WPEC Subgroup-B on Formats and Processing

DRAFT Work Plan Proposal

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1. Background

At the last WPEC meeting at JAERI in June 2000 it was proposed that A. Trkov would lead the WPEC Subgroup-B on Formats and Processing. The letter from C. Dunford to D. Muir of 29 November 2000 implied that the proposal was adopted.

Since this is a new assignment there is no progress report, but the Subgroup-B objectives, goals and work plan are presented for discussion. Through exchange of e-mails a few open problems were identified. Some specific items to be addressed are listed.

2. Objectives

The objectives of the subgroup are:

- To identify the needs for improvements and to suggest new extensions to the evaluated nuclear data file format definitions in a co-ordinated manner.
- To suggest standardised procedures for data file verification and validation, together with the appropriate software tools.

3. Outcomes

The expected outcomes are:

- To have a document defining procedures and scope of evaluated nuclear data file verification and validation tasks. The scope should be structured into levels so that one or more levels of data verification and validation can be executed in sequence independently. This would provide end-users with precise information on the scope of data testing (i.e. the user would know what kind of errors are definitely NOT present in the file).
- To have a library of codes for data verification and validation. The idea is not to create a new library, but to identify and make use of what is already available, supplementing the list with new developments only when needed.

4. Specific Items for discussion

4.1 Error in kinematics equations in the ENDF manual

The equations listed in Appendix-E of the ENDF-6 formats manual are wrong.

4.2 Unit-base and corresponding point interpolation of MF6 energy distributions on incident particle energy

Consider a hypothetical reaction with a 0.1 *MeV* threshold and at 1 *MeV* an isotropic flat energy distribution from 0 to 1 *MeV* outgoing particle energy.

- Linear interpolation on incident particle energy at 0.5 *MeV* gives an unphysical distribution with a narrow step near zero outgoing energy and a small distribution extending beyond reasonable maximum energy loss. The integral is conserved.
- Suppose that the distribution at threshold is approximated by a flat distribution of width 10^{-5} *eV*. Due to normalisation the distribution function value is 10^{+5} at this energy. At the energy of 1 *MeV* the distribution is 10^{-6} for outgoing particle energies between 0 and 10^{6} *eV*. Unit base interpolation gives the distribution 0.5×10^{5} over the interval of 0 to 0.5×10^{6} *eV* outgoing particle energy. The integral is 2.5×10^{10}.

According to ENDF-6 rules it is implicit that the distributions should be normalised to 1 after integration over the energy AND the angle. In practice this may be cumbersome and some code developers may not be aware of the potential danger of straightforward interpolation without renormalization.

It would be a good idea to add explicit guidelines on the procedures for implementing the unit base and corresponding point interpolation laws, emphasizing the potential dangers of improper use, as illustrated by the above example.

4.3 ENDF Utility Codes

A new version of the codes is to be released (Ref. C. Dunford).

4.4 Formatting of activation cross-sections.

The format for storing the activation cross-sections in MF=3/9 or in MF=10 was discussed in connection with the European Activation File (EAF). Although format rules allow MF=3 and MF=10 to co-exist, the approach in EAF is to allow only one due to the potential danger of double counting in NJOY when both are present. Strictly, this is an internal EAF and not a general ENDF rule (Ref. J.P Sublet, R. Forrest, A. Koning).

4.5 Supplement to the ENDF Pre-Processing Codes

A set of codes was prepared or updated, which are relevant and useful for data verification studies. They will be made available to users as a "Supplement to the ENDF

Pre-Processing Codes". The beta version is available upon request for testing purposes and includes the following codes.

GETMAT	is a simple utility for retrieval of selected materials from a master library in ENDF format.
MRGMAT	is a utility to merge evaluated data files into a single library. Unlike MERGER of the PrePro codes, MRGMAT is material oriented. It will replace entire material files (without checking individual reactions) and produce an output library file sorted by MAT in ascending order.
ENDTAB	is a retrieval code to extract cross sections (including differential and double differential ones) from ENDF files. The output is written in two-column PLOTTAB "curves" format. The code uses the DXSEND package to do the retrieval.
SIXTAB	converts correlated energy/angle distributions in ENDF MF6 Law-1 representation into tabular Law-7 representation. Note that the output file is intended for plotting and not as a substitute for the original file, since the conversion process is not complete and exact.
X4TOC4	is an extension of the original code by D.E. Cullen to convert EXFOR data into computational C4 format for plotting purposes.
C4SORT	sorts EXFOR data in computational format by MAT/MF/MT numbers and by the incident particle energy of the first point in a data set. This is convenient when plots are produced with the PLOTC4 code.
PLOTC4	is an extension of the original code by D.E. Cullen to plot EXFOR data in computational format and compares them with the corresponding data in an ENDF file, if requested. The main enhancement is that differential and double differential data can also be compared. The code uses the DXSEND package to do the data retrieval.
DXSEND	is a package of routines for retrieving cross sections from an ENDF file. Cross sections from MF3 as well as double differential cross sections from MF4,5,6 are processed.
STARPLOT	if a graphical interface package to produce PostScript files from the graphics programs. It is based on original work by G.C. Panini and D.E.Cullen.

Additional requirements are:

- The LEGEND code of the PrePro sequence is used to process MF4 data. Some files that were extended to intermediate energies use dual representation (Legendre polynomial and pointwise). The version of LEGEND in PrePro-2000 can not deal with this situation. The author of Pre-Pro codes D.E. Cullen provided a patch. Without this patch the data retrieved later by DXSEND (and the codes using it) are unphysical (i.e. isotropic distribution is assumed).
- A pre-checking code for ENDF files. The need is illustrated by the following practical example:
    - A new partial evaluated data file is produced that needs to be subjected to the verification procedure.

- CHECKR does not run unless the file follows precisely the syntax to the last detail. For example, checking of a section is terminated if the sequence numbers in columns 76-80 do not conform or if a dictionary section is missing, which is often the case in partial evaluations since there are other codes like STANEF that do this. A possible solution is to run STANEF before CHECKR.
- Trying to run STANEF results in a crash if there are trivial errors in the file, which we are trying to locate and remove. This is a "catch-22" situation.

A code (PRECHK) is needed that would check the syntax of an ENDF file in a simple manner, making sure that SEND, FEND, MEND and TEND records are present, the MAT/MF/MT numbers are in sequence (issuing warnings on not terminating the file scanning) and that TAB1, TAB2, CONT etc. records have the correct syntax with respect to variable types, array lengths, etc.