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A code package to produce ACE-formatted files for MCNP calculations

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1. Contents

1. Introduction

Nuclear data processing covers the gap between evaluated nuclear data and final users. During decades the code package NJOY [1] has been extensively used to process data for applications. It is a very comprehensive package, easy to use and allows to process data for continuous energy Monte Carlo simulations and multi-group transport calculations. Most of the nuclear data libraries available for applications have been generated using a version of NJOY. A few years ago, the version NJOY-99 was updated to version NJOY-2012.

The methods and procedures of NJOY were continuously patched in a well-coordinated international effort, but the main physical and mathematical models were not essentially changed from the original ones. It is worthy to mention, that the use of the same data processing methods and coding strongly reduces the probability to identify problems due to the processing itself (common failure mode).

It is also well known from benchmark analysis that processing methods have impact on transport integral parameters, like multiplication factors and resonance integrals, therefore it is important to verify, validate and optimize processing methods and algorithms.

Recently, the codes CALENDF [2], GRUCON [3] and FRENDY [4] have been developed to process evaluated nuclear data for applications. This opens the possibility to carry out an intercomparison exercise between different processing methods and codes.

On the other hand, the PREPRO pre-processing code package is freely available for nuclear data processing [5]. It includes codes for linearizing, reconstructing and Doppler-broadening evaluated nuclear data. Additionally, the codes LEGEND and SPECTRA can prepare linearly interpolable tabulated angular and energy distributions starting from data in the ENDF/B format given on MF=4 and MF=5 respectively [6]. More recently, the code URRFIT from URR-PACK system [7] has made it possible to prepare self-shielded cross section data in the unresolved resonance region.

It was considered worthwhile to extend the capabilities of the PREPRO package to prepare nuclear data for Monte Carlo calculations to be included into the intercomparison exercises. The code package ACEMAKER is a complement to the PREPRO codes to generate continuous-energy ACE formatted files for Monte Carlo simulations.

The package ACEMAKER prepares linearly interpolable tabulated energy-angle distributions from data in ENDF/B format given on MF6 and finally generates an ACE-formatted file for Monte Carlo calculations.

This report summaries the main features and input data needed for ACEMAKER and also describes how to use the PREPRO and URR-PACK packages with ACEMAKER to prepare nuclear data in ACE-format for MCNP [8] calculations.

2. Processing flow using packages PREPRO and ACEMAKER

To produce a continuous-energy ACE-formatted data file for Monte Carlo calculations using the PREPRO, URR-PACK and ACEMAKER packages the following sequence of codes should be called:

Figure 1: Main processing flow

LINEAR: Linearize cross section data as required for the rest of modules.
RECENT: Reconstruct cross section from resonance parameters.
SIGMA1: Doppler broaden cross sections.
FIXUP: Correct format and cross sections, define cross sections by summation and prepare cross sections on a unified energy grid as required by DOACE.
GROUPIE: Calculate self-shielding data, multiband parameters and multi-group cross sections. Multiband parameters are required by URRFIT to prepare self-shielding data in the unresolved resonance range.
URRFIT: Extrapolate cross section moments from resolved resonance range to unresolved resonance range to define self-shielding and 2 band parameters.
MERGER: Retrieve or combine evaluated data. It is required to insert unresolved self-shielding data using extended ENDF/B format sections MF2/MT152 and MF2/MT153 into an ENDF-formatted tape as required by DOACE.
LEGEND: Check and convert Legendre coefficients and tabulated distribution into linearly interpolable tables (MF4) as required by DOACE.
SPECTRA: Convert model and general tabulated data into linearly interpolable spectra (MF5) as required by DOACE.
SIXLIN: Convert and prepare linearly interpolable tabulated energy-angle distributions from ENDF-formatted file MF6 as required by DOACE.
DICTIN: Update reaction dictionary (MF1/MT451).
DOACE: Prepare continuous energy ACE-formatted files for Monte Carlo calculations.
The package ACEMAKER includes the codes SIXLIN and DOACE, the URR-PACK contains URRFIT and the rest of modules belongs to the code package PREPRO.
The description of methods and input options of PREPRO and URR-PACK modules are presented in references [5] and [7] respectively. The main features and inputs options for SIXLIN and DOACE are given in the following sections.

3. Code package name

The code package name is ACEMAKER. It consists of two codes: SIXLIN and DOACE. The codes are written in FORTRAN language.

4. Purpose of ACEMAKER

The purpose of the ACEMAKER code package is to generate continuous energy ACE formatted files for Monte Carlo calculations from evaluated nuclear data files in ENDF/B format preprocessed by the PREPRO package.

The ACEMAKER package contains two codes:

1. SIXLIN: To prepare linearly interpolable tabulated energy-angle distributions from ENDF-formatted file MF6.
2. DOACE: To prepare continuous energy ACE-formatted files for Monte Carlo calculations.

5. Functionalities of ACEMAKER

5.1. SIXLIN code

The code SIXLIN prepares tabulated linearly interpolable energy-angle distribution from ENDF-formatted MF6 file, which is provided to represent the distribution of reaction products in energy and angle. The use of MF6 is recommended when the energy and angular distributions of the outgoing particles are coupled or when so many reaction channels are open that it is difficult to provide separate reactions. Different representations (LAWs) are available [6]:

Table 1: Representation of the distribution function on MF6.

LAW	Description
0	Unknown distribution
1	Continuum energy-angle distribution: LANG=1: Legendre coefficients LANG=2: Kalbach-Mann systematics LANG=11-15: Tabulated angular distribution with (LANG - 10) interpolation scheme
2	Two-body reaction angular distributions
3	Isotropic-two-body distribution
4	Recoil distribution of a two-body reaction
5	Charged-particle elastic scattering
6	n-body phase-space distribution
7	Laboratory angle-energy distribution

SIXLIN converts continuum energy-angle distribution given by Legendre coefficients (LAW=1/LANG=1) and laboratory angle-energy distribution (LAW=7) to continuum energy-angle distribution given by linearly interpolable tabulated data (LAW=1/LANG=11or12). Additionally, SIXLIN linearizes continuum energy-angle distribution given by Kalbach-Mann systematics or by non-linearly interpolable tabulated data (LANG≠12). Table 2 shows the representations that can be found on MF6 file after SIXLIN preprocessing:

Table 2: Representation of the distribution function on MF6 file after SIXLIN preprocessing.

LAW	Description
0	Unknown distribution
1	Continuum energy-angle distribution: (LEP=1 or LEP=2) LANG=2: Kalbach-Mann systematics LANG 11 = constant interpolable angular distribution LANG=12: linearly interpolable tabulated angular distribution
2	Two-body reaction angular distributions
3	Isotropic-two-body distribution
4	Recoil distribution of a two-body reaction
5	Charged-particle elastic scattering
6	n-body phase-space distribution

SIXLIN copies all the data from the input ENDF-formatted tape to the output tape with the exceptions of MF1 and MF6 files. Most of the data on MF1 are also copied to the output tape, but three lines of text are added at the end of the descriptive records (HSUB) to document the work performed by SIXLIN. No attempt is made to update the directory records, if it is required, code DICTIN from the PREPRO pre-processing package can be used for this purpose.

The code SIXLIN only processes MF6 file data. For LAW=0, 2, 3, 4, 5 and 6 the data are copied without any change to output tape. In case of LAW=1 and LAW=7 the data are converted and linearized as described above.

The methods and procedures used for linearizing data are described in Ref. [9]. The code requires the maximum tolerance allowed for linearization, which is read as input data.

In order to convert Legendre coefficient data (LAW=1/LANG=1) to linearly interpolable tables, first tabulated data is generated in a very dense grid and then a thinning procedure is applied to obtain a linearly interpolable tabulated energy-angle distribution.

The SIXLIN output tape contains all the original data in ENDF/B format with the data converted and linearized on MF6, ready to be used by DOACE code.

5.2. DOACE code

The code DOACE is used to prepare continuous energy ACE-formatted files for Monte Carlo calculations starting from ENDF-formatted evaluated nuclear data files. The input evaluated nuclear data file should be previously processed according to the sequence shown on Figure 1. Cross sections and fission neutron yields should be represented as linearly interpolable tabulated data. Cross section data should be Doppler broadened to the working temperature. The cross section should be given on a unified energy grid and summation cross sections should be consistent with partial components. If required, the self-shielding in the unresolved resonance range should be included into the special

sections MF2/MT152 and MF2/MT153. Angular distributions from MF4 and energy distributions from MF5 should be given as linearly interpolable tables, and energy-angle distribution from MF6 should also be linearized. On MF6, file data for Legendre coefficients (LAW=1/LANG=1) and laboratory angle-energy (LAW=7) are not allowed. For continuum energy-angle distribution just LAW=1/LANG=2, 11 or 12 are expected.

Summarizing, the code DOACE is a formatting converter code to generate a continuous energy ACE-formatted file from an ENDF-formatted evaluated data file, previously processed by PREPRO, URR-PACK and SIXLIN modules (Figure 1).

The ACE format stands for "a Compact ENDF" for the MCNP code and is also used by other continuous-energy Monte Carlo codes (e.g. SERPENT). The ACE format applies to several different classes of data, but this version of the code DOACE just prepares continuous-energy neutron data, excluding thermal scattering law data.

A detailed description of the ACE format can be found in Refs [8] and [10]. Here, a brief description is presented for the sake of completeness. There are Type 1 (text/ASCII) and Type 2 (binary) ACE formatted libraries. DOACE only produces Type 1 data files. Conversion to binary should be performed by using a utility program.

Three main arrays are associated with each ACE formatted data table. The NXS array contains various counters and flags, The JXS array contains pointers and the XSS array contains all the data. The array XSS is divided into data blocks. Continuous–energy neutron transport tables contain the following blocks:

1. ESZ: Contains the main energy grid and the total, absorption and elastic cross sections as well as the average heating numbers. The ESZ block always exists.
2. NU: Contains prompt, delayed and/or total fission neutron yields as a function of incident energy. The NU block exists only for fissionable materials.
3. MTR: Contains a list of ENDF/B format MT numbers for all neutron reactions other than elastic scattering. The MTR block exists for all materials that have reactions other than elastic.
4. LQR: Contains a list of kinematic Q-values for all neutron reactions other than elastic scattering. The LQR block exists for all materials that have reactions other than elastic.
5. TYR: Contains general information about the reaction type of a reaction for all neutron reactions other than elastic scattering. It includes the number of secondary neutrons and whether the secondary neutron angular distributions are in the laboratory or center-of-mass reference system. The TYR block exists for all materials that have reactions other than elastic.
6. LSIG: Contains a list of cross-section locators for all neutron reactions other than elastic scattering. The LSIG block exists for all materials that have reactions other than elastic.

7. SIG: Contains cross sections for all reactions other than scattering. The SIG block exists for all materials that have reactions other than elastic.
8. LAND: Contains a list of angular-distributions locators for all reactions producing secondary neutrons. The LAND block always exists.
9. AND: Contains angular distributions for all reactions producing secondary neutrons. The AND block always exists.
10. LDLW: Contains a list of energy-distribution locators for all reactions producing secondary neutrons except for elastic scattering. The LDLW block exists for all materials that have reactions producing secondary neutrons other than elastic.
11. DLW: Contains energy distributions for all reactions producing secondary neutrons except for elastic scattering. The DLW block exists for all materials that have reactions producing secondary neutrons other than elastic.
12. GPD: Contains the total photon production cross section tabulated on the ESZ energy grid and a 30x20 matrix of secondary photon energies. The GPD block exists only for those older evaluations that provide coupled neutron/photon information.
13. MTRP: Contains a list of MT numbers for all photon production reactions (neutron in – photon out). The MTRP block exists if there are photon production reactions.
14. LSIGP: Contains a list of cross-section locators for all photon production reactions. The LSIGP block exists if there are photon production reactions.
15. SIGP: Contains cross-sections for all photon production reactions. The SIGP block exists if there are photon production reactions.
16. LANDP: Contains a list of angular-distribution locators for all photon production reactions. The LANDP block exists if there are photon production reactions.
17. ANDP: Contains photon angular distributions for all photon production reactions. The ANDP block exists if there are photon production reactions.
18. LDLWP: Contains a list of energy-distribution locators for all photon production reactions. The LDLWP block exists if there are photon production reactions.
19. DLWP: Contains energy-distribution for all photon production reactions. The DLWP block exists if there are photon production reactions.
20. YP: Contains a list of MT identifiers of neutron reaction cross sections required as photon production yield multipliers. The YP block exists if there are photon production reactions.
21. FIS: Contains the total fission cross section tabulated on the ESZ energy grid. The FIS block exists if the material is fissionable and JXS(21)≠0.
22. UNR: Contains the unresolved resonance range probability tables. The UNR block exists if self-shielding data in the unresolved resonance energy range are available, JXS(23)≠0.

The blocks ESZ, NU, MTR, LQR, TYR, LSIG, SIG, LAND, AND, LDLW, DLW, FIS and UNR are enough for neutron transport calculations. The current version of DOACE (July 2017) only prepares ACE-formatted data for neutron transport.

The energy grid of ESZ block is copied from the energy grid of the total cross section. The use of FIXUP guarantees that all cross sections are using the same energy grid. The main cross sections of ESZ block are simply prepared from the linearly interpolable tabulated data on MF3 file.

The NU block is prepared from MF1/MT=452,455 and 456. Data is given as linearly interpolable tables.

The MTR, LQR, LSIG and SIG blocks are basically prepared from MF3 files, where all cross section data have been previously linearized.

The TYR block is prepared from file MF3 and the general description of outgoing secondary neutrons from files MF4, MF5 and MF6.

Reactions like elastic scattering and discrete level inelastic scattering (two body scattering) are completely described by their reaction cross sections, Q-values and angular distributions in the center-of-mass system (CM). For these reactions the angular distributions are obtained from MF4 and are then converted into cumulative density functions (CDF) and the corresponding probability density functions (PDF) as a function of the scattering cosine (LAW=4 for scattering cosine [10]). The CDF and PDF functions versus cosine values are stored in the AND block using a set of pointers stored in the LAND block.

Uncorrelated energy distributions are stored in the DLW block using an appropriated set of pointers stored in the LDLW block. The data are taken from MF5 file and are converted into a cumulative density function (CDF) and the corresponding probability density function (PDF) as a function of secondary energy (LAW=4 for secondary energy [10]).

Correlated energy-angle distributions are also stored in the DLW and LDLW blocks from evaluated nuclear data presented on MF6 file using different representations:

1. Kalbach-Mann continuum energy-angle distribution (ENDF-LAW=1/LANG=2) is represented by LAW=44, which is an extension of LAW=4 (Refs [8], [10]). For each incident energy (E_i), there is a pointer to a table of secondary energies ($E'_{i,k}$), probability density function ($PDF_{i,k}$), cumulative density function ($CDF_{i,k}$), pre-compound fractions ($r_{i,k}$) and angular distribution slope values ($a_{i,k}$). Unlike, LAW=4, LAW=44 includes a correlated angular distribution associated with each incident energy E_i as given by the Kalbach-Mann parameters $r_{i,k}$ and $a_{i,k}$.
2. Tabulated continuum energy-angle distribution (ENDF-LAW=1/LANG=11 or 12) is represented by LAW=61 (Refs [8], [10]), which is also an extension of LAW=4. For each incident energy (E_i), there is a pointer to a table of secondary energies ($E'_{i,k}$), probability density function ($PDF_{i,k}$), cumulative density function ($CDF_{i,k}$), and pointers to tabulated angular distributions $L_{i,k}$. Unlike LAW=4, LAW=61 includes a correlated angular distribution associated with each incident energy E_i as given by the angular distribution located using pointers $L_{i,k}$. Therefore, the sampled emission angle depends on the sampled emission energy. If the secondary distribution is given using histogram interpolation, the angular distribution located at $L_{i,k}$ is used to

sample the emission angle. If the secondary distribution is specified as linear interpolation between energy points, $L_{i,k}$ is chosen by selecting the bin closest to the randomly sampled cumulative distribution function (CDF) point. If $L_{i,k}=0$, the angle is sample from an isotropic distribution.

3. N-body phase space distribution (ENDF-LAW=6) is represented by LAW=66, where the data are read from MF6 file and conveniently stored in the DLW and LDLW blocks.

Given that code SIXLIN was used previously, laboratory angle-energy distribution (ENDF-LAW=7) was converted to energy-angle tabulated data (LAW=1).

DOACE takes advantage of previous linearization of MF6 data to prepare the cumulative density functions (CDF).

The FIS block is prepared from fission cross section data on MF3 file, if required.

The UNR block is prepared from evaluated data found on the MF2/MT152 and MF2/MT153 special sections, which were generated by GROUPIE/URRFIT/MERGER. The tables provide a cumulative density function versus total cross section values. The probability tables also include conditional probability distributions that give values for scattering, fission, capture and heating for each particular value of the total.

The main output of DOACE is a continuous-energy ACE-formatted file for neutron transport calculations using MCNP.

6. Input and output data for ACEMAKER package

6.1. SIXLIN input and output data

The input data for SIXLIN is read from the SIXLIN.INP input text file. Table 3 summaries SIXLIN input data and format.

Table 3: Input data description for SIXLIN

Line	Format	Data	Description
1	(2I11,E11.0)	ISEL, IMON, XSMIN	ISEL: MAT/ZA selection option ISEL=0, MAT number (default) ISEL=1, ZA number IMON: Printing option IMON=0, Minimum (default) IMON=1, Maximum YMIN: Minimum y-coordinate value for linearization. Default= $1x10^{-30}$ barn
2	(A72)	INPUTFILE	INPUTFILE: Input ENDF formatted file name. (Default: ENDFB.INP)
3	(A72)	OUTPUTFILE	OUTPUTFILE: Output ENDF formatted file name. (Default: ENDFB.OUT)
4	(2I11)	LLOWER, LUPPER	LLOWER: Lower MAT or ZA limit LUPPER: Upper MAT or ZA limit (Default: LLOWER=LUUPER=0) (First MAT or ZA found)
5	(E11.0)	TOLMAX	TOLMAX: Relative maximum tolerance for linearization. (Default: $1x10^{-2}$)

The output of SIXLIN is an evaluated nuclear data file with a pre-processed MF6 file. The default output file name is ENDFB.OUT. During SIXLIN running output messages are written depending on the value of IMON on the default output device, usually the console, which can be redirected to any file using the piping features of the operating system.

6.2. DOACE input and output data

The input data for DOACE is read from the DOACE.INP input text file. Table 4 summaries DOACE input data and format.

The output of DOACE is a continuous-energy ACE-formatted nuclear data file for MCNP calculations. The default output file name is ACE.OUT. During DOACE running output messages are written depending on the value of IMON on the default output device, usually the console, which can be redirected to any file using the piping features of the operating system.

Table 4: Input data description for DOACE

Line	Format	Data	Description
1	(2I11)	ISEL, IMON	ISEL: MAT/ZA selection option ISEL=0, MAT number (default) ISEL=1, ZA number IMON:Printing option IMON=0, Minimum (default) IMON=1, Maximum
2	(A72)	INPUTFILE	INPUTFILE: Input ENDF formatted file name. (Default: ENDFB.INP)
3	(A72)	OUTPUTFILE	OUTPUTFILE: Output ACE-formatted file name. (Default: ACE.OUT)
4	(2I11)	LLOWER, LUPPER	LLOWER: Lower MAT or ZA limit LUPPER: Upper MAT or ZA limit (Default: LLOWER=LUUPER=0) (First MAT or ZA found on input)
5	(A3)	IDSUFF	IDSUFF: ID suffix for ZAID (default=.00) The ZAID= 1000xZ+A+IDSUFF+c, for continuous-energy fast data. Example: U-235 and IDSUFF=.31 for fast data ZAID=92235.31c

7. Availability

The ACEMAKER package is distributed by the IAEA Nuclear Data Section on request. It is also freely available at its web page: http://www-nds.iaea.org.

8. Final comments and recommendations

The package code ACEMAKER has been developed as a complement to PREPRO and URR-PACK code systems for preparing continuous-energy ACE-formatted data files for neutron transport calculations using MCNP. The code package is freely available at IAEA Nuclear Data Section.

It is strongly recommended to continue the verification and validation process as part of the quality assurance program. An ACE-formatted library should be prepared to solve a set of well-known neutron transport benchmark problems.

Further development of the ACEMAKER system should include capabilities for processing photon, charge particle production, damage and heating cross section data.

9. References

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