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Translated ENDF formatted data at LLNL

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Translated ENDF formatted data at LLNL

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Abstract

The LLNL Computational Nuclear Physics (CNP) Group announces the release of translated ENDF/B-VI, ENDF/B-VII, JEFF-3.1, JENDL-3.3 and other neutron incident evaluated reaction data libraries to LLNL users.

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Database Name	Projectiles	Reference	Part of this release?
BROND-2.2	n	[1]	N
CENDL-2.1	n	[2]	Y
CENDL-3 Fission Product Library	n	[3],[4]	Y
ENDF/B-V	n	[5]	N
ENDF/B-VI	n	[6]	Y
ENDF/B-VII	$n, p, d, t, {}^3\text{He}, \gamma$	[7]	Y, n only
IAEA Photonuclear Library	γ	[8]	N
JEFF-3.0	n	[9]	Y
JEFF-3.1	n, p	[10]	Y, n only
JENDL-3.2	n	[11]	N
JENDL-3.3	n, α, γ	[12]	Y, n only
Maslov Actinide Library	n	[13]	Y

Table 1: Libraries used in testing and contained in this release. Although this release focused on neutron reaction data, other libraries were translated as part of code testing.

1 Introduction

The LLNL Computational Nuclear Physics (CNP) Group is pleased to announce the first release of translated ENDF/B-VI, ENDF/B-VII, JEFF-3.1, JENDL-3.3 and other neutron incident evaluated reaction data libraries to LLNL users. The complete list is given in Table 1. This represents a multi-year effort to extend LLNL’s “From ENDF To ENDL” (a.k.a. **fete**) to handle ENDF charged particle, photonuclear data and the newest additions to the ENDF format. In the process, many evaluation “bugs” were identified and corrected. The translated data are available on LLNL’s LC systems in ascii format at `/usr/gapps/data/nuclear/translated` on LLNL’s LC systems and on the CNP web page <http://nuclear.llnl.gov> and in processed forms on LLNL’s LC systems at `/usr/gapps/data/nuclear/processed`.

There are significant differences between the ENDF and ENDL formats, both in terms of complexity and scope of the formats. All ENDL data is presented in point-wise linearly interpolated tables. On the other hand, ENDF data are presented in a variety of manners, depending on the reaction and quantity in question. The two formats also differ in the arrangement of the data in the databases. Data in the ENDF format are divided into materials (abbreviated MAT), which are further divided into “Material Files” (abbreviated MF). An MF is one type of reaction data (e.g. MF=3 is tabular cross section data). These MF’s are subdivided into “Material Tapes” (abbreviated MT) which contain the data for individual reactions. Thus, MT=16 MF=3 contains $(n, 2n)$ reaction cross section data while MT=18 MF=3 contains the total (n, f) reaction cross section. By contrast, ENDL requires that reactions and nuclei be sorted into nesting directories first according to projectile (e.g. **yi01** means incident neutron), then nuclide (e.g. **za001002** means $Z=1$ and $A=2$ so we have deuterium), then reaction. The data for each reaction has several numbers associated with it, namely **yo** to denote the outgoing particles, **C** to denote reaction type and **I** to denote reaction property.

As a result of these differences between ENDF and ENDL formats, translating ENDF formatted ASCII data into ENDL formatted ASCII data and then into processed **mcf** and **ndf** files suitable for use in LLNL applications is a complicated multi-step process. The entire process can be summarized as: acquire a database, reorganize the database, preprocess the database, translate the database, check results, compute energy depositions, and process it to binary files.

In the following subsections, we will explore each step. We assume some familiarity with unix or related systems. In addition, we will discuss the codes used in this process, their use and their requirements. Because the ENDL and ENDF library format requirements differ in some rather dramatic ways, we will discuss these differences as well as the imperfections (and bugs!) in the libraries.

2 Producing the ENDL libraries

This section details how we prepared the libraries for the LLNL community. The section is divided into subsections describing each step in the process of acquiring and processing the libraries:

1. Acquire a database
2. Reorganize the database
3. Preprocess the database
4. Translate the database
5. Check results
6. Compute energy depositions
7. Process it to binary files

2.1 Acquiring data libraries

The ENDF formatted data is available in several places, both locally at LLNL and on the internet. There are several modern databases that use the ENDF format: ENDF/B-VI [6], JENDL-3.3 [12], JEFF-3.0 [9], BROND-2.2 [1], and CENDL-2.1 [2]. ENDF/B-VI, JENDL-3.3, and JEFF-3.0 are the most up to date and are the main targets of our translation effort. All three of these databases are available on the web, both in raw and point-wise (i.e. preprocessed) form. Since the preprocessing stage can take quite a bit of time (several hours to a day or more, depending on your hardware), we recommend downloading the preprocessed data. ENDL requires that the data be Doppler broadened to 300 degrees Kelvin, so care must be taken to download the correct database. The raw ENDF formatted data is posted on the LC computer clusters at LLNL in `/usr/gapps/data/nuclear/untranslatedENDF/`.

Our database Subversion projects all share a common organization:

```
ENDFLib/  
  originals/  
    (original files, organized like we found them)  
  conversionScript.py  
  yi01/  
    za001001/  
    .  
    .  
    .  
  yi02/  
    .  
    .  
    .
```

In these projects, the original files are kept in the `originals/` directory and these originals are unpacked and rearranged into the `yi0x/` subdirectories as described in the next section.

2.2 Database preparation

The ENDF format specification makes no requirement as to how the data is arranged in the library, so each nuclear data library is shipped in a different form. In the case of the ENDF format, the data may be lumped into one “tape,” hence the need for “splitting” the database with some code. The ENDL standard directory layout [27] is as follows:

```

my_db/yi01/za001001/endl.orig
      /za001002/endl.orig
      .
      .
      .

```

Here, the `endl.orig` file is the raw, unprocessed evaluation for one nuclide.

Once this is done, we preprocess each `orig` file to produce a `prepro` file. The `prepro` file differs from the original file in that:

- All resonances are expanded into a linear-linear interpolable form
- All data sections in the cross section files are merged into one section
- All cross sections are heated to 300 K (this requirement may be changed in the future)

This is mainly an automated process using the `prepro2004.py` script which controls Red Cullen’s `linear`, `recent` and `sigma1` codes [14]. This step is detailed in Appendix A. After this step, the database will appear as:

```

my_db/yi01/za001001/endl.orig
      "      /endl.prepro
      /za001002/endl.orig
      "      /endl.prepro
      .
      .
      .

```

2.3 Translating a database

We translate the data with `fete` [15]. Since `fete` operates on one isotope at a time, we use the `procdb.py` script to automate translation of an entire database. Once the data is translated (and repaired, if needed) we compute the energy depositions using the new C++ version of `endep`: `endepC++` [16].

Both `fete` and `endepC++` (as well as the checking and repair codes discussed later) rely on the masses and other parameters in the `bdf1s` file. In particular, the `bdf1s` file contains group boundaries, fluxes, nuclear masses, half-lives, various physical and conversion constants, and atomic excitation levels. A copy of the `bdf1s` file is included in the `src/` directory of the `fete` package, however it is not kept up to date. The most up-to-date version of this file contains the 2003 mass evaluations from Audi, *et al.* [17]. This file can be found in `/usr/gapps/data/nuclear/bdf1s.Audi_etal.2003.12.22` on LLNL’s LC computer systems. This is the version of the `bdf1s` file used to generate the libraries discussed in this note.

2.4 Repairing the translated data

After the ENDF formatted data are translated into ENDL format, there are still many that fixes must be made. First, since the inception of the ENDF format, the mass tables used for the nuclei have changed several times. This means that there is a mismatch between actual and evaluated Q values and thresholds for most reactions in most nuclei. Secondly, the ENDF format and ENDL format have different completeness requirements (see Section 3). These means that we must patch evaluations to ensure that they meet the completeness requirements of ENDL and delete extra parts of the evaluations that are irrelevant in ENDL and may even confuse application codes. Thirdly, we must resolve some legacy formatting problems, such as breakup data in ENDF. Finally, even though the ENDF evaluations are often very high quality, there are occasional mistakes that must be repaired.

We performed the repairs on the translated data using the `fixENDF.py` script [18]. This is a `fudge` [19] script that fixes a variety of issues:

- Sets Q values according to the new mass tables compiled by Audi, *et al.* [17]. Shifts reaction thresholds so that they are consistent with the new Q values. This is detailed in appendix B.
- Fills in missing data when possible. For discrete excitations, it creates isotropic angular distributions (I=1 files) for the outgoing particle. For outgoing gammas from neutron capture, it uses `nxgam.py` [20] to generate I=9 and I=4 gamma distributions. For other reactions, it attempts to substitute either angular (I=1) and energy-angle (I=3) distribution files or Legendre-expanded energy-angle (I=4) distribution file from other evaluated data libraries.
- Removes (yi,Xyo) files if the outgoing particle data is incomplete.
- Performs a variety of “special fixes” for specific isotopes in specific libraries. The complete list is given in Table 2 and summarized here:
 - Converts special break-up data (stored as S=9 data) into I=0,1, and 3 data. See Appendix C for details on this process.
 - Splits degenerate levels
 - Removes activation only evaluations
 - Repairs non-trivial C number misassignments
 - Averages outgoing distributions if multiple distributions are given for specific outgoing particle
- Records what happens to an evaluation in the `documentation.txt` file (this is done also by `fete` and `endepC++`)

Table 2: List of special fixes applied to various databases.

Database	Projectile	Isotope	Nature of fix
BROND-2.2	n	za002003	Changed C numbers: $(n, 2n)2p$ data misfiled. It should really be $(n, 2np)p$ data.
		za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za008016	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za064000	Increased endl data field precision to account for finely binned data.
		za073181	Increased endl data field precision to account for finely binned data.
CENDL-2.1	n	za002003	Changed C numbers: $(n, 2n)2p$ data misfiled. It should really be $(n, 2np)p$ data.
		za002003	Removed extra outgoing particle distributions for C=29 with X4=1. They are copies of the regular outgoing distributions.
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za009019	Averaged outgoing neutron I=4 files for C = 12.
		za040000	Increased ENDL data field precision to account for finely binned data.
ENDF/B-VI	n	za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za005010	Refiled the C=40, S=9 data. It has incorrectly assigned LR flags in the ENDF data.
		za005010	Process breakup data (ENDF LR>0 data or ENDL S=9 data).
		za006000	Changed C numbers: $(n,n3a)$ data misfiled. It should really be $(n,n2a)a$ data.
		za006000	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za007014	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za009019	Averaged outgoing neutron I=4 files for C = 12.

Table 2: List of special fixes applied to various databases.

		za012024	Deleted, it is for activation only.
		za019041	Deleted, it is for activation only.
		za022046	Deleted, it is for activation only.
		za022047	Deleted, it is for activation only.
		za022048	Deleted, it is for activation only.
		za022050	Deleted, it is for activation only.
		za028059	Deleted, it is for activation only.
		za037085	Removed all files with $C = 26$. Evaluation uses special break-up flag (LR=1) which is not translated correctly.
		za037085	Removed all files with $C = 54$. Evaluation uses special break-up flag (LR=1) which is not translated correctly.
		za040000	Increased endl data field precision to account for finely binned data.
		za040095	Split degenerate level energies.
		za095242m	Split degenerate level energies.
ENDF/B-VII	n	za001001	Fixed missing residual data for $C=46$.
		za001002	Fixed missing residual data for $C=46$.
		za003006	Fixed missing residual data for $C=42$.
		za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za005010	Refiled the $C=40$, $S=9$ data.
			It has incorrectly assigned LR flags in the ENDF data.
		za005010	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za006000	Changed C numbers: $(n, n3a)$ data misfiled.
			It should really be $(n, n2a)a$ data.
		za006000	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za007014	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za009019	Averaged outgoing neutron I=4 files for $C = 12$.
		za060144	Increased ENDL data field precision to account for finely binned data.
		za095242m	Split degenerate level energies.
		za095242m1	Split degenerate level energies.
JEFF-3.0	n	za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za005010	Refiled the $C=40$, $S=9$ data.
			It has incorrectly assigned LR flags in the ENDF data.
		za005010	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za007014	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za008016	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za009019	Averaged outgoing neutron I=4 files for $C = 12$
		za063151	Removed all files with $C = 55$
JEFF-3.1	n	za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za005010	Refiled the $C=40$, $S=9$ data.
			It has incorrectly assigned LR flags in the ENDF data.
		za005010	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za006000	Changed C numbers: $(n, n3a)$ data misfiled.
			It should really be $(n, n2a)a$ data.
		za006000	Refiled the $C=40$, $S=9$ data. It has incorrectly assigned LR flags in the ENDF data.
		za006000	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).

Table 2: List of special fixes applied to various databases.

		za007014	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za009019	Averaged outgoing neutron I=4 files for C = 12.
		za021045	Split degenerate level energies.
		za063151	Removed all files with C = 55.
JENDL-3.3	<i>n</i>	za002003	Increased max. outgoing γ energy because of rather high energy line.
		za003006	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za003007	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za006000	Processed breakup data (ENDF LR>0 data or ENDL S=9 data).
		za006000	Changed C numbers: (<i>n, n3a</i>) data misfiled. It should really be (<i>n, n2a</i>) <i>a</i> data.
		za040095	Split degenerate level energies.

2.5 Checking the translated data

After the data is translated and repaired, we perform some simple validation checks using the `check.py` script [21]. This script ensures that the data satisfies ENDL format and completeness requirements as well as performs some basic physics checks. In particular, it does:

- Checks that stated Q matches Q value computed from C number and projectile, target and product masses.
- Ensures that all probability distributions are properly normalized.
- Checks to see that the data is complete, as per ENDL requirements.
- Checks that data with thresholds have thresholds that match what can be computed from the Q value.
- Checks that all points are in order and that there are no double values.
- Ensures that all cross sections, multiplicities and probability densities are positive.
- Checks that all data headers match over an isotope.
- Parses the errors reported by `fete` and `endepC++` so that they may be correlated with other problems in the data.

After this basic testing, the data undergoes more rigorous testing in simulations of critical assemblies as described by Pruet *et al* [22]. We present a limited set of these tests in Table 4. The full results of this testing will be reported elsewhere.

2.6 Final processing

Before the translated data may be used in applications, they must be processed into a format suitable for either LLNL's Monte-Carlo or deterministic codes. In either case, we start this final processing by computing the energy depositions with the `endepC++` code. After this, we use either `mcfgen` [24] for the Monte-Carlo

Database	Projectile	Isotope	Nature of Issue
BROND-2.2	n	za003006	LAW 3 option is not implemented for MF 6 data in fete .
		za003007	Special break-up data using non-standard form of pseudo-level representation.
		za008016	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
		za017000	Anisotropic γ angular distributions for de-excitation cascades in MF=12 not implemented in fete .
		za030000	Uses LO = 3 for MF = 12 data. Evaluation documentation states this is BROND only feature.
		za041093	($n, 2n$) to an isomer (MT = 26) does not have an ENDL equivalent and is deprecated in ENDF/B-VI.
		za050000	Kalbach representation used for outgoing particle distributions for reactions on a natural target. Kalbach representation requires a well defined Z and A and there is no well defined A for a natural target.
CENDL-2.1	n	za095235	Interpolation type 4 for 1d tabular data is not implemented in fete .
		za024000	Kalbach representation used for outgoing particle distributions for reactions on a natural target. Kalbach representation requires a well defined Z and A and there is no well defined A for a natural target.
		za026000	Same problem as za024000.
		za029000	Same problem as za024000.
ENDF.B-VI	n	za005010	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
		za037085	Cannot determine C number when LR=1 in MF=3; we must process MF=6 file to determine outgoing particles.
ENDF.B-VII	n	za005010	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
JEFF-3.0	n	za004009	Non-standard MT assignments used in the ENDF file. The documentation is not detailed enough to allow us to unscramble the MT's.
		za005010	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
		za008016	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
JEFF-3.1	n	za004009	Non-standard MT assignments used in the ENDF file. The documentation is not detailed enough to allow us to unscramble the MT's.
		za005010	Cannot process special breakup reactions with LR=40 ($e\bar{e}$ pair formation) in cross section file.
		za022046	The outgoing gamma spectrum from the decay out of the continuum for (n, γ) reactions has all of the outgoing energies set to 0 MeV. This bug means that energy cannot be conserved for this reaction.
		za022047	Same problem as za022046.
		za022048	Same problem as za022046.
		za022049	Same problem as za022046.
		za022050	Same problem as za022046.
JENDL-23.3	n	za023000	Kalbach representation used for outgoing particle distributions for reactions on a natural target. Kalbach representation requires a well defined Z and A and there is no well defined A for a natural target.

Table 3: List of evaluations with unfixed or unfixable problems.

Assembly Name	Experimental k_{eff}	Ref. [23] C/E Ratio	Our C/E Ratio
Jezebel	1.000 ± 0.002	0.9969	0.9971
Godiva	1.000 ± 0.001	1.0033	1.0043
Flattop-25 ¹	1.000 ± 0.003	0.998	0.999
Jezebel-233 ²	1.000 ± 0.001	1.0041	1.0052

Table 4: The measured k_{eff} values for several critical assemblies compared to benchmark calculations performed by Okumura *et al.* (Ref. [23]) using the original JENDL-3.3 library and the MVP transport code and performed by us using our translation of the JENDL-3.3 library data and the AMTRAN transport code.

data or `ndfgen` [25] for the deterministic data. In this first release of the data, only room temperature data is being released.

The Monte-Carlo data are stored in the appropriate `mcf` file, eventually containing temperature broadened cross-sections on a temperature grid including room temperature and 11 logarithmically spaced temperatures from 0.1 eV to 10 keV. The elastic neutron E' - μ distributions are not broadened because they are computed on the fly within the Monte-Carlo access routine `mcapm`. Both continuous energy and 175 Group (`gid=6`) data are stored.

The deterministic data (or S_n) are stored in a series of `ndf` files. Each file corresponds to one temperature. In this first release, there will only be the room temperature file. Eventually, we will release temperature broadened cross-sections on a temperature grid including 0.02 eV and 0.031 eV (straddling room temperature) and 15 logarithmically spaced temperatures from 0.1 eV to 100 keV. Only the neutron elastic E' - μ distributions will be broadened. The data is stored in 230 energy groups (`gid=7`) along with their group weights.

3 Data library requirements

Unfortunately, because ENDF and ENDL formats serve slightly different purposes, they require different levels of completeness of the data in the libraries. The most widely used ENDL formatted library, ENDL99, is used to support simulations in a variety of LLNL programs [26]. Because it serves several programs, ENDL99, users can track of neutrons, gammas, and all charged particles in their transport simulations. Therefore, the ENDL format requires that there be enough data present in the database to support tracking of all interesting particles [27]. The ENDF libraries primarily support simulations for the nuclear reactor community. Thus, ENDF formatted libraries are guaranteed to support neutron tracking [28]. In the latest release of ENDF/B-VII[7], there have been vast improvements in the support for both gamma and charged particle tracking. Both the various ENDF libraries and the ENDL library have activation sublibraries (e.g. ENDF/A, JEFF-3.1A for ENDF and radchem for ENDL).

A library suitable for activation studies has very simple requirements. Namely, we need the cross section, $\sigma_i(E)$, as a function of incident energy for all reactions i in which target's Z or A changes.

A library suitable for transport simulations requires significantly more information:

- $\sigma_{\text{tot}}(E)$, the total cross section, so that we can determine if a reaction occurs.
- $\sigma_{\text{elas}}(E)$, the elastic cross section, so that we can scatter off a target nucleus.
- $\sigma_i(E)$ for all reactions i in which the target's excitation, Z or A changes
- $P(E|\mu)$, the outgoing particle angle cosine probability density, for a two-body reaction in which we can determine the energy E' of the outgoing particle from kinematics, for all outgoing particles, that we are tracking. This is given in the ENDL I=1 file or the ENDF MF=4 file.
- $P(E|\mu, E')$ for all other reactions, for all outgoing particles, that we are tracking.
 - In ENDL, all tracked particles need either
 - * $P(E|\mu, E') = P_{I=1}(E|\mu) \times P_{I=3}(E, \mu|E')$, Product of angular distribution and joint energy-angle distribution.

- * $P(E|\mu, E') = P_{I=4}(E|\mu, E')$, Joint energy-angle distribution (expanded in Legendre polynomials).
- In ENDF,
 - * For n 's: either
 - $P(E|\mu, E') = P_{MF=4}(E|\mu) \times P_{MF=5}(E|E')$, Product of angular distribution and joint energy-angle distribution.
 - $P(E|\mu, E') = P_{MF=6}(E|\mu, E')$, Joint energy-angle distribution.
 - * For $p, d, t, {}^3\text{He}$, and α 's: $P(E|\mu, E') = P_{MF=6}(E|\mu, E')$, Joint energy-angle distribution.
 - * For γ 's: either
 - $P(E|\mu, E') = P_{MF=14}(E|\mu) \times P_{MF=15}(E|E')$, Product of angular distribution and joint energy-angle distribution.
 - $P(E|\mu, E') = P_{MF=6}(E|\mu, E')$, Joint energy-angle distribution.
- Multiplicity, $M(E)$, for all reactions in which the number of outgoing particles of a particular type is not constant or not known from the reaction itself (i.e. the reaction is inclusive on this particular particle). In ENDL, the γ multiplicity is stored in the I=9 files while the fission $\bar{\nu}$ is stored in the I=7 files. In ENDF, the γ multiplicity is stored in the MF=12 file or as a production cross-section in MF=13 while the fission $\bar{\nu}$ is stored in the MF=1, MT=452, 455 and 456 files.
- The Q value and intermediate level excitation, if any, for all reactions. From these, and the outgoing particle data, we can compute the energy deposited locally to the reaction products. In ENDL, these are stored in the file headers of every file corresponding to a specific reaction. In ENDF, these are stored in the beginning of the MF=3 file.

Both ENDL and ENDF formats have a series of other requirements. ENDL requires:

- No levels in lists of discrete excitations be degenerate.
- All outgoing particles with only angular distributions have distributions in the center of mass frame, otherwise the angular and energy-angle distributions must be given in the lab frame.
- All cross sections must be “heated” to room temperature. Sometimes this is 300 K, other times it is 296 K.
- There can be no discontinuities. This means jumps and delta functions must be widened in the translation.

ENDF requires:

- Resonance parameters for incident neutrons with $E < 100$ keV.
- All cross sections must not be “heated,” so that we don’t wash out the resonances.

4 Concluding Remarks

Currently, charged particle incident data are available in several libraries. However, not all neutron evaluations have complete charged particle data so it is not clear whether the entire charged particle and neutron induced reaction network can be modeled with any library other than ENDL99. To combat this problem, we must first assess the completeness of libraries containing charged particle incident data and then devise a strategy for “completing” the data evaluations. This strategy may comprise adopting the missing parts from ENDL99 or from simulations using the EMPIRE or TALYS nuclear reaction modeling codes.

In this release, all data are truncated above incident energies of 20 MeV. This cut-off is sufficient for current LLNL needs. Future homeland security and other applications may require the higher energy particle production data contained in many ENDF evaluations. Currently **fete** does not support translation of all

of the particle production data. Furthermore, the ENDL format does not support more exotic produced particles such as pions, etc. The proposed XENDL nuclear data format should address this short-coming.

Setting aside these short-comings, there are still several issues that remain unresolved or partially resolved in this work. First, there is some confusion in the ENDF format specification for how to treat the Q value if the residual of a reaction is an isomer. This should be resolved in the Nov. 2006 CSEWG meeting at Brookhaven National Lab., but that will not be in time for this data release. Second, ENDF occasionally uses the “Method of corresponding points” for interpolating over multi-dimensional tables. This scheme is not explained clearly in the ENDF manual, so it is not implemented correctly either in `fete` nor in NJOY [30]. Finally, the databases themselves often have out-of-date or even wrong data. Fortunately, the data are updated regularly and problems are corrected. In addition, there are several sources for “bug lists”:

- “Known Errors and Deficiencies in ENDF/B-VI” page at <http://www.nndc.bnl.gov/csewg/errors.html>.
- “NJOY 99 Issue Tracker,” page at <http://t2.lanl.gov/codes/njoy99/Issues.html>.
- D.A. Brown and G. Hedstrom, “Possible problems in ENDF/B-VI.r8,” LLNL Report UCRL-CONF-200686 (2003).
- “Known deficiencies in ENDF/B-VIIb2,” page at <http://www.nndc.bnl.gov/exfor2/4web/problems.html>.
- “JEFF-3.0 Feedback,” page at <http://www.nea.fr/html/dbdata/jeff3feedback/welcome.html>.
- “JEFF-3.1 Feedback,” page at <http://www.nea.fr/html/dbdata/jeff3feedback/feedback-31.html>.
- “Defects of JENDL-3.3,” page at <http://wwwndc.tokai-sc.jaea.go.jp/jendl/j33/j33prob.html>.
- CEA’s nuclear data listserver archive at <http://www.nea.fr/listsmh/>.

Whatever your problem is with an evaluation, always be sure to check the `documentation.txt` file provided in each ENDL `za` directory. This file contains all of the errors and warnings produced in the translation by `fete` and calculation of the energy depositions by `endepC++`, all of the changes performed by `fixENDF.py`, and a copy of the original ENDF documentation.

Future work is possible per customer request:

- Fix BROND-2.2
- Work around “unfixable” problems
- Translate charged-particle and γ incident data: JENDL-3.3, JEFF-3.1, ENDF/B-VII, IAEA Photonuclear database
- Translate other (legacy) libraries: JENDL-3.2, ENDF/B-V
- Implement the special features used in activation libraries in `fete`
- Translate High energy (incident energy from 20-200 MeV) libraries
- Create Elemental evaluations
- Translate Future libraries: CENDL-3, BROND-3
- Create TART formatted libraries

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A Preprocessing ENDF Data

There are several steps to convert the ENDF/B-VI database into a form suitable for translation: 1. split the database into individual nuclei, 2. preprocess the database to get it into a pointwise form and 3. Doppler broaden the data to 300 degrees Kelvin.

We have developed a Python script, `prepro2004.py`, to automate the preprocessing of ENDF formatted files. The script requires one argument - the directory containing the split ENDF data:

```
prepro2004.py <za>
```

The script launches three codes sequentially for each evaluation file - `linear`, `recent` and `sigma1`. There are three input files used by these codes called `LINEAR.INP`, `RECENT.INP` and `SIGMA1.INP`. The explicit directions and descriptions for these codes are in the `DOCUMENT/` directory. The default input files have been set to linearize the data to a tolerance of 0.1%, expand resonance data to 0.1% tolerance and heat to 300 degrees Kelvin with a final tolerance of 0.5%. The heating is applied only to the cross sections, not to the angular distributions or energy distributions. The final preprocessed output file for each isotope is named `endf.prepro` and these files are read by `fete`.

There are several common features to the preprocessing codes. These programs only use the ENDF format, but can handle data in any version of the ENDF format. They assume that the data is correctly coded in the ENDF format and perform no error checking. In particular they assume that the redundant information on each line is correct. Sequence numbers are ignored on input, but will be correctly output on all lines. The format of section MF=1, MT=451 and all sections of MF=3 must be correct. The program copies all other sections of data as plain text and is insensitive to their correctness. In the current versions of these codes, all MF=3 energies will be output in 'f' (instead of 'e') FORTRAN format in order to allow energies to be written with up to 9 digits of accuracy. In previous versions this was an output option. However use of this option to compare the results of energies written in the normal ENDF convention of 6 digits to the 9 digit output from this program demonstrated that failure to use the 9 digit output can lead to large errors in the data just due to translation of the energies to the ENDF format.

A.1 Preprocessing code – linear

The purpose of this program is to convert ENDF MF= 3, 23 and 27 data to linear-linear interpolable form. Any section that is already linear-linear interpolable will be thinned. Entire evaluations are output, not just the linearized data cross sections, e.g. angular and energy distributions are also passed to the output file. The default input parameter file, `LINEAR.INP`, sets the output tolerance of 0.1% for the entire incident neutron energy range.

A.2 Preprocessing code – recent

The purpose of this this program is to reconstruct the resonance contribution to the cross section in linearly interpolable form, add in any linearly interpolable background cross section and output the result in the ENDF format. The cross sections outputted by this program are linearly interpolable over the entire energy range.

The resonance contribution is calculated for total (MT=1), elastic (MT=2), capture (MT=102) and fission (MT=18), added to the background (if any) and output. In addition, if there is a first-chance fission (MT=19) background present the resonance contribution of fission will be added to the background and output. If there is no first chance fission background present the program will not output MT=19.

The formats and conventions for reading and interpreting the data varies from one version of ENDF to the next. However, if the section (MF=1, MT=451) describing the data is present, it is possible for this program to distinguish between data in the IV, V and VI versions of the ENDF format and to use the appropriate conventions for each ENDF version (see, subroutine `file1` for a description of how this is done). If the data description section is not present, the program assumes the data are in the VI version of the format. Users are encouraged to insure that the data description section (MF=1, MT=451) is present in all evaluations.

All energies are read in double precision (by special FORTRAN I/O routines) and are treated in double precision in all calculations. Entire evaluations are output, not just the reconstructed MF=3 cross sections, e.g. angular and energy distributions are also included. The default input parameter file is called `RECENT.INP` and sets the output tolerance to 0.1% for the entire incident neutron energy range.

A.3 Preprocessing code – `sigma1`

The purpose of this program is to Doppler broaden neutron-induced cross sections. Each energy range of the cross section (MF=3) data is read from the ENDF file. The data is Doppler broadened, thinned and output in ENDF format. All cross sections that are used by this program must be tabulated and linearly interpolable in energy and cross section. In the unresolved resonance region it is not possible to exactly define the energy dependence of the cross sections. The average widths and spacings given in ENDF are only adequate to define average values of the cross sections. Therefore, all cross sections in the ENDF format for the unresolved region are really average values which cannot be Doppler broadened using the `sigma1` method (which requires tabulated, linearly interpolable, energy dependent cross sections). Therefore,

- All tabulated points within the unresolved resonance region are copied, without modification or broadening. Adoption of this convention allows subsequent programs to properly define self-shielded, Doppler broadened cross sections in the unresolved resonance region.
- Cross sections are extended as $1/v$ below the upper energy limit of the resolved resonance region and above the lower energy limit of the continuum region (i.e. into the unresolved resonance region).

This convention guarantees a smooth behavior close to the unresolved resonance region boundaries. Entire evaluations are output, not just the broadened MF=3 cross sections, e.g. angular and energy distributions are also included. The default input parameter file, `SIGMA1.INP`, is set up to heat the isotopes to 300 degrees Kelvin and output the cross sections using a 0.5% tolerance.

B Setting Q values and thresholds

Recently, Audi, Wapstra, *et al.* produced a new nuclear mass table evaluation [17]. The new masses are often very close to what is quoted in the original ENDF files that we translated. However, this is not the case in general, especially for the older evaluations based off of very old mass tables. As a result, nearly all evaluations contain threshold reactions where the threshold “is not quite right.” We have developed a simple procedure to fix this data and we describe it in this appendix.

We begin by determining the best-guess value for the Q value. For reactions other than fission, we can compute the Q from the mass tables simply by knowing the masses of all reactants and products. We use the ground state masses here. For fission, we take the Q value stated in the ENDF or ENDL file with which we are working.

Knowing the ground state Q value and the discrete level excitations, if any, we can compute what the reaction threshold should be. For many outgoing charged particle reactions, there is an effective threshold caused to the Coulomb barrier of the residual nucleus. This may cause cross-sections and other data to become significant only at incident energies far above the actual threshold.

Once we know what the threshold should be, we check each data file for a reaction. If the data starts at incident energies above threshold, then we do nothing, even if the starting energy is far above threshold as is the case for outgoing charged particle reactions. If the data starts below threshold, we only adjust the data if it starts below the threshold minus an adjustable tolerance. If we must adjust the data, we compute $\Delta E = \text{new } E_{th} - \text{old } E_{th}$. With ΔE , we begin at the first incident energy in a data set and shift it up in energy by ΔE . If this point moves above another point, then we shift this next point in the same manner. We continue this until we either do not move a point past another or we exhaust the entire dataset. Since ΔE is typically small, we have only ever had to shift the first few points in any one dataset. This procedure is illustrated in Fig. 1.

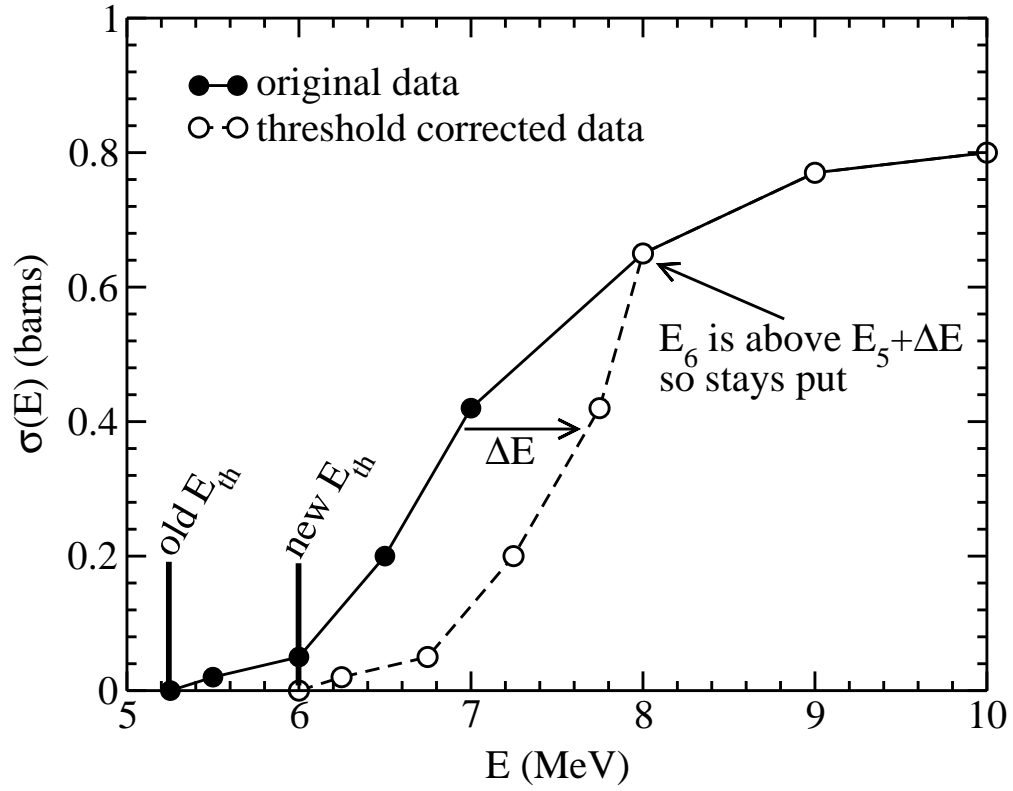


Figure 1: Illustration of our process for shifting thresholds to match the correct Q values. In this plot, points 1 - 3 were all below the new threshold. Because of the size of ΔE , the first 5 points needed to be shifted. Point 6 did not need to be shifted because the new position of point 5 remained below point 6.

C Break-up reactions in legacy ENDF and the LR flag

Outgoing neutrons from reactions on light targets often exhibit strong energy-angle correlations in their outgoing spectrum. These reactions typically lead to several particles in the final state, i.e. they are of the form $n + A \rightarrow n + A' + \text{“stuff”}$. Since ENDF’s focus is on neutron transport, only the outgoing neutron spectrum, $d\sigma(E)/d\mu dE'$, needs to be stored. This is typically handled using MF=6 data in ENDF. However, historically this was not always the case as the MF=6 format was only introduced in the mid-1980’s.

In the mid to late 1970’s, several evaluations were performed at Los Alamos by P.G. Young and others using an innovative scheme for representing this correlated data. Since they could not use MF=6 files, they represented the data by a series of “pseudo-levels” designed to produce outgoing neutrons with an energy-angle distribution that mimics the true distribution. The trick was to treat the reaction as a multiple step break-up reaction where the intermediate state proceeds through the break-up of a residual nucleus in the excited “pseudo-level.” The excitation energy and widths of the “pseudo-levels” are chosen so as to produce the correct E' for the outgoing neutron. These “pseudo-levels” were flags with the LR flag. Additionally, the LR flag notifies the user what other particles are produced in this reaction. This scheme was later adopted in several evaluation by Chiba and others from JAERI (now the Japanese Atomic Energy Agency).

In the next section, we detail how this scheme works in ENDF. Following this, we describe how we translate this data in to ENDL format using `fudge`. Finally, we detail some tests we ran to ascertain the faithfulness of our translation.

C.1 The ENDF data

The “pseudo-level” representation was introduced as a way to represent the the neutron spectrum, $d\sigma(E)/d\mu dE'$, without relying on the MF=6 file. The trick is to view the desired reaction as a two-step process: $n + A \rightarrow n + A^* \rightarrow n + A' + \text{“stuff”}$. One then tunes the excitation level and width of the intermediate state of the target A in order to produce the desired outgoing neutron distribution. We will now describe in detail what is stored in the ENDF files when using the “pseudo-level” representation and how one can use it to construct the neutron spectrum, $d\sigma(E)/d\mu dE'$.

In the “pseudo-level” scheme, data for a particular channel is broken up into several MT’s, each corresponding to a different “pseudo-level” and into MF=3 (cross-section) and MF=4 (outgoing angular distribution, in the center of mass frame) files. These data are flagged with a non-zero LR flag in the header of the cross-section file (MF=3). The LR flag plays two roles. First, it notifies the user of the data that this is a special break-up reaction. Second, its value specifies the identities of the emitted particles comprising the non-neutron “stuff” in the last step of the reaction. When the “pseudo-level” scheme is used, the LR flags are used exclusively in the MT range corresponding to discrete level excitations (MT=51-91 for (n, n') reactions).

The cross-section for populating the i^{th} level, $\sigma_i(E_{lab})$, is given in the appropriate MF=3 file. With the cross-section data, one can compute the probability of populating i^{th} level:

$$P(E_{lab}|i) = \sigma_i(E_{lab})/\sigma(E_{lab}).$$

The probability of emitting neutron (or equivalent) into angle-cosine, μ , from i^{th} pseudo-level as function of incident energy E in cm frame, $P_i(E_{lab}|\mu_{cm})$, is given in the appropriate MF=4 file. From this, we can compute the total probability of a neutron being emitted into a particular μ_{cm} :

$$P(E_{lab}|\mu_{cm}) = \sum_i P(E_{lab}|i)P_i(E|\mu_{cm}).$$

From discrete level, outgoing neutron energy well defined in center of mass frame:

$$E'_{cm} = \left(\left(\frac{m_A}{m_n + m_{A^*}} \right) E_{lab} - QI \right) \left(\frac{m_{A^*}}{m_n + m_{A^*}} \right).$$

Here, $QI = Q + E_i$ the the modified Q value defined in the ENDF documentation [28]. Note, this is independent of μ_{cm} . However, each level has a width ΔE_i so QI varies in range $Q + E_i \pm \Delta E_i$ [31]. Together,

this allows us to compute $P(E_{lab}, |E'_{cm})$:

$$P(E_{lab}, |E'_{cm}) = \sum_i \frac{P(E_{lab}|i)}{\Delta E_i} [\theta(E'_{i-} - E'_{cm}) - \theta(E'_{i+} - E'_{cm})]$$

Here the “ \pm ” signs refer to the extremes that QI can take as we vary E_i over the level width ΔE_i . Using this scheme one makes a histogram in E' by making a series of “pseudo-levels” of finite width.

From these, the neutron spectrum can be computed in the cm frame:

$$\frac{d\sigma(E_{lab})}{d\mu_{cm}dE'_{cm}} \equiv \sigma(E_{lab})P(E|\mu_{cm}, E'_{cm}) = \sigma(E_{lab})P(E_{lab}, |E'_{cm})P(E_{lab}|\mu_{cm})$$

In the cm frame, the outgoing energy and angle are uncorrelated. Note $E_{lab} = \frac{(m_n + m_A)^2}{m_A^2} E_{cm}$. The outgoing neutron spectrum is related to the invariant neutron production spectrum by assuming azimuthal symmetry of the outgoing neutrons:

$$\frac{E' d^3 \sigma(E)}{d^3 p'} = \frac{E' d^2 \sigma(E)}{\pi dp'_z dp_T'^2} = \frac{\sqrt{E'}}{\pi (2m_n)^{3/2}} \frac{d^2 \sigma(E)}{dE' d\mu}.$$

Here p'_z , p'_T and p' are the outgoing particle’s momentum. Thus, if we have the neutron spectrum in one reference frame, we can boost it to any frame.

C.2 Converting ENDF data into ENDL

From these, we effectively have $P(E_{lab}|\mu_{cm})$ and $P(E_{lab}, \mu_{cm}|E'_{cm}) = P(E_{lab}|E'_{cm})$, in the cm frame. Unfortunately, ENDL requires them in the lab frame. Rewriting the outgoing energy and angle cosine is straightforward. Boost velocity that goes from lab to cm is

$$\beta = \sqrt{2m_n E_{cm}} / (E_{cm} m_n / m_A + m_A) \approx \sqrt{2m_n E_{lab}} / (m_n + m_A).$$

So, we find

$$E'_{cm} \approx E'_{lab} + \frac{m_n^2 E_{lab}}{(m_n + m_A)^2} - 2\mu_{lab} \frac{m_n}{m_n + m_A} \sqrt{E_{lab} E'_{lab}}$$

and

$$\mu_{cm} \approx \mu_{lab} \sqrt{\frac{E'_{lab}}{E'_{cm}}} - \frac{E_{lab}}{E'_{cm}} \left(\frac{E'_{lab} + m_A}{m_n + m_A} \right)$$

Boosting the probability distributions takes a little more work since, independently, they are not Lorentz invariant. Working from the invariant neutron spectrum above, we find the Jacobian of the transformation. This relates the outgoing probabilities in both frames via:

$$P(E_{lab}|\mu_{lab}, E'_{lab}) = \sqrt{\frac{E'_{cm}}{E'_{lab}}} P(E|\mu_{cm}, E'_{cm}).$$

Using our results for the outgoing probability density in the cm frame, we find,

$$P(E_{lab}|\mu_{lab}) = \int dE'_{lab} \sqrt{\frac{E'_{cm}}{E'_{lab}}} P(E_{lab}|\mu_{cm}) P(E_{lab}, \mu_{cm}|E'_{cm})$$

and

$$P(E_{lab}, \mu_{lab}|E'_{lab}) = \sqrt{\frac{E'_{cm}}{E'_{lab}}} P(E_{lab}|\mu_{cm}) P(E_{lab}, \mu_{cm}|E'_{cm}) / P(E_{lab}|\mu_{lab})$$

We have coded these results as a special post-translation fix in the translation effort.

C.3 Validation

We have attempted to validate our reconstruction of the data. However, our efforts were only partially successful. Most evaluations using this “pseudo-level” representation were performed using R-matrix fits to all available data. Unfortunately, there is not a lot of double differential (that is $E' - \mu$) data available. Furthermore, it is not entirely clear if our interpretation of the Q value of the “pseudo-levels” is correct given the sparse evaluation documentation. Given this, we chose to validate the ${}^6\text{Li}(n, nd)\alpha$ evaluation in ENDF/B-VII, where there is both double differential data and plots from an older ENDF evaluation with which to compare our evaluation. In both cases, the comparisons are fair, but agreement not spectacular and are shown in Figs. 2–4. It is possible that the evaluation has changed dramatically between ENDF/B-VII and the Stewart-Young evaluation which we compare against in Figs. 2 and 4.

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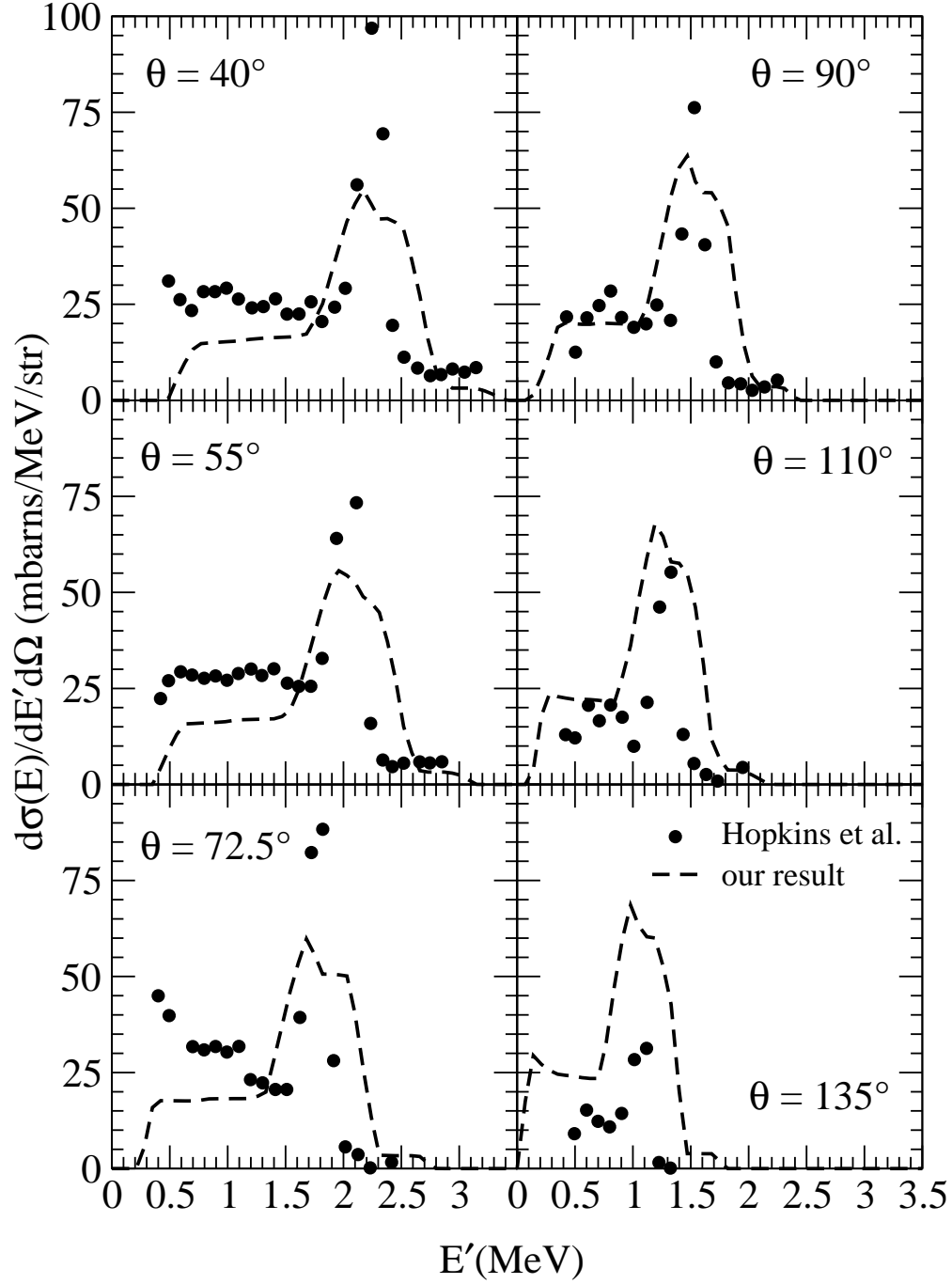


Figure 2: Plot of the ${}^6\text{Li}(n, nd)$ cross section at 4.83 MeV reconstructed from the ENDF/B-VII za003006 evaluation [32] (which uses the “pseudo-level” scheme) compared to the data of Hopkins *et al* [33], upon which the ENDF/B-VII evaluation is based. Agreement is pretty good: we match the location of all of the peaks in the data and nearly match the overall size and shape of the data.

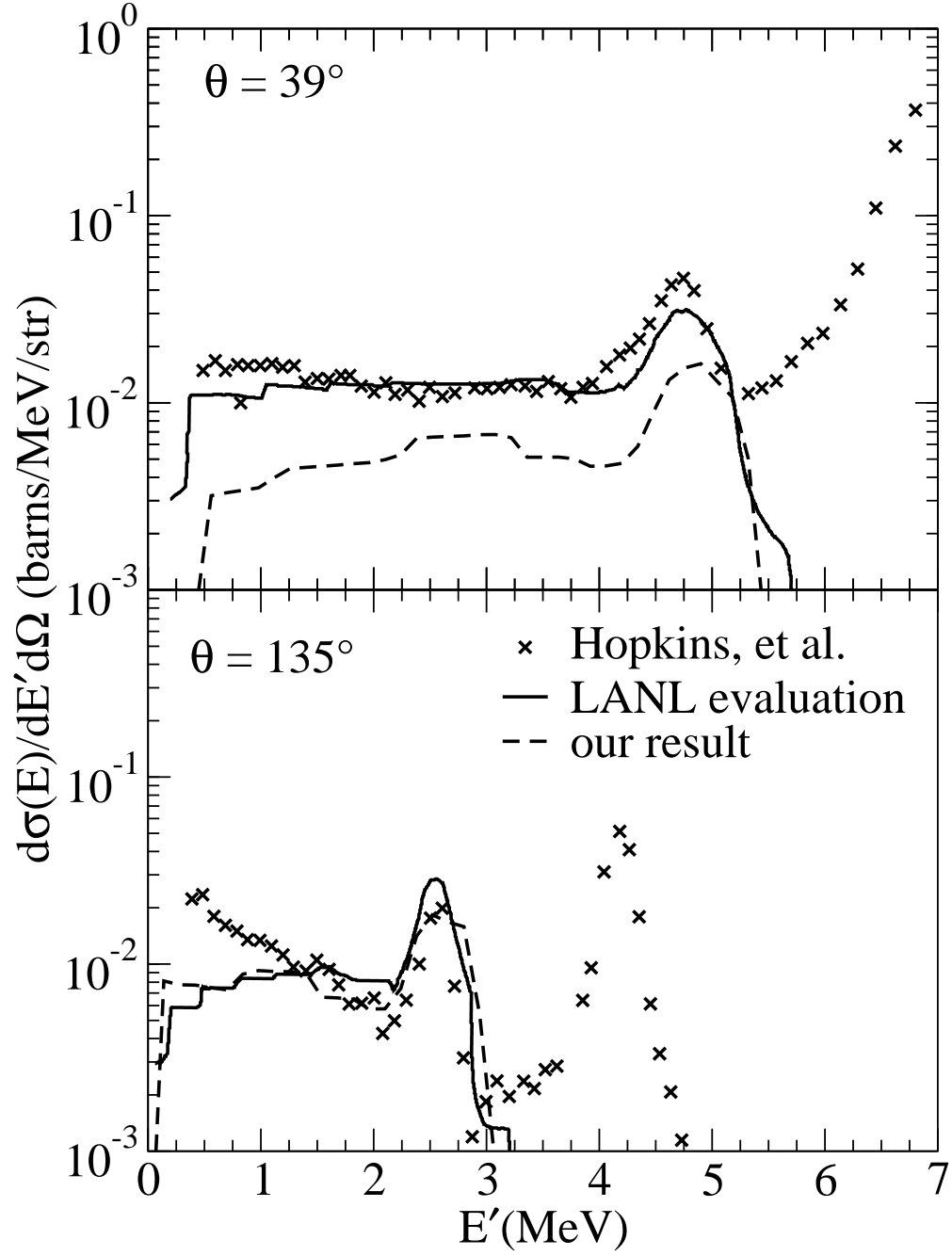


Figure 3: Plot of the ${}^6\text{Li}(n, nd)$ cross section at 7.5 MeV reconstructed from the ENDF/B-VII za003006 evaluation [32] (which uses the pseudo-level scheme) compared to the original evaluation by Stewart and Young [34]. Here, agreement is only fair: while we match the shape of the Stewart-Young evaluation, we only match the magnitude of it at forward angles.

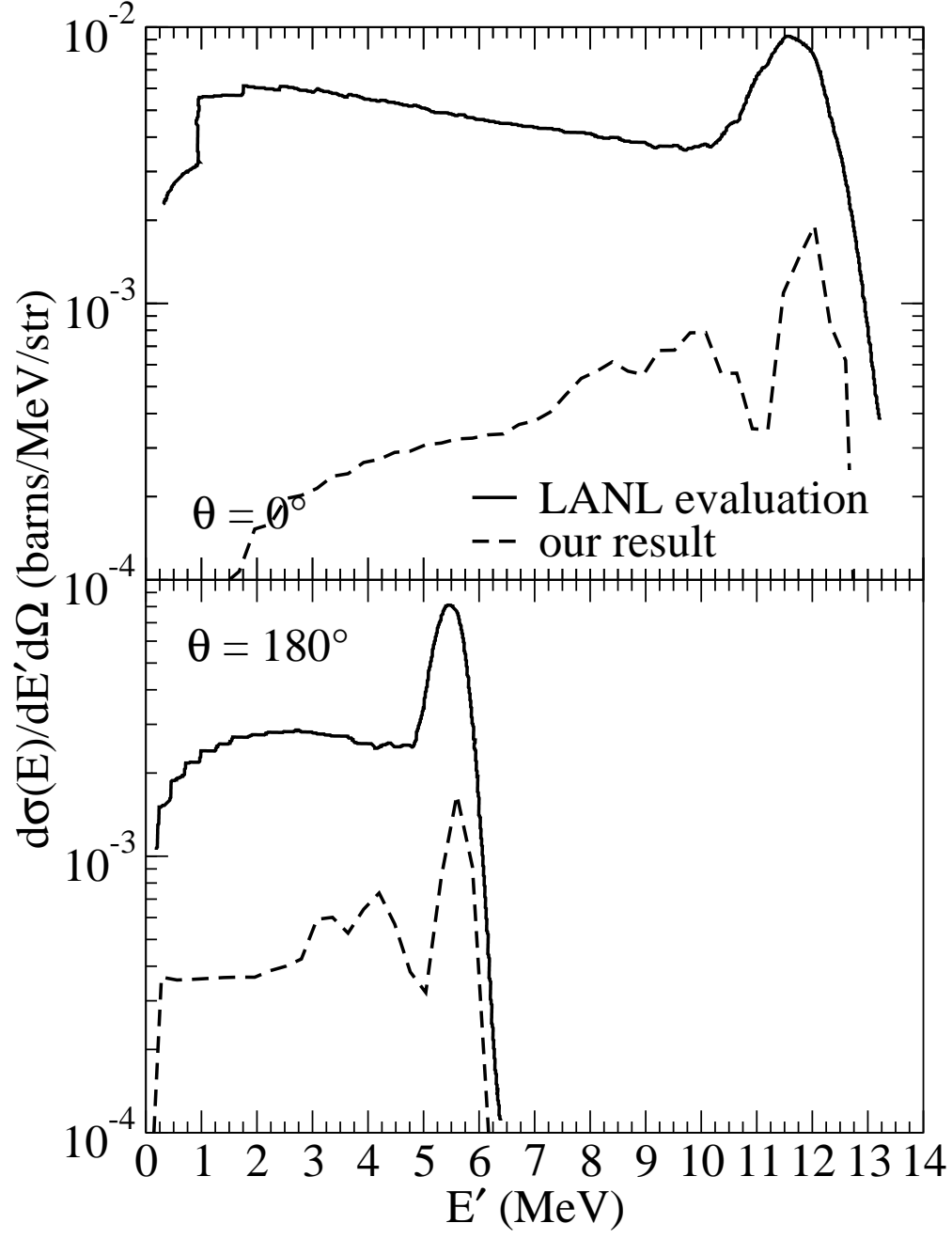


Figure 4: Plot of the ${}^6\text{Li}(n, nd)$ cross section at 14.2 MeV reconstructed from the ENDF/B-VII za003006 evaluation [32] (which uses the pseudo-level scheme) compared to the original evaluation by Stewart and Young [34]. Here the agreement is rather poor: our peaks only match the peaks in the Stewart-Young evaluation, but not the shape or magnitude of the curve.

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