User's Guide to `fete`: From ENDF To ENDL

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(Dated: February 9, 2006)

This guide describes how to run the `fete` ENDF to ENDL translation code and outlines some of the general features of the translation process. In particular, this guide details how to install the code and supporting scripts, how to prepare an ENDF formatted database for translation, how to translate the database, and how to check the translated database. This guide also explains how `fete` treats each ENDF reaction and data type.

Contents

I. INTRODUCTION

This guide is a description of the LLNL Computational Nuclear Physics (CNP) Groups's "From ENDF To ENDL" (a.k.a. `fete`) code. `fete` translates nuclear reaction data from the ENDF [1] to Livermore's internal ENDL [2] format. There is a companion document to this manual which describes the entire database preparation process [3]. ENDF is the name we give to the international standard data format used in ENDF/B-VI, ENDF/B-VII, JEFF-3.1, JENDL-3.3 and other evaluated nuclear data libraries [4]. Because of the significant difference in both format and content, the translation process is a complicated multi-step process.

The two formats differ in the arrangement of the data in the databases as well as the data formatting itself. ENDF sublibraries are labeled jointly by the type of data stored and by the incident particle. 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. The ENDF data itself is presented in a variety of manners, depending on the reaction and quantity in question.

By contrast, ENDL requires that reactions and nuclei be sorted into nesting directories first according to projectile (the YI number, e.g. `yi01` means incident neutron), then nuclide (e.g. deuterium, with Z=1 and A=2, is specified by `za001002`), then reaction. Table I shows the mapping of ENDF sublibrary to ENDL YI number. The data for each reaction has several numbers associated with it: YO denotes the outgoing particles, C denotes reaction type and I denotes the data type. The ENDL C and I numbers are analogous to the ENDF MF

and MT numbers, respectively. However, we caution that the mapping from (MF,MT) to (C,I) is not this straightforward as we see in Tables II and III. Finally, all of ENDL data is presented in point-wise interpolated tables in contrast to the complicated manner of ENDF data.

In this note, we will first cover the installation and use of `fete`. Second, we will detail the translation process and highlight issues of which a user should be aware. Finally, we will discuss some of the outstanding issues in the translation: the extensions that ENDL will need in order to support the rest of the ENDF format and information for locating and reporting bugs in the format specifications and in the databases. This manual also contains an appendix detailing some of the mathematical issues encountered in translating ENDF double differential data. This note does not go into the detailed workings of the code. This is covered in the `fete` Code Reference [**?**] documentation that accompanies the source code distribution.

II. INSTALLATION AND USE

A. Getting `fete`

You may obtain `fete` in several ways:

- `fete` is available as a tarball on Livermore's CNP Group web page `http://nuclear.llnl.gov/` [5]. The tarball unpacks to a directory called `fete/`.
- Inside LLNL, `fete` is available from the CNP Group's Subversion repository located at `oban.llnl.gov:/usr/gapps/svnRepos/ndg/fete`.
- `fete` is installed on LLNL's LC cluster in `/usr/apps/fete/`.

B. Building `fete`

If you download `fete` from the web or check it out of our source code repository, then you will need to build it. Inside the `fete/` directory, there are several subdirectories:

- `doc/Code_Reference`: `Doxygen` generated source code reference. This is a series of html pages.
- `doc/Users_Guide`: this manual, in pdf, ps and tex formats.
- `src`: the source code for `fete`
- `examples`: some sample inputs to test the code

To build the package on a Unix, Linux or MacOSX system, enter the main project directory (`fete/`) and type "`make`." If compilation went well, an executable file called `fete` will be left in the `src/` directory. We recommend moving this executable file to some place in your environment's path. There are two macros you may find useful to override while building the package: `CXX` (the C++ compiler) and `CXXFLAGS` (any flags to pass to the C++ compiler).

The documentation files may also be regenerated at any time by moving to the `doc/` subdirectory and typing "`make`." If you wish to do this, you will need LaTeXfor the *User's Guide to* `fete` and `Doxygen` for the `fete` *Code Reference*.

C. Setting up the environment

`fete` requires one auxiliary file: the `bdfls` file. The `bdfls` file contains a variety of data required by several of the codes maintained by the CNP group. In particular, the `bdfls` file contains group boundaries, fluxes, nuclear masses, half-lives, various physical and conversion constants, and atomic excitation levels. `fete`, `endep` [6] and `fudge` [7] all require the masses.

A copy of the `bdfls` file is included in the `src/` directory of the `fete` package, however it is not kept up to date. You will need to set the `$BDFLSPATH` environment variable to point to the `bdfls` file. If you do not set this variable, `fete` will attempt to load the `bdfls` file from the '.' directory.

D. Running `fete`

Running `fete` is fairly straightforward. If you have an file ENDF formatted file called `endf.prepro` in your current directory, simply type "`fete`." We have defined several command line options which you may use to tune `fete`'s behavior. The most important of these are:

- `-help`: Print the `fete` usage message and all of the command line options.
- `-f endf_file`: Translate the file named `endf_file` instead of the default `endf.prepro`, e.g.
  ```
  > fete -f n+Ca40.endf
  ```
- `-p options_file`: Use the settings in the options file `options_file` instead of the default settings. See the next paragraph.

The settings that control how the translation proceeds can be overridden on the command line or in the `fete_options.inp` file. These settings are described in Section III and listed in Table IV. Each option may be set on the command line by prepending a "`-`" to the option, e.g.

NSUB[a]	IPART[b]	ITYPE	Sub-Library Name	YX	Incident Particle
0	0	0	Photo-nuclear data	7	γ
1	0	1	Photo-induced fission product yields	7	γ
3	0	3	Photo-atomic interaction data	7	γ
4	0	4	Radioactive decay data	0	n/a
5	0	5	Spontaneous fission product yields	0	n/a
6	0	6	Atomic relaxation data[c]	n/a	n/a
10	1	0	Incident-neutron data	1	n
11	1	1	Neutron-induced fission yields	1	n
12	1	2	Thermal neutron scattering data	1	n
13	1	3	Electro-atomic interaction data	9	e
10010	1001	0	Incident-proton data	2	p
10011	1001	1	Proton-induced fission yields	2	p
10020	1002	0	Incident-deuteron data	3	d
10030	1003	0	Incident-triton data	4	t
20030	2003	0	Incident-^{3}He data	5	^{3}He
20040	2004	0	Incident-alpha data	6	α

[a] NSUB = 10 * IPART + ITYPE.
[b] IPART = 1000 * Z + A for the incident particle. Thus, γ-induced reactions have the same IPART as spontaneous reactions.
[c] Has no ENDL equivalent.

TABLE I: ENDF sub-library designator to ENDL YX (i.e. YI or YO) mapping. Data from different sub-libraries with the same ITYPE are distinguished in ENDL by differing C numbers. Currently only ITYPE's 0 - 2 are translated by `fete`.

```
> fete -tol_1d 0.001 -mf5_tol 0.000025
```

Each option may also be listed in the `fete_options.inp` file directly and a sample `fete_options.inp` is provided in the `src/` directory. Additionally, the `-p` option allows you to override the name of the `fete_options.inp` file:

```
> fete -p n+Ca40_options.inp
```

Note that `fete` can translate the ENDF/B-VI version of the ENDF format in both it's preprocessed and original forms. `fete` can also translate data from all types of incident particles. However, `fete` can no longer translate the ENDF/B-V version of the ENDF format.

III. TRANSLATION DETAILS

In this section, we discuss what is involved in the actual translation. We start with the treatment of reaction cross sections. Then we discuss angle, energy, and joint energy-angle distributions for massive particles (not gammas). Following this, we discuss gamma data, delayed fission neutrons, charged-particle data and, our treatment of Q values. You are encouraged to consult Tables II and III while reading this section.

A. General information on the reaction data in ENDF.

1. *MF=1 (Documentation & Delayed Particles From Fission)*

The MF=1 file documents the contents of the evaluation and, in MT=455-460, contains delayed particle data from fission. The treatment of delayed fission neutron information is detailed in Subsection III D. The delayed photon data is not yet translated.

The documentation contained in the MF=1 file is placed in the `documentation.txt` file in the same directory as the other translated ENDL formatted data. The `documentation.txt` file also contains any error messages or warnings generated by `fete` during the translation process. This may be turned off by setting the `skip_logging` flag to a number greater than 0. These messages are logged in `documentation.txt` to aid in tracking down problems in the translated data.

2. *MF=2 (Resonance Data)*

The MF=2 data gives the resonance parameters. We preprocess this data with Red Cullen's `recent` code to convert this information to tabular cross sections [8]. This table is combined with the MF=3 cross section data to form the actual cross section for the reaction.

MF	Description	I
1	General information	n/a[a]
2	Resonance parameter data	0[b]
3	Reaction cross sections	0
4	Angular distributions for massive emitted particles	1
5	Energy distributions for massive emitted particles	4
6	Energy-angle distributions for emitted particles (γ's or massive particles)	3 or 4
7	Thermal neutron scattering law data	n/a[c]
8	Radioactivity and fission-product yield data	n/a[a]
9	Multiplicities for radioactive nuclide production	n/a[a]
10	Cross sections for radioactive nuclide production	n/a[a]
12	Multiplicities for photon production	9
13	Cross sections for photon production	0
14	Angular distributions for photon production	4[d]
15	Energy distributions for photon production	4
23	Photo-atomic interaction cross sections	0
27	Atomic form factors or scattering functions for photo-atomic interactions	941
30	Data Covariances obtained from parameter covariances and sensitivities	n/a
31	Data covariances for nubar	n/a
32	Data covariances for resonance parameters	n/a
33	Data covariances for reaction cross sections	n/a
34	Data covariances for angular distributions	n/a
35	Data covariances for energy distributions	n/a
39	Data covariances for radionuclide production yields	n/a
40	Data covariances for radionuclide production cross sections	n/a

[a]MT=451 delayed neutron data is handled separately.
[b]Translated into pointwise data using Red Cullen's `recent` code.
[c]Not implemented in ENDL yet.
[d]Only if not isotropic; if isotropic, this file is ignored since the ENDL default is isotropic.

TABLE II: ENDF MF numbers and their rough ENDL equivalent.

3. MF=3 (Cross Section Data)

The MF=3 file gives tabular cross section data. As a second preprocessing step, we use Red Cullen's `sigma1` code to Doppler broaden the data to room temperature. The corresponding ENDL file is flagged by I=0.

B. Data on massive particles, ordered by MF number.

1. MF=4 (Outgoing Angular Distributions)

The MF=4 file gives angular distributions for outgoing particles. This is most commonly used for discrete 2-body reactions and it consists of coefficients for Legendre expansions in the center-of-mass frame. ENDL also uses the center-of-mass frame for such data, but it only has a piecewise-linear representation. We approximate the Legendre expansions by piecewise-linear functions. The corresponding ENDL file is flagged by I=1. Note that the sum of the Legendre expansion is sometimes negative for certain outgoing angles and when this happens, we replace these unphysical values by zero.

Interpolation of this data with respect to energy of the incident neutron is usually straightforward, since linear interpolation of Legendre coefficients is equivalent to linear interpolation of the sum of the Legendre series. For some targets, e.g. ^{238}Pu (za094238), ENDF/B-VI uses log-linear interpolation for the Legendre coefficients. We expand the data to linear-linear interpolation.

In some cases the MF=4 data consists of tabular angular distributions in the laboratory frame. In these cases energy distributions are also given and the two distributions are regarded as uncorrelated. The translation of this data to ENDL is no problem because ENDL uses the same conventions. Such tabular data in MF=4 is "archival data," in the sense that new evaluations for ENDF/B-VI and ENDF/B-VII are supposed to provide double differential (joint energy-angle) distributions.

MT	Description	C
1	(n,total)	1
2	(z,elastic)	10
3	(z,non-elastic)	55[a]
4	(z,n)	11[b]
5	(z,anything)	n/a[c]
10	(z,continuum)	n/a[c]
11	(n,2nd)	32
16	(z,2n)	12
17	(z,3n)	13
18	(z,f)	15
19	(n,f) – 1^{st} chance fission.	n/a[d]
20	(n,nf) – 2^{nd} chance fission.	n/a[d]
21	(n,2nf) – 3^{rd} chance fission.	n/a[d]
22	(z,nα)	26
23	(z,n3α)	36
24	(z,2nα)	33
25	(z,3nα)	16[e]
27	(n,abs)	n/a[c]
28	(z,np)	20,21[f]
29	(z,n2α)	27
30	(z,2n2α)	n/a
32	(z,nd)	22
33	(z,nt)	24
34	(z,n^{3}He)	25
35	(z,nd2α)	n/a
36	(z,nt2α)	n/a
37	(z,4n)	14
38	(n,3nf) – 4^{th} chance fission.	n/a[d]
41	(z,2np)	29
42	(z,3np)	16[e]
44	(n,n2p)	17
45	(n,npα)	34
50	(z,n[0]) – excitation of g.s.	11[b,g]
51-90	(z,n[n]) – excitation of nth excited state	11[b,g]
91	(z,n[c]) – excitation to continuum	11[b,g]
101	(n,disappearance)	n/a[c]
102	(z,γ)	46
103	(z,p)	40
104	(z,d)	41
105	(z,t)	42
106	(z,^{3}He)	44
107	(z,α)	45
108	(z,2α)	37
109	(z,3α)	n/a
111	(z,2p)	18
112	(z,pα)	48
113	(z,t2α)	42[h]
114	(z,d2α)	n/a
115	(z,pd)	19
116	(z,pt)	39
151	(n,resonance)	n/a
201	(z,Xn)	56
202	(z,Xγ)	55
203	(z,Xp)	50
204	(z,Xd)	51
205	(z,Xt)	52
206	(z,X^{3}He)	53
207	(z,Xα)	54
208-218	Various meson and antiparticle production σ's	n/a
251-253	Various elastic neutrons scattering parameters.	n/a
301	Energy release for total and partial σ's.	n/a
451	Heading or title information (MF=1 only).	n/a[i]
452	(z,f) $\bar{\nu}$ total (prompt plus delayed) fission.	15[j]
454	(z,f) Independent fission product yields.	15[j]
455	(z,f) $\bar{\nu}$ for delayed fission.	15[j]
456	(z,f) $\bar{\nu}$ for prompt fission.	15[j]
457	(z,f) Radioactive decay data.	n/a
458	(z,f) Energy release in fission for incident n's.	15[j]
459	(z,f) Cumulative fission product yields.	15[j]
500	Total charged particle stopping power.	n/a
501	Total photon interaction σ.	70
502	Photon coherent scattering.	71
504	Photon incoherent scattering.	72
505	Imaginary scattering factor.	n/a
506	Real scattering factor.	n/a
515	Pair production, electron field.	n/a
516	Pair production.	74
517	Pair production, nuclear field.	n/a
522	Photoelectric absorption.	73
534-572	Various subshell photoelectric σ's.	n/a
600	(z,p[0])	40
601-648	(z,p[n])	40
649	(z,p[c])	40
650	(z,d[0])	41
651-698	(z,d[n])	41
699	(z,d[c])	41
700	(z,t[0])	42
701-748	(z,t[n])	42
749	(z,t[c])	42
750	(z,^{3}He[0])	44
751-798	(z,^{3}He[n])	44
799	(z,^{3}He[c])	44
800	(z,α[0])	45
801-848	(z,α[n])	45
849	(z,α[c])	45
851	Lumped reaction covariances.	n/a

[a] If MF=12–15, then the outgoing γ's are lumped in the C=55 file, otherwise the data is discarded since it should be stored with individual reactions. The non-γ data is discarded since it is purely derived data.
[b] If the `sum_inelastic` option is set then use the MT=4 data (lumping all γ data into the C=55 file), otherwise use the MT=51–91 data.
[c] Purely a derived file, so it is not needed.
[d] Only total fission data is stored in ENDL.
[e] Below $E_{\rm inc} = 20$ MeV, only ^{7}Li has this reaction and $^7\mathrm{Li}(n,3np)\alpha \equiv {}^7\mathrm{Li}(n,3n\alpha)p$
[f] ENDF does not distinguish whether the proton or neutron is emitted first.
[g] Level excitation functions stored in S=1 type files in ENDL.
[h] Below $E_{\rm inc} = 20$ MeV, only ^{10}B has this reaction and $^{10}\mathrm{B}+n \rightarrow t+{}^8\mathrm{Be}^* \rightarrow t+2\alpha$
[i] ENDL does not yet have a slot for documentation, however `fete` creates a file called `documentation.txt` containing the MT=451 data.
[j] Delayed fission information is stored in S=7 type files in ENDL.

TABLE III: ENDF MT numbers and their rough ENDL equivalent.

Key	Value	Description
Interpolation Options		
tol_1d	0.005	Relative accuracy of 1-d list interpolation
cut_off_1d	0.001	Suspend tol_1d below this absolute value (arb. units)[a]
tol_2d	0.015	Relative accuracy of 2-d list interpolation
cut_off_2d	0.003	Suspend tol_2d below this absolute value (arb. units)[a]
dE_tol	0.01	Maximum incident energy difference for 2-d lists (MeV)
log_log_tol	0.005	Relative error in converting log-log to lin-lin
3d List Options		
num_mu_3d	12	2*num_mu_3d+1 = number of μ bins in 3d expansion
num_E_in_3d	12	Number of incident energies for 3d expansion
MF=5 Options (see Section III B 2)		
num_mf5_bins	32	Number of equiprobable energy bins
mf5_shift	0.00002	Amount by which the first distribution is above threshold[b]
mf5_tol	0.00001	Energy tolerance used when evaluating parametric data in ENDF files (MeV)
mf5_weight_tol	0.001	Tolerance in total probability when summing multiple MF=5 models
Other Options For Specific Types Of Data		
sum_inelastic	0	If = 0, use the MT=51–91 individual inelastic data[c]; otherwise, use the MT=4 total inelastic data
Kalbach_i10	0	If > 0, calculate the I=10 average energy (see Section III B 3)
split_gammas	0	If > 0, split discrete gammas from continuum using S=3 (see Section III C)
skip_gammas	0	If > 0, skip translation of all outgoing gamma data (see Section III C)
fission_Q	0	If > 0, use ENDF fission Q value, otherwise subtract Q for delayed fission decays (see Section III D)
max_Coulomb_mu	0.94	Sets maximum scattering cosine, μ, to tabulate data for Coulomb scattering. This allows us to avoid the small-angle singularity in the Rutherford scattering cross-section (see Section III E).
General Processing Options		
skip_date	1	If > 0, don't bother processing evaluation's date field
skip_logging	1	If > 0, don't bother logging Unimplemented, Warning and SevereError messages to the documentation.txt file
message_level	0	If = 0, all messages reported; if ≤ 1, Info and Unimplemented messages are not reported but Warning and SevereError messages are reported; if > 1, only SevereError messages are reported.
endl_datafield_precision	8	Precision saved in ENDL files
max_n_energy	20.0	Maximum energy for incident neutrons in ENDL files (MeV)
max_cp_energy	30.0	Maximum energy for incident charged particles in ENDL files (MeV)
max_g_energy	30.0	Maximum energy for incident gammas in ENDL files (MeV)
max_list_size	500	Maximum length of a 1-d list

[a] For cross section data, this has units of barns; for multiplicities and probabilities, this has no units.
[b] $E_{\rm shift} = E_{\rm thresh}(1 + \texttt{mf5\_shift})$.
[c] The accompanying γ data is lumped into the C=55 file.

TABLE IV: Default parameters for the fete code. The parameter names are not case-sensitive.

2. MF=5 (Outgoing Energy Distributions)

The MF=5 file contains energy distributions of the outgoing particles. This data is often in laboratory coordinates as is the ENDL equivalent data (I=4). When the data is presented as an interpolatable table, the translation to ENDL format is trivial.

Unfortunately, it is more common for ENDF MF=5 data to be given as a table of parameters to use in some formula. Thus, the energy distribution may be given by a single temperature evaporation model:

$$CE' \exp[-E'/\Theta]$$

for $0 \le E' \le E'_{\max}$. Here, E' is the energy of the outgoing particle, and values of Θ (the effective evaporation temperature in MeV) are given in the MF=5 file for various values of the energy of the incident neutron. The value of $E'_{\max}$ is determined by energy conservation, and the constant C is chosen to make the total probability be one. We expand this a formula into a piecewise-linear interpolation table, accurate to an amount specified by `mf5_tol`.

The translation code has a cutoff, `cut_off_1d`, so that we do not impose accurate piecewise-linear interpolation in the exponentially small tail. Specifically, if the energy probability density is denoted by $p = f(E')$ and if $p_{\max}$ is the maximum value of p, then accurate interpolation is not enforced when $f(E') < \texttt{cut\_off\_1d} * p_{\max}$.

What makes translation of this functional ENDF data to ENDL format difficult is the interpolation with respect to the energy of the incident neutron. The usual prescription in ENDF is to derive such energy distributions by linear interpolation of the values of Θ. Some ENDL processing codes (e.g. `ndfgen` code [9]) use unit-base interpolation while others (e.g. `mcapm` [10]) use equally-probable energy bins, a mathematically similar procedure [12].

We have found that the unit-base interpolation scheme is usually not compatible with the linear interpolation of the function parameters, e.g. Θ, used by ENDF. We therefore chose to ensure that linear interpolation of the equally-probable bin boundaries in `mcapm` is consistent with linear interpolation of the function parameters in ENDF.

Another complication of translating ENDF energy distributions comes from the ENDF option of representing the data as a weighted average of some number of functional formulas,

$$p = \sum_{i=1}^{N} w_i f_i(E').$$

For example, for an (n, 2n) reaction, with different formulas for the energy distributions of the two outgoing neutrons. Because we expand out all of the functional data, different data types may have different accuracy. We have implemented a quality assurance test on the summed probability. The option `mf5_weight_tol` sets the acceptable tolerance on the summed probability.

3. MF=6 (Outgoing Energy–Angle Distributions)

The MF=6 files contain double differential (joint energy-angle) distributions. ENDL has two options for representing such data: I=4 files giving the joint distributions as Legendre expansions in the laboratory frame:

$$p(E,\mu) = \sum_n c_n(E) P_n(\mu)$$

and I=3 files containing tables of joint distributions (again in the laboratory frame). ENDF allows both of these options and adds the ability to represent data by a formula.

When an ENDF evaluator uses Legendre expansions we can copy it directly to an ENDL I=4 file as this data is always in laboratory coordinates. When an evaluator uses a table of double differential data, we must first boost to the laboratory frame if necessary and then "transpose" the data. We must transpose the data before copying it into an I=3 file because the ENDF column ordering is E, E' then μ whereas ENDL's is E, μ then E'.

The most common MF=6 model used in the latest ENDF-formatted libraries is the Kalbach-Mann formula [11]. We evaluate the formula for the number of outgoing angles and energies specified by the `num_mu_3d` option. In the future we hope to automate these parameter choices. One area of difficulty with Kalbach-Mann data is that it is in center-of-mass coordinates. Because the double differential distributions are probability densities, the conversion from center-of-mass to laboratory coordinates includes multiplication by the Jacobian of the transformation. See Appendix A. Another trouble with Kalbach-Mann data is that the function parameters are given as histogram data in the center-of-mass frame. There is no way to make an exactly faithful representation in the laboratory frame.

As a check on the accuracy of the translation of the Kalbach-Mann data, we have implemented a calculation of the average energy of the outgoing particles. The standard approach within ENDL is to use the `endep` code to integrate the double differential data in laboratory coordinates. The new method of calculating the average energy uses integration of the ENDF data in center-of-mass coordinates. You can use the new method by setting the `Kalbach_i10` option. With the current default values of the number of energies and angles to use in the translation, the disagreement in the two approaches is typically about 2%. We expect that this figure would be improved with a better method for selecting the ENDL data points.

Finally, we need to mention that double differential probability densities are normalized differently in ENDF and ENDL. ENDF double differential data is normalized such that $\int_0^\infty \int_{-1}^1 p(E,\mu)\, d\mu\, dE = 1$ assuming $p(E,\mu) = 0$

whenever (E, μ) is outside the range of validity of the data. ENDL double differential data is normalized such that $p(E, \mu) = P_1(\mu)P_3(E, \mu)$ where P_i is the probability density in the I=i file. The individual P_1 and P_3 files are normalized so that $\int_0^\infty P_3(E, \mu)\, dE = 1$ for each value of μ and $\int_{-1}^1 P_1(\mu)\, d\mu = 1$. Again, we use the convention that $P_1 = 0$ and $P_3 = 0$ outside the domain of validity of the data.

C. Gamma data

In ENDF the information on emitted gammas is given in files with MF numbers 12 through 15. This data has been the most difficult to put into ENDL format because the ENDL format is more constraining than the ENDF format.

In ENDL, it was customary to lump the gamma information into two categories: (n,γ) and (n,Xγ) (the C=46 and C=55 files). In fact, there are only 7 isotopes in ENDL that have gamma files other than C=55 and C=46 and all of them are light isotopes. The majority of these isotopes have gamma data only for inelastic scattering. Otherwise for $(n, n'\gamma)$ discrete data, it was assumed that the decay would proceed via a single jump to the ground state. In ENDF it is customary to leave the gamma data with the associated reaction. We have chosen not to combine all of the ENDF gamma data into C=55 files, but to keep it with the reactions.

For some targets and certain combinations of reactions, many ENDF-formatted libraries do have total gamma data. For gammas from inelastic scattering, the combined data is given in MT=4 files. ENDF may also combine gamma data from any reactions having MT=3 files. In our translation we join such gamma data and write it to C=55 ENDL files.

1. MF=12 (Multiplicity) and MF=13 (Cross Section Data)

The MF=12 and MF=13 ENDF data is closely related. For a given reaction, an MF=12 file gives the multiplicity of emitted gammas, while an MF=13 file gives the product of the multiplicity with the reaction cross section (the gamma production cross section). In ENDL the C=55 file with I=0 gives the gamma production cross section, while for individual reactions only the gamma multiplicity may be given (an I=9 file). Thus, if ENDF has MF=13 data for a given reaction, we have to divide by the cross section to produce and ENDL I=9 file, while if ENDF has MF=12 for a combination of reactions, we have to multiply by the cross section to produce an ENDL C=55 file.

There are two wrinkles we encounter when processing the MF=12 and MF=13 data. First, the MF=12 or MF=13 files may give detailed information on the γ decay chains. For the translation to ENDL we have to accumulate this information into files of energy distributions and multiplicities. Second, ENDL's mechanism for handling discrete and continuum gammas (S=3 files) requires more detail than is present in the ENDF data files. The problem with the ENDL S=3 option is that it requires those channels with continuum gammas and those with different discrete excitation levels each be treated as separate reactions, having their own cross section and outgoing energy distributions. To deal with this problem, we introduced a `split_gammas` option. If set, we split the discrete lines out from the continuum gammas in the individual reactions. Otherwise, we convert the discrete lines to a continuum distribution with approximate δ-functions at the lines. This scheme also handles the case where an ENDF evaluator represents continuum gamma distributions as a set of discrete lines with frequencies dependent upon the energy of the incident neutron.

We comment that the ENDL unit-base interpolation never made sense for gamma distributions represented as approximate δ-functions, and fortunately there were are few targets in ENDL99 which have such data. It does make sense to interpolate equally-probable bins for this data, and that is how the translation code is written.

2. MF=14 (Angular Distributions)

The MF=14 files contain information on angular distributions for gammas. These are usually isotropic, and in ENDL the convention is that a distribution is isotropic if no angular information is given. There are a few reactions in the ENDF-formatted libraries for which the MF=14 data is Legendre coefficients. We convert this data to ENDL I=4 format with Legendre expansions.

3. MF=15 (Energy Distributions)

The MF=15 files are for energy distributions of continuum gammas. The corresponding continuum gamma multiplicity is given as the last table in the MF=12 file, or the gamma production cross section is the last table in the MF=13 file.

D. Delayed neutrons

For delayed fission neutrons in ENDF/B-VI some of the multiplicity data is in the MF=1 MT=455 file and some in the MF=5 MT=455 file, so we need to handle them together.

The MF=1 MT=455 file starts with a list of the time constants for delayed fission neutrons. In ENDL format the delayed neutron data is identified by C=15 (fission), along with S=7 (delayed neutrons). The data corresponding to the different time constants is put into different ENDL blocks, with the time constant located in the x[1] slot. This is an extension of the ENDL format,

which originally had only one variety of delayed fission neutron.

For C=15 and S=7 we usually produce an I=7 delayed neutron multiplicity file, with separate blocks corresponding to the different time constants. ENDF may also give energy distributions for delayed fission neutrons. In that case we write a corresponding C=15, S=7, I=4 ENDL energy distribution file.

E. Incident charged particles

Translating ENDF's charge particle data is straightforward. For the most part, this data is contained in MF=6 data using the LAW=5 option. LAW=5 data is basically the differential cross-section for charged particle scattering rather than the usual outgoing energy-angle distribution. We produce normalized particle distributions from this data in the angular range $\mu \in (-1, \texttt{max\_Coulomb\_mu})$.

F. Treatment of Q values

The treatment of Q values in ENDL and ENDF is different is a few subtle, but important ways. To complicate the matter, the ENDF manual [1] is not clear on how to treat isomer targets and how to treat the Q value for fission.

1. QI and QM in ENDF vs. Q and ELEVEL in ENDL

ENDL rules regarding Q values are straightforward [2]. There are three fields that more or less determine everything, although one field (X1) has meaning that depends on the ENDL S number. In the first row of the header of each file, one specifies the ELEVEL which is the excitation level of the target. This is how one specifies an isomer target in ENDL. On the second line of the header, we write the Q value for the ground state. We do this whether or not the target is actually in the ground state. Finally, for S=1 data, the X1 field of the second line of the header caries the excitation level of the product. The energies of all of these fields are given in MeV.

In ENDF, things are a little more murky. In ENDF, there are actually two Q values, QI and QM. QM is the Mass-difference Q value, defined as the target and projectile masses minus the mass of the residual nucleus and masses of all other reaction products. That is, for a+A→b+c+...+B, QM=[(ma+mA)-(mb+mc+...+mB)]×(amu/eV) if the masses are in amu. On the other hand, QI is the "Reaction" Q value for the (lowest energy) state defined by the given MT value in a simple two-body reaction or a breakup reaction. QM is defined as the residual nucleus (or intermediate system before breakup) minus the energy of the excited level in this system. One uses QI=QM for reactions with no intermediate states in the residual nucleus and without complex breakup. The trouble with the current ENDF documentation is that it is not clear which masses to use in the case of an isomer target. We have found examples where the isomer's excitation energy is and is not added to the mass in the calculation of QI and QM [13].

C	Reaction
16	(n, 3n p)
17	(n, n 2p)
18	(n, 2p)
19	(n, p d)
36	(n, n 3α)

TABLE V: Reactions added to ENDL.

Our solution, as we proposed at the Oct. 2005 CSEWG meeting [14] is as follows. In general, the masses used in the calculation of QM and QI should correspond the rest masses of the target and residual nuclei. If the target or residual is in the ground state, the rest mass is just the nuclear mass. If the target or residual is an isomer, the rest mass is the nuclear mass plus the excitation energy of the nucleus, which should be specified in the ELIS field in the MF=1 MT=451 file.

2. Q values for fission

In ENDF, the Q value for fission is the energy released per fission minus the neutrino energy. In ENDL, we also subtract off the energy of the delayed neutrons, emitted β's and delayed photons. The `fete` flag `fission_Q` defaults to the ENDL behavior, but setting it to 1 makes `fete` follow ENDF recommendations.

IV. CONCLUSIONS

Throughout this manual we have dealt with the detailed differences between ENDF and ENDL. As a result of these differences, we have had to add several new reactions to ENDL and these are summarized in Table V. Interestingly, there is one case where ENDL has more information than ENDF. In ENDL, (n, np) and (n, pn) reactions are treated as separate reactions if energy distributions are given only for the outgoing neutron and proton. This is done because the average energy for the gammas and the residual differs slightly depending on the order of particle emission. ENDF has just one reaction, which we treat as (n, np).

Finally we mention that work that we have yet to do. Most serious issues that remain are:

1. Not all downstream codes have been updated to handle discrete gamma data and delayed fission neutron data.

2. ENDF has uncertainties and covariances for several evaluations now, but ENDL has no way to represent either.

3. `fete` does not translate radioactive decay and fission product yields and cross-sections (MF=8-10) yet.

4. `fete`'s treatment of isomer target/projectiles is not very obvious (different Q values are used denote the different channels).

5. `fete` has not been updated to handle the ENDF format additions made at the 2005 CSEWG Meeting [14], namely

   (a) post-fission β-delayed γ data (ENDL has no way to represent this yet),

   (b) relativistic kinematics for light particle reactions,

   (c) treatment of Q values is "confused" in ENDF, especially for isomer target/projectiles as mentioned in Section III F.

In addition to these problems, the databases themselves often have out-of-date or sometimes even wrong data. Fortunately the data is updated regularly and problems are corrected. There are several sources for "bug lists":

- NNDC's "Known Errors and Deficiencies in ENDF/B-VI" page at `http://www.nndc.bnl.gov/csewg/errors.html`.
- NJOY's "NJOY 99 Issue Tracker" page at `http://t2.lanl.gov/codes/njoy99/Issues.html`.
- CEA's nuclear data listserver archive at `http://www.nea.fr/listsmh/`.
- 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.jaeri.go.jp/jendl/j33/j33prob.html`.
- D.A. Brown and G. Hedstrom, "Possible problems in ENDF/B-VI.r8" LLNL Report UCRL-CONF-200686 (2003).

Consumers of both our translated data and `fete` itself are encouraged to check there and the `documentation.txt` files within each evaluation to track down issues in their data.

Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

APPENDIX A: DOUBLE DIFFERENTIAL DATA IN ENDF

For joint probability distributions of the energy and direction cosine of emitted particles (double differential data), it is common in ENDF [1], Chap. 6 for the data to be given in terms of the Kalbach [11] parameterization. A complicating factor is that this representation is in the center-or-mass coordinate system, while double differential data in `ENDL` is in the laboratory frame. Because we are dealing with a probability density, the transformation formula is

$$p_{\mathtt{lab}}(E_{\mathtt{lab}}, \mu_{\mathtt{lab}}) = p_{\mathtt{cm}}(E_{\mathtt{cm}}, \mu_{\mathtt{cm}}) J(E_{\mathtt{cm}}, \mu_{\mathtt{cm}}) \tag{A1}$$

Here, $p_{\mathtt{lab}}$ and $p_{\mathtt{cm}}$ are the probability density in, respectively, laboratory and center-of-mass coordinates, $E_{\mathtt{lab}}$ and $E_{\mathtt{cm}}$ are the energies of the emitted particle, $\mu_{\mathtt{lab}}$ and $\mu_{\mathtt{cm}}$ are the direction cosines of the emitted particle relative to the incident particle, and J is the Jacobian of the mapping from center-of-mass to laboratory coordinates. In Eq. (A1), the dependence of $p_{\mathtt{cm}}$ and the Jacobian, J, on $E_{\mathtt{cm}}$ and $\mu_{\mathtt{cm}}$ is parametric so we must compute $E_{\mathtt{cm}}$ and $\mu_{\mathtt{cm}}$ from $E_{\mathtt{lab}}$ and $\mu_{\mathtt{lab}}$ in practice. The Jacobian must be included, because the probability of finding emitted particles within a region of energies and cosines is the integral of p over that region.

`fete` assumes that the ENDF double differential is given for particles emitted in all directions $-1 \le \mu_{\mathtt{cm}} \le 1$ for a range of energies $E_{\mathtt{min}} \le E_{\mathtt{cm}} \le E_{\mathtt{max}}$ with $E_{\mathtt{min}} \ge 0$. That is, in center-of-mass coordinates we have a rectangle with $\Omega_{\mathtt{cm}} = \{(E_{\mathtt{cm}}, \mu_{\mathtt{cm}}) : E_{\mathtt{min}} \le E_{\mathtt{cm}} \le E_{\mathtt{max}}, -1 \le \mu_{\mathtt{cm}} \le 1\}$. In practice, we always have $E_{\mathtt{min}} = 0$.

The steps involved in finding the probability density in laboratory coordinates are as follows. (1) Find the domain $\Omega_{\mathtt{lab}}$ in laboratory coordinates corresponding to the region $\Omega_{\mathtt{cm}}$ where we have data. (2) For a point $(E_{\mathtt{lab}}, \mu_{\mathtt{lab}})$ in $\Omega_{\mathtt{lab}}$ find its image $(E_{\mathtt{cm}}, \mu_{\mathtt{cm}})$ and evaluate the probability density $p_{\mathtt{cm}}(E_{\mathtt{cm}}, \mu_{\mathtt{cm}})$. (3) Compute $J(E_{\mathtt{cm}}, \mu_{\mathtt{cm}})$ and use (A1) to calculate the probability density in the laboratory frame. Let us expand on these concepts.

1. The domain in the laboratory frame

When ENDF data is given in center-or-mass coordinates, it is assumed that the mapping to laboratory coordinates is to be done according to Newtonian mechanics [1], p. 6.5. It is also assumed that the target nucleus is at rest. Consequently, if the masses of the target, projectile, and ejected particle are denoted by, respectively, $M_{\mathtt{targ}}$, $M_{\mathtt{proj}}$, and $M_{\mathtt{eject}}$, then a stationary ejected particle in the center-of-mass frame ($E_{\mathtt{cm}} = 0$) has energy

$$E_0 = \frac{M_{\mathtt{proj}} M_{\mathtt{eject}}}{(M_{\mathtt{targ}} + M_{\mathtt{proj}})^2} E_{\mathtt{in}} \tag{A2}$$

in the laboratory frame if the incident particle has (lab frame) energy $E_{\mathtt{in}}$. The direction of such a particle is

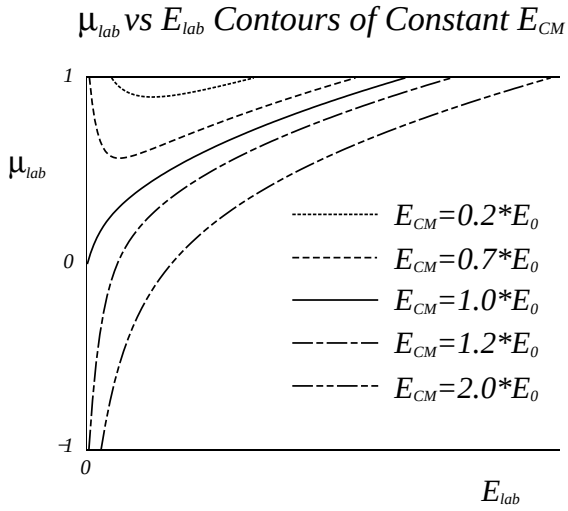

FIG. 1: Mapping center of mass energy and angles into the laboratory frame. Here the center of mass energy, E_{cm}, is given in units of the kinetic energy of the center of mass system, E_0.

forward, $\mu_{\mathtt{lab}} = 1$.

For particles emitted with positive energy, the mapping from center-of-mass to laboratory coordinates is given by

$$E_{\mathtt{lab}} = E_0 + E_{\mathtt{cm}} + 2\mu_{\mathtt{cm}}\sqrt{E_0 E_{\mathtt{cm}}}, \tag{A3}$$

$$\mu_{\mathtt{lab}} = \mu_{\mathtt{cm}}\sqrt{\frac{E_{\mathtt{cm}}}{E_{\mathtt{lab}}}} + \sqrt{\frac{E_0}{E_{\mathtt{lab}}}}. \tag{A4}$$

Some curves of $(E_{\mathtt{lab}}, \mu_{\mathtt{lab}})$ for constant E_0 and $E_{\mathtt{cm}}$ for $-1 \le \mu_{\mathtt{cm}} \le 1$ are shown in Figure 1. Note that the direction of emission in the laboratory frame is always forward ($\mu_{\mathtt{lab}} > 0$) if $E_{\mathtt{cm}} < E_0$.

In the case that the ENDF data is for $0 \le E_{\mathtt{cm}} \le E_{\mathtt{max}}$, there are 3 possibilities for the domain $\Omega_{\mathtt{lab}}$ depending on the size of $E_{\mathtt{max}}$ relative to E_0. If $E_{\mathtt{max}} < E_0$, then we have only forward emission in the lab frame, and $\Omega_{\mathtt{lab}}$ is a disk-shaped region bounded by the line $\mu_{\mathtt{lab}} = 1$ and a curve as in Figure 1 with $\mu_{\mathtt{lab}} > 0$. In this case, the minimum value of $\mu_{\mathtt{lab}}$ is $\min \mu_{\mathtt{lab}} = \sqrt{1 - \frac{E_{\mathtt{max}}}{E_0}}$. If $E_{\mathtt{max}} = E_0$, the region $\Omega_{\mathtt{lab}}$ is bounded below by the curve starting at the origin in Figure 1. This is because the point with $E_{\mathtt{cm}} = E_0$ and $\mu = -1$ maps to $E_{\mathtt{lab}} = 0$. Finally, if $E_{\mathtt{max}} > E_0$, then backward emission is possible in the lab frame and $\Omega_{\mathtt{lab}}$ is bounded by a curve as in Figure 1 with $-1 \le \mu_{\mathtt{lab}} \le 1$.

If we find that $E_{\mathtt{min}} > 0$ and $E_{\mathtt{min}} \le E_{\mathtt{cm}} \le E_{\mathtt{max}}$ for the `ENDF` data, then $\Omega_{\mathtt{lab}}$ is the difference between two of the domains described in the previous paragraph.

2. Center-of-mass probability density

For given $(E_{\mathtt{lab}}, \mu_{\mathtt{lab}})$ in $\Omega_{\mathtt{lab}}$, we may invert Eqs. (A3)–(A4) to get

$$E_{\mathtt{cm}} = E_0 + E_{\mathtt{lab}} - 2\mu_{\mathtt{lab}}\sqrt{E_0 E_{\mathtt{lab}}}, \tag{A5}$$

$$\mu_{\mathtt{cm}} = \mu_{\mathtt{lab}}\sqrt{\frac{E_{\mathtt{lab}}}{E_{\mathtt{cm}}}} - \sqrt{\frac{E_0}{E_{\mathtt{cm}}}}. \tag{A6}$$

We insert these values of $(E_{\mathtt{cm}}, \mu_{\mathtt{cm}})$ into the formulas appropriate to the ENDF data [1], Chap. 6.

3. The Jacobian

The Jacobian of the mapping from center-of-mass to laboratory coordinates can be derived several different ways and the result is:

$$J(E_{\mathtt{cm}}, \mu_{\mathtt{cm}}) = \sqrt{\frac{E_{\mathtt{lab}}}{E_{\mathtt{cm}}}}. \tag{A7}$$

Note that this Jacobian has a singularity due to the fact that we have $E_{\mathtt{lab}} = E_0$ and $\mu_{\mathtt{lab}} = 1$ for $E_{\mathtt{cm}} = 0$ and all directions $-1 \le \mu_{\mathtt{cm}} \le 1$. Small perturbations cover so much more area in the center-of-mass frame than in the laboratory frame that we have $J(0, \mu_{\mathtt{cm}}) = \infty$ for $-1 \le \mu_{\mathtt{cm}} \le 1$. This is not a serious difficulty because differentiation of (A5)–(A6) shows that $J(E_{\mathtt{cm}}, \mu_{\mathtt{cm}}) \sim \frac{1}{\sqrt{E_{\mathtt{cm}}}}$ as $E_{\mathtt{cm}} \to 0$, which is an integrable singularity. The Jacobian also has a zero for $E_{\mathtt{cm}} = E_0$ and $\mu_{\mathtt{cm}} = -1$. This is because the corresponding energy in the laboratory frame is $E_{\mathtt{lab}} = 0$ and the direction is arbitrary, $-1 \le \mu_{\mathtt{lab}} \le 1$.

APPENDIX B: LLNL DISCLAIMER

[1] Cross Section Evaluation Working Group, "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," Ed. V. McLane, C.L. Dunford, P.F. Rose, Brookhaven National Laboratory Report BNL-NCS-44945, (1997).

[2] B. Beck, T. Hill, D. McNabb, "ASCII format specifications for the Evaluated Nuclear Data Libraries (ENDL)," in preparation; R. J. Howerton, R. E. Dye, P. C. Giles, J. R. Kimlinger, S. T.Perkins, and E. F. Plechaty, "Omega: A Cray 1 executive code for LLNL nuclear data libraries", Lawrence Livermore National Laboratory Report UCRL-50400, Vol. 25 (1983).

[3] D.A. Brown, "Translated ENDF Data at LLNL," in preparation. LLNL Report, UCRL's pending.

[4] Evaluated Nuclear Data File `http://www.nndc.bnl.gov/nndc/endf/`; Japanese Evaluated Nuclear Data Library `http://wwwndc.tokai.jaeri.go.jp/jendl/j33/j33.html`; Joint European File `http://www.nea.fr/html/dbdata/data/evaluated.htm`.

[5] LLNL Computational Nuclear Physics Group page `http://nuclear.llnl.gov/`.

[6] G.W. Hedstrom "An explanation of the ENDEP code," Lawrence Livermore National Laboratory Report UCRL-ID-151609 (1999).

[7] B. Beck, "For UpDating ENDL (`fudge`)," manual in preparation.

[8] D. Cullen, `prepro2004` Computer Code available from `http://www-nds.iaea.org/ndspub/endf/prepro/`.

[9] Beck B., "LLNL's Deterministic Transport Access Routines and Data: Documentation for the Nuclear Data Files (ndf) and the libndf.a access routines," Lawrence Livermore National Laboratory Report UCRL-MA-147647 (2002).

[10] Hedstrom G., Cox L., and Perkins S., "The Content and Structure of MCF Files," Lawrence Livermore National Laboratory Report UCRL-ID-127438, Rev. 1 July (1997).

[11] C. Kalbach, "Systematics of continuum angular distributions: Extensions to higher energies," Phys. Rev. C **37** (1988) 2350–2369.

[12] G. Hedstrom, LLNL Report, pending UCRL assignment.

[13] D.A. Brown, "Sorting out Q values, threshold energies and level excitations in ENDL and ENDF," LLNL Report UCRL-TR-216790 (2006).

[14] Proceedings of the CSEWG & USNDP Meetings, BNL, November 8-11, 2005, Edited by Pavel Oblozinsky, National Nuclear Data Center, BNL.