

The High-Energy Intra-Nuclear Cascade Liège-based Residual (HEIR) nuclear data library

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Abstract. It is standard practice for nuclear data files to include tabulated data for distinct reaction channels for incident energies up to 20-30 MeV. Above these energies, the assumptions implicit in the definition of individual channels break down and event generators are typically used within codes that simulate nuclear observables in applications. These offer robust simulation of the physics but increase the computational burden. So-called 'high-energy' nuclear data files have been produced, but the well-known libraries are more than a decade old and rely upon models developed many years before their release. This presentation describes a modern library with a high level of production automation that offers regular updates as the models it is based upon are improved.

The most recent versions of the intra-nuclear cascade and de-excitation models available within Geant4 were used to generate tabulated data of residual nuclide production. For the first released library, the INCL++5.3 and ABLA version within Geant4 v10.3 were used to calculate over 10^{12} incident protons over 2095 target isotopes with incident energies up to 1 GeV. These were collated into tabulated data in the international-standard ENDF-6 format. The resulting files were provided as group-wise files and were distributed as HEIR-0.1 with the FISPACT-II version 4.0 release.

A second library, HEIR-0.2, has been generated using the new INCL++6.0 and C++ translation of the ABLA07 model available within Geant4 v10.4. Simulations were performed using incident protons, neutrons, deuterons and π^\pm . An improved agreement is observed in the comparison to experimental data not only between the two versions, but against the other well-known high-energy nuclear data files and models available within Geant4. This benchmark includes mass and isotopic distributions, as well as incident-energy dependent cumulative and independent cross sections from the EXFOR database.

1 Introduction

The simulation of activation-transmutation requires complete nuclear data, including all reaction channels for both stable isotopes and any reaction products that may undergo subsequent reactions during the irradiation. While some general-purpose nuclear data libraries, such as TENDL [1] and the JENDL High Energy 2007 File (JENDL/HE-2007) [2], have extended up to hundreds of MeV and even GeVs, intra-nuclear cascade and coupled de-excitation models are commonly used from energies starting at 20-200 MeV due to their superior accuracy [3].

Following a study into the models available within Geant4 [4], it was found that the Intra-Nuclear Cascade Liège (INCL) [5] and ABLA03 [6] models provided the best agreement with several experiments considered and they were used to create a full reaction data library in the ENDF-6 format [7], which was named the High-Energy Intra-Nuclear Cascade Liège-based Residual (HEIR) nuclear data library [8].

2 Upgrading HEIR with improved models

One benefit of a purely model-based nuclear data library is that new versions may be easily created using the most recent models. Since the creation of the first prototype HEIR-0.1 library, a new INCL-6.0 version and C++ translation of the ABLA07 [9] code were integrated into Geant4. Following the approach taken with HEIR-0.1, calculations were performed with 1 million incident particles for each stable isotope and 100 000 for each unstable isotope with a half-life above 1 second. The FISPACT-II [10] 162-group energy grid from 30 MeV to 1 GeV was used for the energy discretisation.

Following the previous study for HEIR-0.1 [8], the HEIR-0.2 data has been compared against well-known measurements, including ^{208}Pb isotopic and mass-distribution data from 1 GeV incident protons, as shown in Figures 1 and 2. The HEIR-0.2 library shows superior agreement with the data against the now decade-old JENDL/HE-2007 [2] and HEAD [11] libraries. The new models provide better agreement with isotopes created

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with large mass difference not caused by fission¹ that were significantly under-predicted with HEIR-0.1.

The ⁵⁶Fe data that was also part of the IAEA spallation models CRP study [13] was also considered with the new HEIR-0.2 data, as shown in Figure 3. As with ²⁰⁸Pb, the ‘deep spallation’ products have an enhanced cross section that broadly improves the agreement with the experimental data.

3 Cumulative residual production cross sections

The EXFOR [16] database contains many cumulative reaction data, particularly for high-energy charged-particle-induced reactions. These were previously not considered for HEIR-0.1 testing due to the need for nuclear decay sub-library processing to calculate the full branching ratio matrix \mathcal{B} , which is required to generate the independent to cumulative matrix, $Q = (1 - \mathcal{B})^{-1}$. Using the SANDY Python package [17], this was easily performed and used to generate cumulative residual product cross sections for comparison with EXFOR. Lead has the largest dataset in EXFOR and the comparison includes more than a hundred products with thousands of datapoints over the 30 MeV – 1 GeV energy range of HEIR-0.2. To summarise this data, as shown in Figure 4, the minimum difference in experimental standard deviations

$$(\min_i[(C - E_i)/\Delta E_i])\forall i \text{ in EXFOR}$$

was calculated for all datasets in the HEIR energy range with linear interpolation between HEIR data points (C) and experimental data in EXFOR (E) with their associated uncertainty (ΔE). 56% of the reaction products had at least one experimental point within 1σ and fewer than 7% of products had no data within 5σ (all of which had only one measurement at one incident energy to compare).

Data that did not include measurements within 30 MeV – 1 GeV, isomeric products and data without uncertainties were excluded, which accounts for 62 of the 193 nuclides with proton-induced lead residual product data in EXFOR. Figure 5 gives an overview of the types of comparisons that are summarised in Figure 4, including:

- those few with significant discrepancy, but only one point (¹³²Cs);
- those with many measurements that universally have some data within 1σ of HEIR-0.2 (⁸⁵Sr);
- cases with multiple, discrepant measurements (⁶⁰Fe);
- those with data outside the HEIR energy bounds and are excluded and marked black in Figure 4 (²⁴Na).

These underline the difficulty in drawing conclusions from such a heterogeneous and complex database, although with moderate effort and approximations trends can be extracted.

¹Sometimes referred to as ‘deep spallation’.

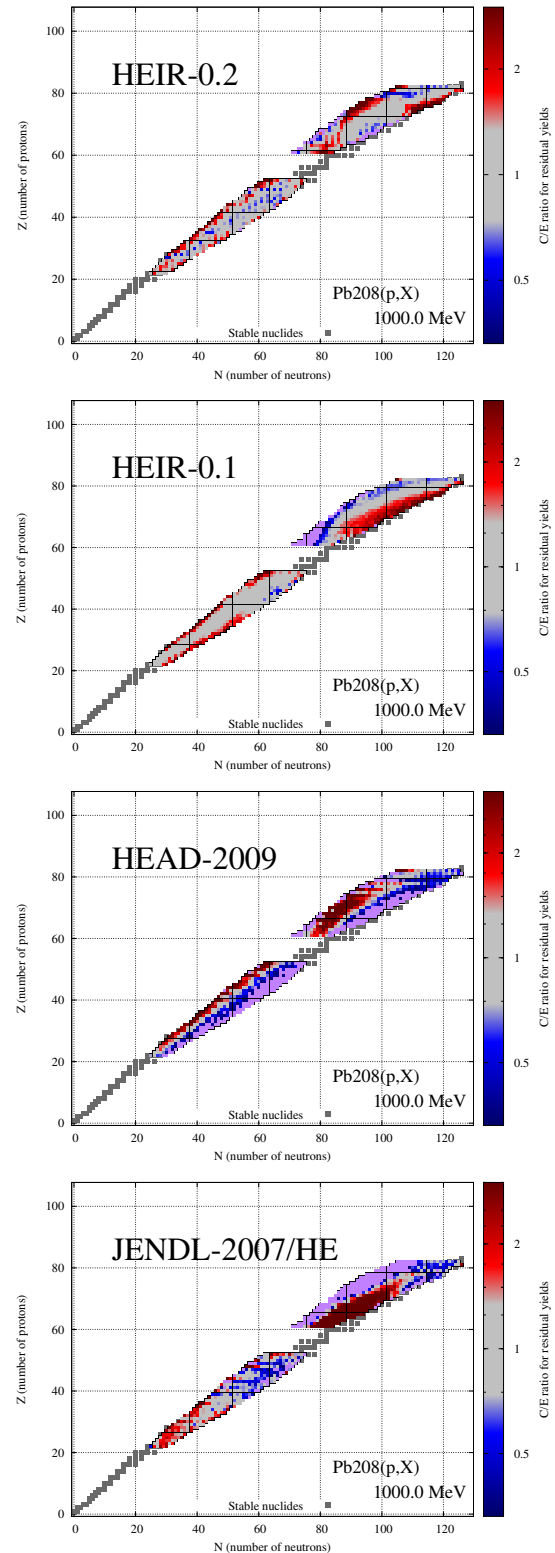


Figure 1. Comparison against EXFOR data of Enqvist et al. [12] of the residual product cross sections from a 1 GeV incident proton on ²⁰⁸Pb in HEIR-0.2/0.1, JENDL/2007-HE and HEAD-2009. Ratios are provided for all documented experimental nuclide product values with a logarithmic scale. Values shown as violet are absent in the nuclear data files.

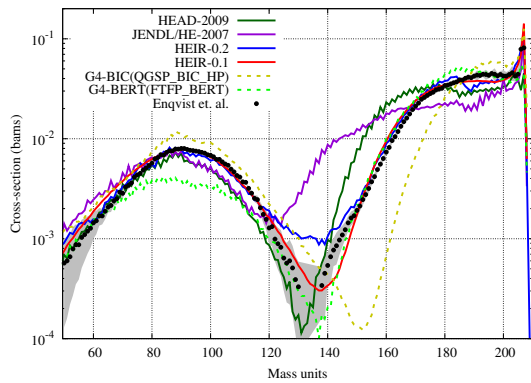


Figure 2. Comparison of nuclear data libraries and other INC/de-excitation models in Geant4 for 1 GeV proton-induced ^{208}Pb residual product cross sections compared with experimental data from Enqvist et al. [12].

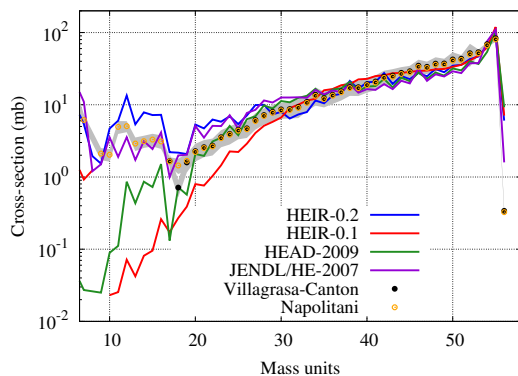


Figure 3. Comparison of nuclear data libraries for 1 GeV proton-induced ^{56}Fe residual product cross sections, compared with experimental data from Villagrasa-Canton et al. [14] and Napolitani et al. [15].

4 Simulation with FISPACT-II

The *raison d'être* of the HEIR project was to perform time-dependent inventory calculations using complete reaction data up to 1 GeV that would complement the low-energy nuclear data libraries that were already available within FISPACT-II. Version 4.0 [18] of FISPACT-II introduced a new functionality to splice low energy with high energy libraries and perform simulations using incident particle spectra provided from Monte-Carlo simulations that may utilise intra-nuclear cascade models. This is shown in Figure 6, where the HEIR library provides the ‘all-energy’ data required for complete activation-transmutation cross section calculations. HEIR-0.2 follows the same ENDF-6 MF=10 construction formats and therefore integrates directly into FISPACT-II to provide the same functionality with improved data.

5 Discussion

It is a challenge to draw conclusions from the thousands of data points over all products, particularly when individ-

ual measurements at one energy from pre-1960 are juxtaposed with hundreds of points covering a range of hundreds of MeV. By using all data sources, including cumulative residual production, mass and isotopic measurements, we may attempt to perform a more comprehensive validation of these complex data.

While HEIR-0.2 improves upon HEIR-0.1 with more modern models and superior agreement with experimental data, the cumulative product data highlights the need to consider a wider incident-energy range and isomeric products to make use of approximately one third of the EXFOR products. The introduction of isomeric states within the de-excitation model is the subject of future work for ABLA development and, when released, may be directly integrated into future HEIR versions. A comprehensive comparison with all EXFOR data and all targets will be the subject of future work to provide the most complete verification and validation exercise possible.

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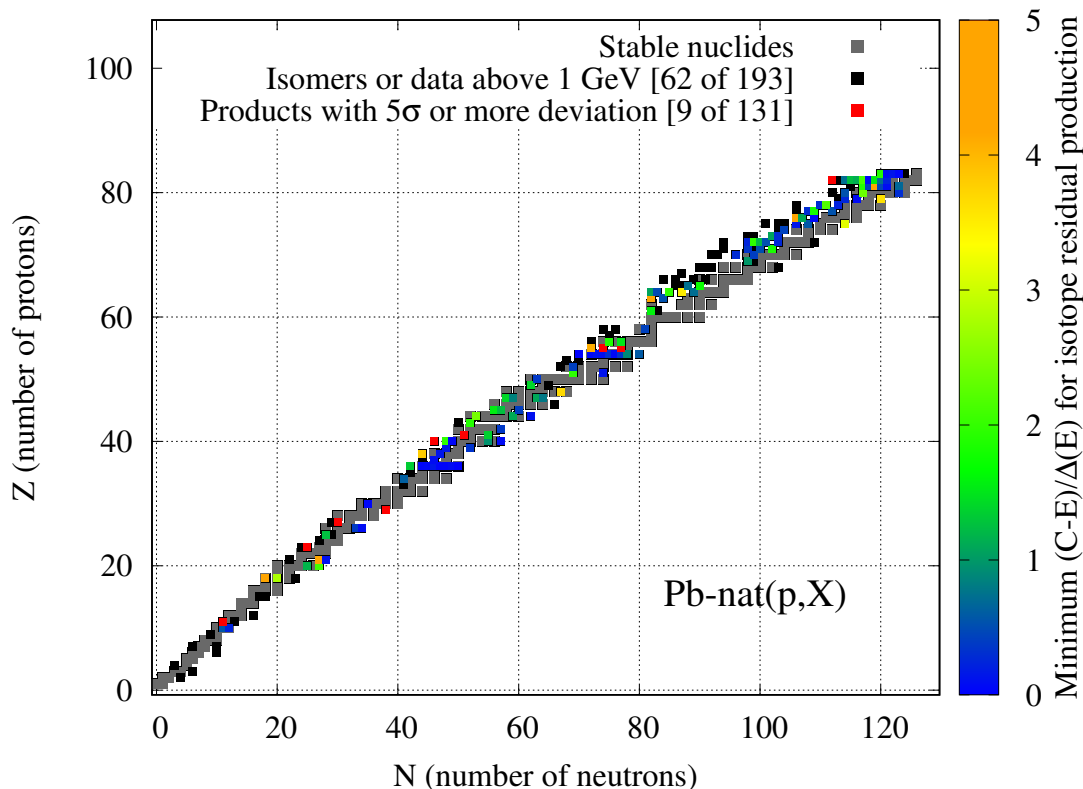


Figure 4. Minimum number of experimental σ deviations between the HEIR-0.2 cumulative residual cross sections and all EXFOR data for proton-induced reactions on ^{nat}Pb over the range of HEIR-0.2 energies. Note that isomeric data and data outside the HEIR-0.2 energy bounds (62 nuclides) are excluded and marked black.

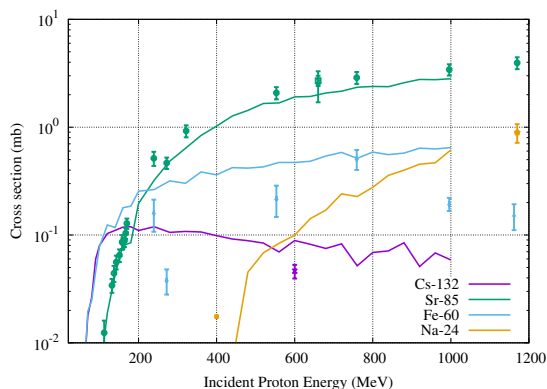


Figure 5. Comparisons of cumulative residual product cross sections of proton on ^{nat}Pb between 30 MeV and 1 GeV between EXFOR (points) and HEIR-0.2 (curves) for four product isotopes: ^{132}Cs , ^{85}Sr , ^{60}Fe and ^{24}Na .

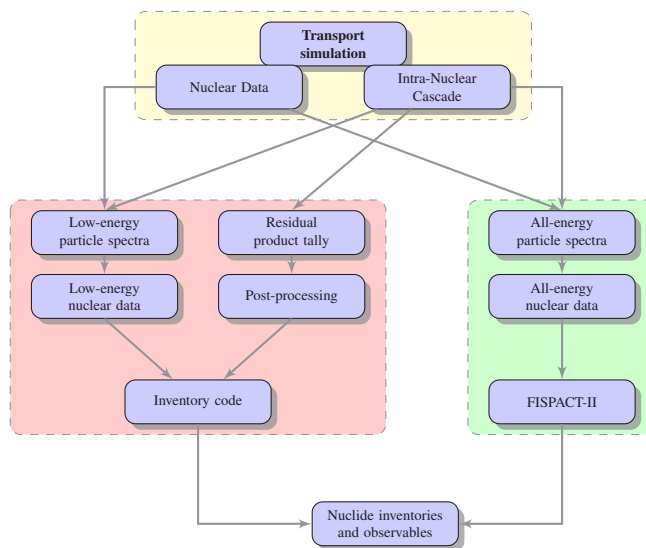


Figure 6. Schematic for activation-transmutation inventory calculations, using a Monte-Carlo transport simulation (yellow), coupled with either (red) separate nuclear data and residual history data or (green) pure nuclear data library calculations.

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