applications, from nuclear energy to nuclear medicine and basic science, rely on transport codes accurately simulate the performance of a given nuclear system. Such codes make use of nuclear data libraries to inform relative probabilities of the many different reaction processes. Therefore, the reliability of nuclear applications is intrinsically tied to the quality of the nuclear reaction data adopted. The ENDF/B library is the main nuclear reaction data library in the United States and it is widely used not only domestically but also internationally [1]. The ENDF/B has had many releases since the first one back in the 1960s, the most recent ones being ENDF/B-VIII.0 [1] in 2018, ENDF/B-VII.1 [2] in 2011, and ENDF/B-VII.0 [3] in 2006.

The recent years have seen many important developments in the evaluation of impactful nuclear data files, warranting the release of a new version of the library, namely the ENDF/B-VIII.1. These updates, many of which are part of the IAEA-coordinated International Nuclear

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Data Evaluation Network (INDEN [4]) collaboration, will be shown in some detail in the sections below. This release is planned to happen in February 2024. There are however, many intermediate tasks that need to be completed before the final release. This includes evaluation reviews and the release of intermediate Beta versions of the library. Both aspects will also be discussed in the sections below.

2 Library infrastructure

In 2023, in support of the ENDF/B library management and related projects, the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) established a repository system [5] using the GitLab platform [6]. This allowed to modernize the version-control approach of evaluation files, keeping track of any individual changes and developments. This streamlines and facilitates the tagging, release and access of Beta versions of the library.

Another important feature implemented through the NNDC GitLab repository is the possibility to create review environments. This facilitated enormously the review of submitted files allowing a direct interaction among evaluators, reviewers and library manager, through cross-referencing posts which allow markdown text, plots and uploaded files. The intention of the review process implemented for ENDF/B-VIII.1 was inspired by the refereeing system carried out by peer-reviewed journals to guide the publication decision of manuscripts. We could not fully replicate the journal system, due to the relatively small pool of nuclear data experts capable of providing constructive reviews in a timely manner. However, this was already a huge step forward in the direction of improving the quality of the release. In past releases, quite often a critical, detailed investigation of a contributed evaluation would happen at much later stages, whereas now issues are found, communicated and corrected much earlier, diminishing the likelihood that they are present in the final release.

Additionally, the NNDC GitLab repository serves also as an integrated logging tool for tracking issues related to the nuclear data files reported by the community. This is particularly useful when used in concert with the review environment, so the issues found can be documented in great detail to be fixed at some point by the collaborative community.

2.1 Continuous integration system: ADVANCE

The Continuous Integration (CI) system called ADVANCE (Automated Data Verification and Assurance for Neutron Calculations Enhancement), developed at the NNDC, had been initially developed as a short-term solution to help with the release of ENDF/B-VII.1. ADVANCE was able to run a series of checking codes on a given evaluated file. However, with the implementation of the NNDC GitLab ENDF repository, it became clear that there was an important potential in integrating both systems.

With this in mind, the ADVANCE system was almost completely re-worked. Since GitLab's CI configuration is controlled by per-project YAML files that, in principle, can be modified by anyone who is part of a given project, a more secure approach had to be developed. To prevent accidental, or even intentional, jeopardizing modifications, all checking codes to be executed are run in Kubernetes cluster of Docker containers behind the BNL firewall. Reverse proxy server (outside the BNL FireWall) secures access from the Internet to GitLab. To implement this we actually had to overcome two requirements that GitLab had not anticipated: 1) computer cluster running codes must be behind firewall; and 2) legacy checking codes need temporary space. To find a solution to this, Gitlab and BNL cyber security engineers had to collaborate with us to resolve issues.

Currently, the ADVANCE system is fully operational and deployed. As soon as any modified data file is uploaded to the repository, it triggers a series of checking and processing

codes that are run in the updated file, leading to a report in markdown format, which allows to combine formatted text with plots. This allows for quick error detection, making it easier to fix them.

3 ENDF/B-VIII.1 Beta releases

It is very useful to tag and distribute intermediate preliminary releases of the library, ahead of the main release. This allows a broader testing of the updates, gauging potential formatting, processing and integral performance issues, with sufficient time to fix them.

3.1 ENDF/B-VIII.1-β1

The first Beta version of ENDF/B-VIII.1 was released on March 1, 2023. It contained updates to the neutrons, fission yields, and alphas sublibraries.

On the neutrons sublibrary, one of the main updates was to the ^{239}Pu file. It started as parallel independent evaluations from different groups which, through some coordination effort, converged to a single collaborative multi-institution file, combining and leveraging the strengths of each approach. Among the many other files submitted, reviewed, and incorporated into ENDF/B-VIII.1-β1, were the product of the INDEN collaboration: ^{235,238}U, ^{54,56,57}Fe, ^{28,29,30}Si, ^{55}Mn, ^{50,52,53,54}Cr, ^{16,18}O, ^{19}F. Among the files included in ENDF/B-VIII.1-β1 outside the INDEN collaboration, it is worth highlighting ^{140,142}Ce (ORNL), ^{103}Rh (RPI/IRSN), ^{6}Li (LANL), ^{9}Be (LANL), ^{234,236}U (LANL), ^{181}Ta (RPI/ORNL/LANL), ^{95}Mo (IRSN/LANL), and ^{156,158,160,161,162,163,164}Dy (ORNL). There were also updates to the unresolved resonance range of some fission products and many other small fixes.

For both spontaneous and neutron-induced fission yields sublibraries, the updates were mostly to uncertainties. As reported in Ref. [7], there were some files in ENDF/B-VIII.0 with cumulative yields that had huge unphysical uncertainty, coming from improper error propagation. These uncertainties were recalculated in Ref. [7] and their corresponding values were updated.

In the alphas sublibrary, the files for ^{9}Be, ^{17}O, and ^{18}O were updated. These files existed before in ENDF/B-VIII.0 but many reactions are being described for the first time. There were also minor updates to ^{4}He to account for minor fixes.

3.2 ENDF/B-VIII.1-β1.1

About a month after the release of ENDF/B-VIII.1-β1, on April 18, 2023, ENDF/B-VIII.1-β1.1 was released, focusing mostly on the Thermal Scattering Law (TSL) sublibrary. The reason for this was that the review process for TSL evaluations proved to be more complex than anticipated and there was the desired of the community to start testing the neutrons sublibrary promptly. ENDF/B-VIII.1-β1.1 incorporated 64 TSL either new or updated files, relative to ENDF/B-VIII.0. These evaluations had been developed mostly by groups in North Carolina State University (NCSU), Naval Nuclear Laboratory (NNL), and ORNL. The large number of contributions caused to exhaust the number of indices allocated to identify each evaluation (MAT numbers, see Ref. [8]), which led to a discussion in the community on how to handle and uniquely identify these contributions.

Additionally, we took the opportunity of the ENDF/B-VIII.1-β1.1 release to incorporate fixes in four files of the neutrons sublibrary to issues uncovered after the release of ENDF/B-VIII.1-β1. These fixes should not impact integral benchmarks, and thus not compromise any validation testing being performed. The files changed were ^{9}Be, ^{54}Cr, ^{235}U, and ^{239}Pu.

3.3 Feedback on ENDF/B-VIII.1-β1/1.1

The Cross Section Evaluation Working Group (CSEWG) [9], which is the body that maintains and coordinates development of the ENDF/B library, convened extraordinarily on April 25-27, 2023, at Lawrence Livermore National Laboratory (LLNL) to discuss results and plans related to the ENDF/B-VIII.1. The meeting, named mini-CSEWG Meeting, focused on needs for the ENDF/B-VIII.1 release, in particular on validation results from multiple institutions from the US and abroad. The preliminary feedback was generally positive with some aspects in need of improvement.

For example, results from testing the Beta release on LLNL pulsed-sphere neutron leakage spectra simulations showed improvements, in particular related to ^{235}U and ^{239}Pu, but also identified areas in need of additional work. There were also results from leakage benchmarks sensitive to stainless steel and its components. The overall results showed that the new library performs much better than ENDF/B-VIII.0, even leading to users from industry to endorse the performance of the new iron and chromium [10] files, as shown in Ref. [11].

Particularly noteworthy were the validation results from LANL which highlighted the performance improvement in LCT and HST critical benchmarks, especially when considering further improvements in the ^{238}U done after ENDF/B-VIII.1-β1.1, which will eventually be part of ENDF/B-VIII.1-β2. In addition to that, it was shared that ENDF/B-VIII.1-β1.1 led to a degradation in performance specifically in depletion benchmarks, likely tied with the ^{239}Pu resonance evaluation. The INDEN evaluators promptly agreed to further investigate and find a proper balance between the PFNS, nubar and resonance contributions. This will eventually be fixed in ENDF/B-VIII.1-β2.

3.4 Expectations for ENDF/B-VIII.1-β2

There are many expected developments to be done for the next Beta release.

For the neutrons sublibrary, we expect to fill exit distributions that are currently non-existent for some reaction channels. This effort is being led by LLNL, LANL, and KAERI. We also anticipate improvements to ^{238}U and ^{239}Pu, motivated by performance in criticality benchmarks, as discussed in Section 3.3. ^{6}Li should also be updated to restore (n,t) cross section below 1 MeV back to standards. We also expect to include in ENDF/B-VIII.1-β2 all submitted files that were not reviewed in time to be included in ENDF/B-VIII.1-β1. This corresponds to important materials such as ^{63,65}Cu, ^{233}U, ^{206,207,208}Pb and others.

For the TSL sublibrary we expect to include fixes and other materials such as polystyrene. For the photonuclear sublibrary we expect to include many evaluations originating from an IAEA-coordinated effort [12]. For some mission-critical materials, however, we expect to maintain their versions from ENDF/B-VIII.0 until a more detailed analysis and comparison is done.

4 Conclusion

We have developed a support infrastructure for the ENDF/B library which allowed us to migrate to a repository system, implement an evaluation review process and track issues. We also integrated the repository with a continuous integration system that runs checking codes and produces reports in an automated, per-commit basis. The process for the next ENDF/B release is moving along well with multiple Beta versions released, while we currently prepare for the next one. Validation feedback is generally positive with specific improvement needs that are already being addressed.

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