International Conference on Nuclear Data for Science and Technology 2010

FROM ENDF TO PENDF: NJOY VERSUS PREPRO

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Received
Accepted for Publication

Evaluated nuclear data are frequently processed using either NJOY or PREPRO to produce application-specific libraries. The processing chain typically consists of a series of modules executed in a particular order or sequence. While some modules in NJOY overlap with those of PREPRO, others do not. It would be advantageous to be able to use the two independent codes complementarily. First, the flexibilities and constraints in a nuclear data processing chain requires outlining. The fact that

– both NJOY and PREPRO are modular;
– intermediate PENDFs are passed from the output of one module as input to the next

allows technical flexibilities such as:

– NJOY and PREPRO modules may be interleaved within the same processing chain;
– for modules without inter-module dependencies, the order of execution does not matter.

On the other hand, the constraints are:

– NJOY requires the various MF-MT pairs for a material to be put in a common energy grid;
– inter-module dependencies require some (but not all) modules to be executed in a particular sequence.

The cost of imposing a common energy grid is investigated along with the interchangeability of selected functionally-similar NJOY and PREPRO modules.

KEYWORDS : FLUKA, NJOY, PREPRO, PENDF, JEFF

1. CONTEXT

Existing work[1–5] on nuclear data processing predominantly centres around the ACE[1] format, the MCNP[6] family and criticality applications. Here, we report the considerations in producing pointwise libraries for FLUKA[7], which is distinct by design:

– with its capability for analog transport in addition to non-analog transport;
– it is general-purpose but sub-critical;
– the interface with nuclear data is not in ACE format.

Implementing analog and correlation between ejectiles are demanding both in terms of data and algorithm. Code development aside, even for end-users demonstrable differences between analog and non-analog transport should not be under-estimated[8, 9].

Evaluated nuclear data[2] (in ENDF format) may be processed using processors[3] to produce pointwise (PENDF) and multigroup (GENDF) libraries. A typical feature of ENDF *tapes*[4] which partly spells the need for processing is the apparent *zero* cross section and *unexpected* discontinuity in the resonance regions. Once processed, the resultant PENDF tapes will have the resonances in place, having been reconstructed using abbreviated data present elsewhere in the same ENDF tape.

PENDF and GENDF libraries, in turn, are passed to Monte Carlo codes[5] for use in pointwise and multigroup transport, respectively. Either may be more appropriate for particle transport calculations, depending on the problem at hand. This work focuses on pointwise libraries.

The dividing line between PENDF/GENDF libraries and a Monte Carlo code is, however, not clear-cut. Some Monte Carlo codes manage or even execute on-the-fly certain processes which overlap with those offered by NJOY[10] and/or PREPRO[11]. The ACE interface cannot be taken as a standard for all Monte Carlo codes.

[1] a file format for MCNP libraries
[2] *e.g.* ENDF, JEFF, JENDL, CENDL, BROND, ROSFOND
[3] *e.g.* NJOY[10], PREPRO[11], AMPX[12]
[4] Throughout this article *tape* (ENDF-6 nomenclature[13]) is used; each *tape* is deliminated by *TEND* records. This is to avoid confusion with *file* which under ENDF6 nomenclature, refers to a specific MF within a *tape*.
[5] *e.g.* MCNP/MCNPX, MARS, FLUKA, GEANT4

Various groups have produced application-specific libraries from evaluated nuclear data; existing reports already detail the chosen processing paths[1–5]. This work does not propose a particular processing sequence; it is not a documentation of the generation of a specific library. Rather, it considers the flexibilities and constraints in formulating a processing path, as well as the associated issues.

1.1 NJOY and PREPRO modules

Some NJOY and PREPRO modules overlap; others do not. Overlaps include that between:

- RECONR$_n$ and the combination of LINEAR$_p$ and RECENT$_p$;
- BROADR$_n$ and SIGMA1$_p$;
- GROUPR$_n$ and GROUPIE$_p$;
- MIXR$_n$ and MIXER$_p$.

Throughout this communication NJOY and PREPRO modules are labelled with subscripts n and p, respectively.

Subsequent modules may be optional. The parallel match between PREPRO and NJOY modules diminishes. Sometimes described as physics add-ons, these include:

- unresolved resonances (UNRESR$_n$ and PURR$_n$)
- damage calculations (GASPR$_n$ and HEATR$_n$)
- thermal treatment (LEAPR$_n$ and THERMR$_n$)
- estimation of radiation quantities (ACTIVATE$_p$ and VIRGIN$_p$).

1.2 Flexibilities and constraints

Given that

- both NJOY and PREPRO are modular by function; and
- the input and output of each module are in PENDF and/or ENDF formats

a processing path need not be restricted to either one of the codes. Instead, modules from both codes may be interleaved *e.g.* by feeding the intermediate output from an NJOY module as input to a PREPRO module, or vice versa.

The processing path, characterised by the sequence of the modules used, is to some extent flexible. Inter-module dependencies draw the limit. Some modules are independent. Reversing the order of some modules will not make a difference. This is because such modules, each with its own dedicated function, operate on and write to different parts of the nuclear data tape. Each part is specified by a MF-MT pair, where MF and MT identify the *data type*[6] and the *reaction type*[7], respectively.

Modules performing add-on functions typically operate and write on different parts of the tape. ACTIVATE$_p$, for example, deletes MF=9 and inserts MF=10; LEGEND$_p$ modifies MF=4; HEATR$_n$ writes to 301≤MT≤450; BROADR$_n$ modifies MT=2 MF=152 and MT=3 MF=1 to 849; UNRESR$_n$ modifies MF=2 MT=152; PURR$_n$ modifies MF=2 MT=152 and 153; GASPR$_n$ modifies MF=3 MT=203 to 207; THERMR$_n$ modifes MF=3 and 6 MT=211. SIXPAK$_p$ does not write to a PENF at all, but output to a separate text file. The order by which selected modules are executed, in this case, is flexible and does not affect the eventual PENDF.

On the other hand, inter-module dependencies require certain modules to be processed before another. Linearisation, uniform gridding (for NJOY) and Doppler broadening/thinning are the core functions and primary steps in the processing path. For instance, in NJOY subsequent modules expect the data to have already been linearised and put in a uniform energy grid. Likewise, ACTIVATE$_p$ assumes that the data have already been linearised.

1.3 Unionisation of energy grid

Whereas PREPRO allows the option[8] of turning on or off the unionisation of energy grid, with NJOY this is mandatory and there is no way of producing PENDFs containing varied energy grids.

1.4 Input parameters and output verbosity

A further feature is PREPRO's emphasis on output verbosity. There is a recommended default for every input parameter; none is required from the user. NJOY, on the other hand, requires the user's active decision on most input parameters.

2. MATERIALS AND METHODS

PREPRO 2007 and NJOY 99.259 were used to process 381 materials from the JEFF 3.1.1 incident neutron sub-library. To compare functionally-parallel core modules, an NJOY run consisting RECONR$_n$ and BROADR$_n$, as well as a PREPRO run consisting LINEAR$_p$, RECENT$_p$, SIGMA1$_p$, FIXUP$_p$ and DICTIN$_p$ were executed for temperature 293 K. For the NJOY run, $1.0e^{-3}$ was set as the fractional reconstruction tolerance to be used when resonance-integral error criterion is not satisfied; $2.0e^{-2}$ the fractional reconstruction tolerance to be used when the criterion is met; $1.0e^{-7}$ the maximum resonance-integral error (in barns) per grid point. For the PREPRO run data were requested to be linearised to within $1.0e^{-3}$ and the options for cross section summation/reconstruction and missing section creation were turned on[9].

To gauge the penalty of putting various MF-MT pairs into a common energy grid, the number of energy points before and after LINEAR and RECENT were recorded.

3. RESULTS AND DISCUSSION

For most of the materials processed, differences between the total cross sections produced from RECONR$_n$-

[6] *e.g.* reaction cross sections, resonance parameter data, atomic relaxation data

[7] *e.g.* (n,total), (n,fission), (n,nα)

[8] via the FIXUP module

[9] without which interpolation and summation aberrations were observed for some materials

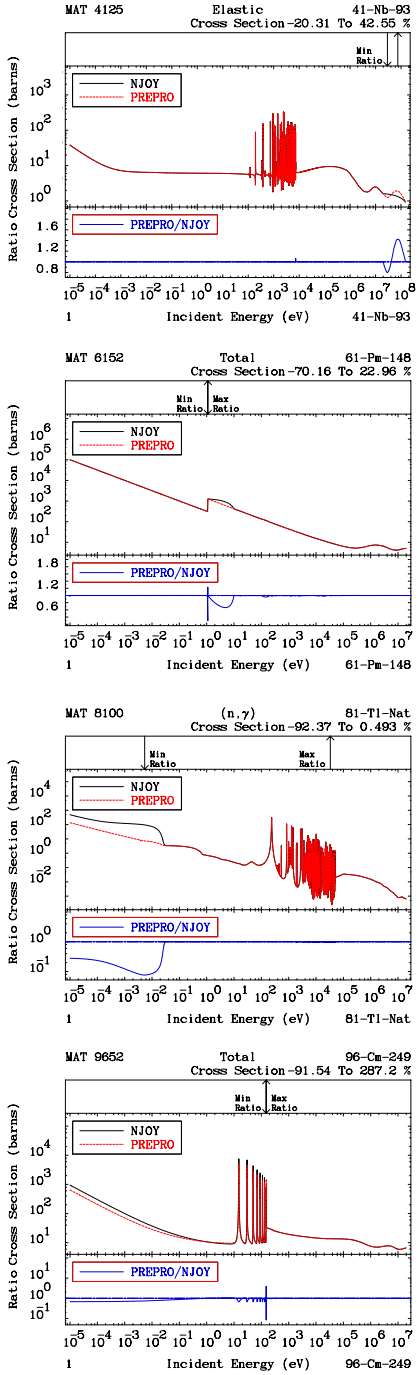

Fig. 1. COMPLOT$_p$ comparison of MF=3 MT=1 produced from two different processing paths: RECONR$_n$-BROADR$_n$ (NJOY) and LINEAR$_p$-RECENT$_p$-SIGMA1$_p$-FIXUP$_p$-DICTIN$_p$ (PREPRO).

BROADR$_n$ (NJOY) and LINEAR$_p$-RECENT$_p$-SIGMA1$_p$-FIXUP$_p$-DICTIN$_p$ (PREPRO) were observed at high-gradient points only. For isolated cases, however, systematic deviations were observed (Fig. 1). That of ^{93}Nb was traced to MT=2; that of ^{nat}Tl to MT=102. Some differences were due to interpolation at resonance region boundaries, some were due to the handling of unexpected characteristics in the original ENDF tape. Each line of investigation and curation is tremendously helpful in highlighting areas requiring further attention.

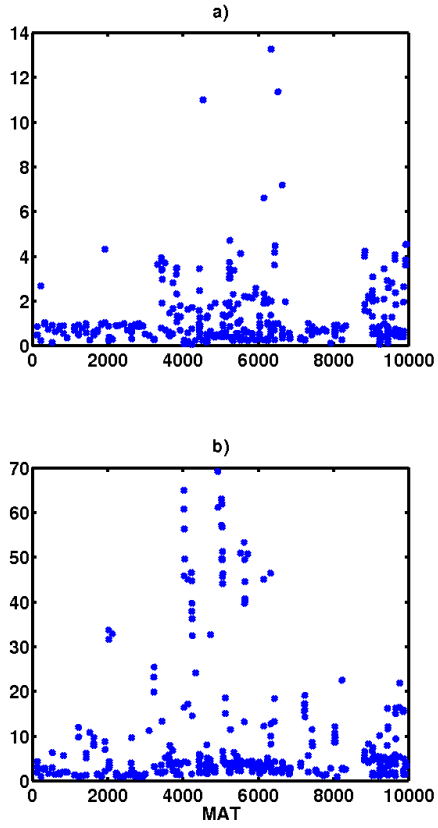

Fig. 2. The after-to-before ratio of energy points for MF=3 MT=1 (total reaction cross section) for various materials (identified by MAT[13]) at a) linearisation; b) unionisation of energy grid. Data are shown for the processing of the 381 materials given in JEFF 3.1.1 incident neutron sub-library.

The unionisation of energy grid is an important consideration in choosing whether to use PREPRO or NJOY for resonance reconstruction and Doppler broadening/thinning. Whereas linearisation may decrease or increase the number of energy points, unionisation of energy grids drastically increases this number by up to almost 70 fold (Fig. 2). Indeed, a common energy grid allows convenient summation of cross sections from individual contributing components. On the other hand, a common energy grid containing redundant intervals (without providing any additional information), if implemented in a Monte Carlo transport code, could impose critical memory and processing penalties which could affect every event and/or every history in every subsequent use of the Monte Carlo code. This is to be considered hand-in-hand with the interpolation steps involved, which could produce a counter-effect.

Fig.3 shows a possible processing path where a non-unionised energy grid is preserved as far as possible before PREPRO hands over to NJOY for physics add-ons. An alternative fix is to run a script at the end of the processing chain to remove the redundant points.

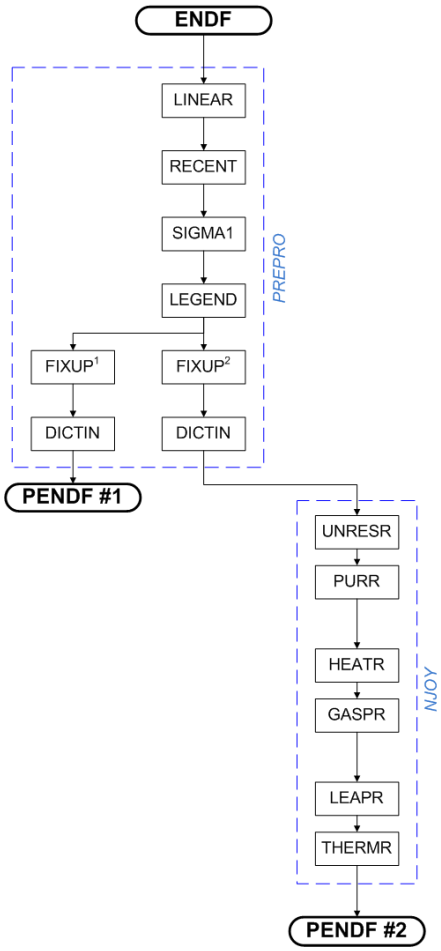

Fig. 3. A processing sequence where two versions of PENDF are produced: one without uniform energy grid and is PREPRO-only; another with uniform energy grid. FIXUP[1] is run with the option not to unionise the energy grid; FIXUP[2] is run with the option to unionise so that the PENDF may be fed into NJOY.

1997 negative cross sections were detected by LINEAR$_p$ in MF=3 MT=2 of ^{24}Mg. These were present before any resonance reconstruction. No negative cross sections were introduced by the modules. Detecting negative values is trivial; we need neither NJOY nor PREPRO for that. The issue is not in the detection but the treatment: what should be done with the negative values. This depends on their origin; zeroing the values is not the ultimate solution. Some tapes contain negative cross sections with an intention e.g. as adjustment to reproduce measured data.

4. CONCLUSION

Modules from NJOY and PREPRO may be technically interleaved within the same processing sequence. PREPRO may be preferred in case a common energy grid is not desirable. The increase in redundant data points varies from ENDF tape to ENDF tape; that for each tape in JEFF 3.1.1 has been catalogued. Functionally-equivalent NJOY and PREPRO modules differ by algorithm and ENDF handling, resulting in systematic deviations for isolated isotopes. The line of investigation is tape-specific and is found to be indispensable in identifying areas requiring special attention and in generating a robust library.

ACKNOWLEDGMENTS

Exchanges with Dermott Cullen and Skip Kahler are greatly appreciated.

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