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ACEMAKER-2.0

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

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Contents

| | |
|--|----|
| 1. Introduction..... | 1 |
| 2. Generating a continuous- energy fast ACE-formatted file using ACEMAKER..... | 2 |
| 3. Generating a thermal ACE-formatted file using ACEMAKER..... | 3 |
| 4. ACEMAKER code package description..... | 3 |
| 5. Purpose..... | 3 |
| 6. Functionalities of SIXLIN, DOACE, DOTSL and ACEMAKER..... | 3 |
| 6.1 SIXLIN code: Convert and linearize MF6 angle/energy distributions..... | 3 |
| 6.2 DOACE code: Prepare fast continuous energy ACE-formatted files..... | 5 |
| 6.3 DOTSL code: Prepare thermal ACE-formatted files..... | 8 |
| 6.4 ACEMAKER: driver module..... | 14 |
| 7. ACEMAKER input and output data by module..... | 15 |
| 7.1 SIXLIN input and output data..... | 15 |
| 7.2 DOACE input and output data..... | 15 |
| 7.3 DOTSL input and output data..... | 16 |
| 7.4 ACEMAKER input and output data..... | 18 |
| 8. Availability..... | 25 |
| 9. Final comments and recommendations..... | 25 |
| 10. References..... | 26 |
| Appendix A..... | 27 |
| Appendix B..... | 29 |

1. Introduction

Nuclear data processing covers the gap between evaluated nuclear data and end users. Over decades, the code package NJOY [1] has been extensively used to process data for applications. It is a very comprehensive package, which is 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 upgraded to version NJOY-2012 and more recently to NJOY-2016 and NJOY21

The methods and procedures of NJOY were continuously patched in a well-coordinated international effort, while the main physical and mathematical models were not essentially changed from the original ones. It is worth mentioning 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 well known from benchmark analysis that processing methods have an 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 offers an opportunity to carry out an intercomparison exercise between different processing methods and codes.

Furthermore, the PREPRO pre-processing code package by D.E. Cullen [5] is freely available for nuclear data processing. 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-6 format given on MF=4 and MF=5, respectively [6]. The code URRFIT from URR-PACK system [7] has made it possible to prepare self-shielded cross section data in the unresolved resonance region. This issue has been implemented in GROUPIE-2019 as a regular option in the PREPRO-2019 package [5].

It was considered worthwhile to develop a code package to extend the capabilities of PREPRO-2019, with the goal of preparing nuclear data in ACE-format for Monte Carlo calculations. The package has been named ACEMAKER. It includes four new modules to generate continuous-energy fast and thermal ACE-formatted files for Monte Carlo simulations.

The ACEMAKER-2.0 package can prepare fast-continuous energy and thermal ACE-formatted files for Monte Carlo calculations from evaluated data in ENDF-6 format. Compared to version 1.0, this version contains some coding improvements for the generation of the fast-continuous energy ACE-formatted files and includes the option for processing the thermal scattering law data in MF7 to produce a thermal ACE-formatted file.

This report summarizes the main features and input data needed for ACEMAKER 2.0 and describes how to use the driver module to prepare nuclear data in ACE-format for MCNP [8] calculations.

2. Generating a continuous- energy fast ACE-formatted file using ACEMAKER

The ACEMAKER driver module calls the following codes from the packages PREPRO-2019 and ACEMAKER to produce a continuous-energy fast ACE-formatted file for Monte Carlo calculations (Fig. 1):

FIG. 1: Main processing flow for fast ACE-formatted files



- LINEAR:** Linearize cross section data as required for the rest of the modules.
- RECENT:** Reconstruct cross section from resonance parameters.
- 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.
- SIGMA1:** Doppler broadens 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-shielded data, two band parameters and probability tables (PTAB) to use in the unresolved resonance range (URR).
- MERGER:** Retrieve or combine evaluated data. It is required to insert unresolved self-shielded data (extended sections MF2/MT152 and MF2/MT153) into an ENDF-formatted tape as required by DOACE.
- DICTIN:** Update reaction dictionary (MF1/MT451).
- DOACE:** Prepare fast continuous energy ACE-formatted files for Monte Carlo calculations for neutrons.

The codes LINEAR, RECENT, LEGEND, SPECTRA, SIGMA1, FIXUP, GROUPIE, MERGER and DICTIN belong to the PREPRO-2019 package. The modules SIXLIN and DOACE are part of the ACEMAKER package, which also includes the driver program ACEMAKER.

The above-mentioned PREPRO-2019 modules are distributed with the ACEMAKER package because the current version of ACEMAKER (version 2.0) has been developed to work with the 2019 version of PREPRO. The use of a different version of PREPRO does not guarantee a correct coupling of two packages.

The PREPRO-2019 methods and input options are presented in Ref. [5]. The method for treating the self-shielding effect in the unresolved resonance region is described in Ref. [7]. The main features and input options for the ACEMAKER package are briefly explained later in this report.

3. Generating a thermal ACE-formatted file using ACEMAKER

The ACEMAKER package uses the module DOTSL for processing the thermal scattering data available in MF7 of the ENDF-6 formatted evaluated nuclear data. The driver code calls the modules MERGER and DOTSL for generating a thermal ACE-formatted file to be used in Monte Carlo simulations. The DOTSL code can also be used in stand-alone mode for processing the thermal scattering law of one material at one temperature at a time, because it does not require any pre-processing task. The use of the DOTSL module in the ACEMAKER framework allows the processing of multiple materials and temperatures in a single ACEMAKER run. The main features of DOTSL are described in Section 6.3.

4. ACEMAKER code package description

The ACEMAKER package includes the codes SIXLIN, DOACE, DOTSL and the driver code ACEMAKER.

5. Purpose

The purpose of the ACEMAKER code package is to generate continuous energy (fast) and thermal ACE formatted files for Monte Carlo calculations from evaluated nuclear data files in ENDF-6 format.

6. Functionalities of SIXLIN, DOACE, DOTSL and ACEMAKER

6.1. SIXLIN code: Convert and linearize MF6 angle/energy distributions

The SIXLIN code prepares tabulated linearly interpolable energy-angle distribution from the 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. Table 1 presents the different representations (LAWs) available for MF6 in the ENDF-6 format [6].

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=11 or 12). 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 in the MF6 file after SIXLIN processing.

TABLE 1: REPRESENTATION OF THE DISTRIBUTION FUNCTION I THE N MF6 FILE

| 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 |

TABLE 2: REPRESENTATION OF THE DISTRIBUTION FUNCTION ON MF6 FILE AFTER SIXLIN PROCESSING

| 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 |

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

The code SIXLIN only processes MF6 file data. Data for LAW=0, 2, 3, 4, 5 and 6 are copied without any change to the 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 are generated in a very dense grid and then a thinning procedure is applied to obtain a linearly interpolable tabulated energy-angle distribution within the requested tolerance.

The SIXLIN output tape contains all the original data in ENDF-6 format with the data converted and linearized in MF6, ready to be used by the DOACE code.

6.2. DOACE code: Prepare fast continuous energy ACE-formatted files

The DOACE code is used to prepare continuous energy ACE-formatted files for Monte Carlo calculations starting from ENDF-formatted evaluated nuclear data files in ENDF-6 format. The input evaluated nuclear data file should be previously processed according to the sequence shown in Fig. 1 above. 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 section 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. In the 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 format converter code to generate a continuous energy ACE-formatted file from an ENDF-formatted evaluated data file, previously processed by PREPRO-2019 modules and SIXLIN.

The ACE format stands for “a Compact ENDF” used by MCNP and others continuous-energy Monte Carlo codes (e.g. SERPENT). The ACE format applies to several different classes of data, but this version of the DOACE code just prepares fast continuous-energy data for incident neutrons.

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

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 XSS array 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 with 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 with 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 information on the reference system (laboratory or center-of-mass). The TYR block exists for all materials with 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 with reactions other than elastic.
7. SIG: Contains cross sections for all reactions other than scattering. The SIG block exists for all materials with 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 with 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 with 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 in case of photon production reactions.
14. LSIGP: Contains a list of cross-section locators for all photon production reactions. The LSIGP block exists in case of photon production reactions.
15. SIGP: Contains cross-sections for all photon production reactions. The SIGP block exists in case of photon production reactions.
16. LANDP: Contains a list of angular-distribution locators for all photon production reactions. The LANDP block exists in case of photon production reactions.
17. ANDP: Contains photon angular distributions for all photon production reactions. The ANDP block exists in case of photon production reactions.
18. LDLWP: Contains a list of energy-distribution locators for all photon production reactions. The LDLWP block exists in case of photon production reactions.
19. DLWP: Contains energy-distribution for all photon production reactions. The DLWP block exists in case of photon production reactions.

20. YP: Contains a list of MT identifiers of neutron reaction cross sections required as multipliers for photon production calculation. The YP block exists in case of 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 $JXS(21) \neq 0$.
22. UNR: Contains the probability tables in the unresolved resonance range. The UNR block exists if self-shielding data in the unresolved resonance energy range are available, $JXS(23) \neq 0$.

The blocks ESZ, NU, MTR, LQR, TYR, LSIG, SIG, LAND, AND, LDLW, DLW, FIS and UNR are sufficient for neutron transport calculations.

The energy grid of the 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 the ESZ block are simply prepared from the linearly interpolable tabulated data in the 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 the MF3 file, 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 the 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 in the MF6 file using different representations:

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

The SIXLIN code previously converted any occurrence of the LAW-7 for describing the angle/energy distribution into the LAW-1 in the MF6 file.

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 in the MF3 file, if required.

The UNR block is prepared from evaluated data found in the MF2/MT153 special section, which were generated by GROUPIE-2019 using the two-band approach. 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 value of the total.

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

6.3. DOTSL code: Prepare thermal ACE-formatted files

The DOTSL module prepares a thermal ACE-formatted file from the thermal scattering law stored in MF7 of the ENDF-6 formatted evaluated nuclear data file. The code processes and formats the evaluated data without calling any other module.

The ACE-format for the thermal scattering law is described in Refs [10, 11]. Here, a brief description is given for the sake of completeness. The ACE-format provides a comprehensive representation of thermal neutron scattering by molecules and crystalline solids. Cross sections and energy/angle data are included in the ACE-tables. For the time being four blocks of data are associated with the thermal scattering law:

1. ITIE block – contains the inelastic thermal scattering cross section as a function of incident energy. The ITIE block always exists.
2. ITCE block – contains the elastic thermal cross section data as a function of incident energy. This block exists in case the material has coherent or incoherent elastic scattering.
3. ITXE Block – contains the coupled energy/angle distribution for the inelastic thermal scattering. The ITXE block always exists.
4. ITCA Block – contains angular distribution for thermal elastic scattering. This block exists if the material has incoherent elastic scattering. For the coherent elastic scattering no angular data are required, because the angular distribution is completely defined by the kinematics and can be easily calculated from the data contained in the ITCE block.

Currently it is assumed that a material always has inelastic thermal scattering and could additionally have incoherent or coherent elastic scattering, but not both. Recently, it has been shown that some materials such as LiH and LiD exhibit both coherent and incoherent elastic scattering in the thermal energy range, therefore a mixed elastic scattering format has been proposed [12].

The DOTSL code is able to both read and process this new mixed format. It saves the data for the incoherent elastic scattering in the ITCE and ITCA blocks and adds a JTCE block for the coherent elastic cross section data. Angular tabulated data are not needed for the coherent elastic scattering as mentioned above.

The ITCE (JTCE) block for the coherent elastic scattering stores the strength function $S(E_i, T)$ at the Bragg edge energies E_i . For the incoherent elastic cross section, the ITCE block contains the incoherent elastic cross section as a function of incident energy E .

In general, the ITXE block for the angle/energy distribution can have three representations, but the DOTSL code only prepares the continuous secondary energy representation (IWT=2 for NJOY). The distribution of outgoing energies for each incident energy is continuous in energy and specified by a probability density function (PDF) and a cumulative distribution function (CDF). The number of outgoing energies for each incident energy is allowed to vary, however, the number of equiprobable cosines should be the same for each combination of incident and outgoing energies. Therefore, for each pair (E_{in}, E_{out}) , the values of the PDF, CDF and N_u equiprobable cosines are stored in the ITXE block.

For the incoherent elastic scattering for each incident energy given in the ITCE block, N_u equiprobable cosines are given in the ITCA block.

Linear-linear interpolation is assumed between adjacent values for all blocks. The DOTSL code sets the following triggers (NXS) and pointers (JXS) for directly accessing the thermal scattering data:

- a. NXS(1)=len2: Length of second block of data (XSS array on the ACE-formatted file)
- b. NXS(2)=IDPNI: Inelastic scattering mode (IDPNI=3)
- c. NXS(3)=NIL: Inelastic angular dimensioning parameter (NIL=NBIN+1)
- d. NXS(4)=NIEB: Number of inelastic exiting energies (NIEB=NBIN for IFENG=2)
- e. NXS(5)=IDPNC: Elastic scattering mode (incoherent=3, coherent=4, mixed=5)

- f. NXS(6)=NCL: Elastic angular dimensioning parameter
(NCL=NBIN-1 for incoherent elastic and NCL=-1 for coherent elastic)
- g. NXS(7)=IFENG: Secondary energy mode (IFENG=2 continuous)
- h. JXS(1)=ITIE: Pointer to inelastic energy table
- i. JXS(2)=ITIX: Pointer to inelastic cross sections
- j. JXS(3)=ITXE: Pointer to inelastic angle/energy distribution
- k. JXS(4)=ITCE: Pointer to elastic energy table
- l. JXS(5)=ITCX: Pointer to elastic cross section data
- m. JXS(6)=ITCA: Pointer to elastic angular distribution

If mixed thermal scattering law is specified, then ITCE, ITCX and ITCA are used for the incoherent elastic scattering and the following two pointers are set for the coherent elastic scattering:

- n. JXS(7)=JTCE: Pointer to coherent elastic energy table
- o. JXS(8)=JTCX: Pointer to coherent elastic cross section data

NBIN represents the number of equiprobable cosines requested by input.

Evaluated nuclear data formats and procedures for thermal scattering law processing are presented in Ref. [6]. The ITIE and ITXE blocks for the inelastic thermal scattering are prepared from the evaluated nuclear data given in the MF7/MT4 section, which contains all the information needed about the thermal scattering law $S(\alpha, \beta, T)$. The double differential inelastic cross section $\sigma_{ine}(E \rightarrow E', \mu, T)$ at temperature T for the main atom can be calculated as:

$$\sigma_{ine}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} e^{-\frac{\beta}{2}} S(\alpha, \beta, T) \quad (1)$$

where E is the incident neutron energy, E' is the outgoing energy of the scattered neutron, μ is the scattering cosine in the laboratory system, σ_b is the characteristic bound inelastic cross section for the nuclide, T is the temperature in Kelvin, β is the dimensionless energy transfer and α is the dimensionless momentum transfer given by:

$$\beta = \frac{E' - E}{kT} \quad (2)$$

$$\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{AkT} \quad (3)$$

k is the Boltzmann's constant and A is the ratio of the scatter mass to neutron mass (AWR). The bound cross section can be calculated from the characteristic free gas cross section σ_f as:

$$\sigma_b = \sigma_f \left(\frac{A+1}{A} \right)^2 \quad (4)$$

The thermal scattering law $S(\alpha, \beta, T)$ describes the binding of the scattering atom in a material and is tabulated as a function of α , β and T in MF7/MT4. The values of $S(\alpha, \beta, T)$ are calculated by interpolation in the α , β space at a given temperature. If the values of α or β are outside the range of the table, the differential scattering cross section can be computed using the short collision time (SCT) approximation

$$\sigma_{ine}^{SCT}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} \left(4\pi\alpha \frac{T_{eff}}{T}\right)^{-\frac{1}{2}} e^{-\frac{(\alpha-|\beta|)^2 T_{eff}}{4\alpha T} - \frac{\beta+|\beta|}{2}} \quad (5)$$

where T_{eff} is the effective temperature for the SCT approximation, which is included in the evaluated nuclear data file in MF7/MT4.

DOTSL expects the requested temperature T to be one of the temperatures included in the MF7/MT4 section. The intermediate temperature should be obtained by interpolating between cross sections and not by interpolating $S(\alpha, \beta, T)$. This task is not performed by DOTSL.

The following steps are completed for preparing the ITIE and ITXE blocks at the requested temperature T :

1. The generation of the incident energy (E) grid: DOTSL generates an incident energy grid in such a way that a cross section that follows a “1/E” behavior can be linearly interpolated between energies within a fractional tolerance TOLE, entered as input. It guarantees smoother dependencies like the “1/v” behavior of inelastic cross section at low thermal energies and the constant behavior at high thermal energies (4 – 10 eV). Additionally, the up-scattering energy distribution $\sigma_{ine}(E \rightarrow E')$ of a free gas follows a “1/E” behavior. For an input tolerance of 0.003, the incident energy grid contains around 130 points. If the fractional tolerance is reduced to 0.001, then the number of points increases up to 215. The analysis of a selected set of benchmarks has shown that this approach produces good results applying fractional tolerances of, or smaller than 0.003 even for oscillating thermal cross sections as in the case of H bound in ZrH. The fractional tolerance TOLE is up to the user. This grid is used to tabulate the integral inelastic cross section $\sigma_{ine}(E)$ in the ITIE block.
2. The adaptive generation of the outgoing energy grid to give $PDF(E, E')$, $CDF(E, E')$ and N_u equiprobable cosines $\bar{\mu}_i^{ine}(E, E')$: DOTSL prepares for each incident energy an initial outgoing energy grid starting from the values of β given by the evaluation of $S(\alpha, \beta)$, with the restriction $E' \geq 0.0 \text{ eV}$. Then, each E' interval is further subdivided by successive halving until the value of $\sigma_{ine}(E \rightarrow E')$ and the angular distribution given by N_u equiprobable cosines are linearly interpolable within the tolerance TOL, entered as input parameter. This procedure guarantees a good description of the entire structure considered in the evaluation. Once the outgoing energy grid has constructed the inelastic cross section ($\sigma_{ine}(E)$) is calculating by integration of $\sigma_{ine}(E \rightarrow E')$, using the trapezoid rule.
3. The adaptive generation of the cosine grid to calculate $\sigma_{ine}(E \rightarrow E')$ and the N_u equiprobable cosines: DOTSL adaptively constructs a cosine grid to calculate the integrals needed to find $\sigma_{ine}(E \rightarrow E')$ and $\bar{\mu}_i^{ine}(E, E')$. In this case, an initial cosine grid is prepared for each value of the incident energy (E) and the outgoing energy (E'), starting from the values of α given by the evaluation of $S(\alpha, \beta)$, considering the restriction $-1.0 \leq \mu \leq 1.0$. Then, as before, each μ interval is subdivided by successive halving until the energy angular distribution $\sigma_{ine}(E \rightarrow E', \mu)$ is linearly interpolable to within a specified tolerance. After that, the values of $\sigma_{ine}(E \rightarrow E')$ and $\bar{\mu}_i^{ine}(E, E')$ are obtained by integration:

$$\sigma_{ine}(E \rightarrow E') = \int_{-1}^1 \sigma_{ine}(E \rightarrow E', \mu) d\mu \quad (6)$$

$$\bar{\mu}_i^{ine}(E, E') = \frac{\int_{\mu_i}^{\mu_{i+1}} \mu \sigma_{ine}(E \rightarrow E', \mu) d\mu}{\int_{\mu_i}^{\mu_{i+1}} \sigma_{ine}(E \rightarrow E', \mu) d\mu} = N_u \frac{\int_{\mu_i}^{\mu_{i+1}} \mu \sigma_{ine}(E \rightarrow E', \mu) d\mu}{\sigma_{ine}(E \rightarrow E')} \quad (7)$$

where μ_i and μ_{i+1} are the lower and upper boundaries of the cosine interval i that fulfill the condition:

$$\int_{\mu_i}^{\mu_{i+1}} \sigma_{ine}(E \rightarrow E', \mu) d\mu = \frac{\sigma_{ine}(E \rightarrow E')}{N_u} \quad (8)$$

and $i = 1, 2, 3, \dots, N_u$

Due to the fact that $\sigma_{ine}(E \rightarrow E', \mu)$ is linearly interpolable in μ , the integrals can be solved analytically.

4. Preparation of the ITIE and ITXE blocks: $PDF(E, E')$ and $CDF(E, E')$ are finally calculated as:

$$PDF(E, E') = \frac{\sigma_{ine}(E \rightarrow E')}{\sigma_{ine}(E)} \quad (9)$$

$$CDF(E, E') = \int_0^{E'} PDF(E, E'') dE'' = \frac{1}{\sigma_{ine}(E)} \int_0^{E'} \sigma_{ine}(E \rightarrow E'') dE'' \quad (10)$$

A thinning process is applied to reduce the number of outgoing energies for each incident energy. The selection criteria applied are:

$$CDF(E, E'_{i+1}) - CDF(E, E'_i) \geq 0.000001 \quad (11)$$

$$\left[\frac{1}{N_u} \sum_{i=1}^{NBIN} \mu_i(E, E'_{i+1}) - \frac{1}{N_u} \sum_{i=1}^{NBIN} \mu_i(E, E'_i) \right] \geq 0.0075 \quad (12)$$

It means that from the original outgoing energy grid the energy E'_{i+1} is not rejected if either of the conditions (11) or (12) is satisfied. The lower (first) outgoing energy is selected using criterion (11), then the next one is the first E' that satisfies inequality (11) or (12) and the same procedure applies successively. This thinning procedure mainly affects the edges of the cumulative distribution.

The inelastic cross section $\sigma_{ine}(E)$ and the coupled energy/angle distribution are saved in the ITCE and ITXE blocks, respectively.

The preparation of the ITCE and ITCA blocks depends on the representation of the thermal elastic scattering ($E=E'$). If the elastic scattering shows an incoherent component, then the differential cross section is given by:

$$\sigma_{ela}^{inc}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2} e^{-2EW'(T)(1-\mu)} \delta(E - E') \quad (13)$$

where:

σ_b is the characteristic bound cross section [barns]

W' is the Debye-Waller integral divided by atomic mass [eV^{-1}]

and all the other symbols have the same meaning as above. The values of σ_b and W' can be obtained from MF7/MT2 of an ENDF-6 formatted evaluation. The integral incoherent elastic cross section $\sigma_{ela}^{inc}(E)$ and the equally probable cosines $\bar{\mu}_i^{inc}(E)$ are analytically obtained by:

$$\sigma_{ela}^{inc}(E) = \frac{\sigma_b}{2} \left(\frac{1 - e^{-4W'E}}{2EW'} \right) \quad (14)$$

$$\mu_i^{inc}(E) = 1 + \frac{1}{2W'E} \ln \left\{ \frac{1 - e^{-4W'E}}{N_u} + e^{-2W'E[1 - \mu_{i-1}^{inc}(E)]} \right\} \quad (15)$$

$$\bar{\mu}_i^{inc}(E) = \frac{N_u}{2W'E} \left\{ \frac{[2W'E \mu_i^{inc}(E) - 1] e^{-2W'E[1 - \mu_i^{inc}(E)]} - [2W'E \mu_{i-1}^{inc}(E) - 1] e^{-2W'E[1 - \mu_{i-1}^{inc}(E)]}}{1 - e^{-4W'E}} \right\} \quad (16)$$

where $\mu_i^{inc}(E)$ represents the upper boundary of the equally probable interval i with $i = 1, 2, 3, \dots, N_u$ and $\mu_0^{inc}(E) = -1$.

The incident energy grid of the inelastic scattering is used to compute $\sigma_{ela}^{inc}(E)$, the incoherent elastic cross section, and the $\bar{\mu}_i^{inc}(E)$ equally probable cosines and the values are stored in the ITCE and ITCA blocks.

In case that the elastic scattering has a coherent component, the coherent elastic differential cross-section $\sigma_{ela}^{coh}(E \rightarrow E', \mu, T)$ can be expressed as:

$$\sigma_{ela}^{coh}(E \rightarrow E', \mu, T) = \frac{1}{E} \sum_{i=1}^{E_i \leq E} s(E_i, T) \delta[\mu - \mu_{ela_i}^{coh}(E)] \delta(E - E') \quad (17)$$

where:

$$\mu_{ela_i}^{coh}(E) = 1 - \frac{2E_i}{E} \quad (18)$$

E_i : Energies of the Bragg edges [eV]

$s(E_i, T)$: Intensity, magnitude proportional to the structure factors [eV.barns]

$\mu_{ela_i}^{coh}(E)$: Characteristic scattering cosines for each set of lattice planes

and the rest of the symbols have the same meaning as above.

The integral coherent elastic section-section can be computed as:

$$\sigma_{ela}^{coh}(E, T) = \frac{S(E, T)}{E} \quad (19)$$

where:

$$S(E, T) = \sum_{i=1}^{E_i \leq E} s(E_i, T) \quad (20)$$

is the cumulative intensity.

The cumulative intensity $S(E, T)$ is given in MF7/MT2 of an ENDF-6 formatted evaluation, which is conveniently represented as stair step function with breaks at the Bragg edge energies using histogram interpolation (INT=1).

If coherent elastic scattering is present, then DOTSL reads the cumulative intensity function $S(E, T)$ at the energies of Bragg edges from MF7/MT2, removes any duplicated value and stores the data in the ITCE block for the pure coherent scatter and in the JTCE block for the mixed thermal scattering law. The angular distribution is not required in this case. If the material is a pure coherent scatter, then additionally NCL is set to -1.

6.4. ACEMAKER: driver module

The ACEMAKER module drives the main calculation flow. It reads the user input options and prepares the necessary input files for all modules that have to be called to produce the ACE-formatted file.

The driver code invokes the calculation sequence presented in Fig. 1 for fast ACE-formatted files or the modules MERGER and DOTSL for preparing thermal ACE-formatted files. An external loop over each case found on the ACEMAKER input file is the outermost cycle. Inside the case loop, the input options are read and setup. Then, an inner cycle is carried out for each material requested by the user in the input data file. If more than one temperature is demanded, an innermost cycle is executed for each temperature inside the material loop. ACEMAKER consistently manages the creation, forwarding and deletion of the data files required for each invoked module.

The modules are called using the FORTRAN-77 standard subroutine *system*. The default path for the executable programs is the \ACEMAKER\exe\ subdirectory, but it could be changed creating the two-line text file *acemaker.cfg* on the working directory. The first line is the PREPRO-2019 full-path for modules MERGER, LINEAR, RECENT, LEGEND, SPECTRA, SIGMA1, FIXUP, DICTIN and GROUPIE. The second line specifies the subdirectory for the modules SIXLIN, DOACE, DOTSL and ACEMAKER. An example of the *acemaker.cfg* file is given in Fig. 2. The character ‘\’ (windows) or ‘/’ (linux) is compulsory at the end of the string as a part of the full path.

FIG. 2. Example of *acemaker.cfg*

```
D:\PREPRO19\  
D:\ACEMAKER\exe\
```

It is also possible to redefine full paths changing the values of the variables *preprod* and *acemakerd* in the corresponding DATA statement on the ACEMAKER main program and recompiling it.

7. ACEMAKER input and output data by module

7.1. SIXLIN input and output data

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

The output of SIXLIN is an evaluated nuclear data file with a processed MF6 file. 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.

TABLE 3: INPUT DATA DESCRIPTION FOR SIXLIN

| Line | Format | Data | Description |
|------|--------------|-------------------|---|
| 1 | (2I11,E11.0) | ISEL, IMON, XSMIN | <p>ISEL: MAT/ZA selection option ISEL=0, MAT number (default) ISEL=1, ZA number</p> <p>IMON: Printing option IMON=0, Minimum (default) IMON=1, Maximum</p> <p>YMIN: Minimum y-coordinate value for linearization. Default= $1.0 \cdot 10^{-30}$ barn</p> |
| 2 | (A72) | INPUTFILE | Input: Input ENDF formatted filename |
| 3 | (A72) | OUTPUTFILE | Output: Output ENDF formatted filename |
| 4 | (2I11) | ILOWER, IUPPER | <p>LLOWER: Lower MAT or ZA limit</p> <p>LUPPER: Upper MAT or ZA limit (Default: ILOWER=IUPPER=0) (First MAT or ZA found)</p> |
| 5 | (2E11.0) | TOLMAX, DXMU | <p>TOLMAX: Relative maximum fractional tolerance for linearization. (Default: 1×10^{-2})</p> <p>DXMU: Maximum value of a cosine interval ($\Delta\mu$) for linearization/reconstruction (Default: 1×10^{-3})</p> |

7.2. DOACE input and output data

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

The output of DOACE is a fast continuous-energy ACE-formatted nuclear data file for MCNP calculations. 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 | (3I11) | ISEL, IMON, MCNPX | ISEL: MAT/ZA selection option ISEL=0, MAT number (default) ISEL=1, ZA number IMON: Printing option IMON=0, Minimum (default) IMON=1, Maximum MCNPX: MCNP trigger MCNPX=0, MCNP (default) MCNPX=1, MCNPX |
| 2 | (A72) | INPUTFILE | Input: PENDF formatted file name |
| 3 | (A72) | OUTPUTFILE | Output: ACE-formatted file |
| 4 | (I11) | IMAT | IMAT: MAT or ZA Default: IMAT=0, it means first MAT found on the input PENDF file |
| 5 | (A4) | SUFF | ID suffix for ZAID on the ACE-file. It should start with a dot ('.'), followed by two digits (XX) for MCNPX=0 and three digits (XXX) for MCNPX=1. (Default: .00) |

7.3. DOTSL input and output data

The input data for DOTSL are read from the DOTSL.INP text file. Table 5 summaries DOTSL input data and formats.

The main output of DOTSL is a thermal ACE-formatted nuclear data file for MCNP calculations. During DOTSL 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. Additionally, the DOTSL.PTL and DOTSL.CUR files are prepared for plotting using PLOTTAB [13]. If DOTSL is used in the ACEMAKER framework, then the files DOTSL.PLT/DOTSL.CUR are renamed as THZAID.SUFFt.plt/THZAID.SUFFt.cur for MCNPX=0 or as THZAID.SUFFnt.plt/THZAIDnt.cur for MCNPX=1 respectively.

TABLE 5: INPUT DATA DESCRIPTION FOR DOTSL

| Line | Format | Data | Description |
|-------|--|--|---|
| 1 | A72 | INPUTFILE | Input: ENDF-formatted file name |
| 2 | A72 | OUTPUTFILE | Output: Thermal ACE-formatted file |
| 3 | I11 E11.0 I11 I11 | MAT TEMP NMIX IMON | MAT: Material number TEMP: Temperature in Kelvin NMIX: Number of atoms types in moderator material (Default =1) IMON: Monitor printing trigger IMON = 0 min. (Default) =1 max. =2 max.+plots |
| 4 | I11 E11.0 E11.0 E11.0 | NBIN ETHMAX TOL TOLE | NBIN: Number of equiprobable cosines for the inelastic and incoherent elastic scattering (Default=16) ETHMAX: Maximum energy for thermal treatment (Default = 4.0 eV) TOL: Fractional tolerance for linearization (Default = 0.001=0.1%) TOLE: Fractional tolerance for preparing incident energy grid (Default = 0.003 = 0.3%) |
| 5 | 5X,A6 7X,A4 I11 I11 | THZAID SUFF MCNPX NZA | THZAID: Thermal ZAID for thermal ACE-formatted file SUFF: ID suffix for ZAID on the ACE-file. It should start with a dot ('.'), followed by two digits (XX) for MCNPX=0 and three digits (XXX) for MCNPX=1. (Default: .00) MCNPX: Trigger to use extended ZAID for MCNPX. 0/1 = MCNP/MCNPX (Default=0) NZA: Number of moderator materials for which the TSL of material MAT is applicable (max. = 16) |
| 6 & 7 | 2(8I7) | (IZA(I),I=1,NZA) | IZA(I): ZA value of moderator material (component) I for which the TSL of material MAT is applicable, given in two lines, 8 values each |

7.4. ACEMAKER input and output data

The input options for running ACEMAKER should be entered on the *acemaker.inp* file. The name is fixed inside the code. The *acemaker.inp* file is a text file containing the input options given by keywords. The first line should be the title of the case. It is followed by a set of keywords, one by line. The keywords should be entered in the first six-character positions. The data fields start in column 7, if needed. Some keywords could require additional lines. It is possible to use lower- or uppercase writing, but not a combination. The last line should contain the card END or end. The complete keyword set is presented in Tables 6 and 7.

TABLE 6: KEYWORD SET FOR ACEMAKER INPUT

| No. | Keyword Columns 1-6 | Data fields From Column 7-80 | Description |
|-----------------|------------------------|---------------------------------|--|
| General options | | | |
| 1 | ace ACE | IACE | Type of ACE-formatted file to be generated IACE=1 fast IACE=2 thermal |
| 2 | endf ENDF | Full filename | ENDF-6 input data filename (character*66) (Default: ENDFB.IN) |
| 3 | mat MAT | NMAT | Number of materials (integer). It should be followed by NMAT lines containing one MAT number according to ENDF-6 conventions (one by line) (Default: NMAT=0, means first material on the ENDF input tape) |
| 4 | temp TEMP | NTEMP | Number of temperatures (integer). It should be followed by NTEMP lines containing one temperature value in Kelvin (one by line) (Default: NTEMP=1, means processing at 293.6 K) |
| 5 | tol TOL | TOL | Maximum fractional tolerance for data processing and linearization (real) (Default: TOL=0.001) |
| 6 | mcpn MCNP | MCNPX | Trigger to use extended ZAID for MCNPX (MCNPX = 0/1 = MCNP/MCNPX, Default = 0) |
| 7 | suff SUFF | SUFF | Suffix for the ZAID on the ACE-file. It should start with a dot ('.'), followed by two digits (XX) for MCNPX=0 and three digits (XXX) for MCNPX=1. (Default: .00) |
| 8 | mon MON | IMON | Printing monitor trigger IMON=0/1 = min./max. print out (Default: IMON=0) |
| 9 | keep KEEP | IKEEP | Intermediate file trigger IKEEP=0/1 = no/keep all intermediate files (Default: IKEEP=0) |
| 10 | end END | | End of case |

| No. | Keyword Columns 1-6 | Data fields From Column 7-80 | Description |
|-----------------|------------------------|---------------------------------|---|
| Fast options | | | |
| 11 | ymin YMIN | FYMIN | Minimum cross section or distribution value of interest for linearization or processing (real) (Default: FYMIN=1.0D-30) |
| 12 | dxmu DXMU | FMUMAX | Maximum cosine interval ($\Delta\mu$) for angle-energy distribution reconstruction or linearization (real) (Default: FMUMAX=0.001) |
| 13 | ptab PTAB | IPTAB | Probability tables (PTAB) in the unresolved resonance region (URR). IPTAB=0/1 = no / ptable (Default: IPTAB=1) |
| 14 | pndf PNDF | IPNDF | PENDF tape trigger IPNDF=0/1 = no / keep PENDF (Default: IPNDF=0) |
| 15 | urr URR | IURR | Trigger to keep the PTAB intermediate file ZAzzzaaa.URR.ENDF from groupie IURR =0/1 = no/yes (Default: IURR=0) |
| Thermal options | | | |
| 16 | nbin NBIN | NBIN | Number of equally probable cosines for incoherent elastic and inelastic scattering (Default: NBIN=16) |
| 17 | ethm ETHM | ETHMAX | Maximum energy for thermal treatment (Default: ETHMAX=4 eV) |
| 18 | eps EPS | EPS | Fractional tolerance for preparing incident energy grid (Default: EPS=0.003) |
| 19 | thdat THDAT | NMATH | Thermal data description by material. NMATH must be equal to NMAT on the MAT keyword (NMATH=NMAT). It should be followed by NMATH sets of NZAM(i)+1 line containing the data presented in Table 7 |

TABLE 7: THDAT KEYWORD DESCRIPTION (IACE=1)

| | | |
|--|----------------------------------|---------------------------|
| | | THDAT NMATH |
| line | 1: | THZAID(1) NMIX(1) NZAM(1) |
| line | 2: | IZAM(1,1) |
| line | 3: | IZAM(2,1) |
| | | ... |
| | | IZAM(j,1) |
| | | ... |
| line | NZAM(1)+1: | IZAM(NZAM(1),1) |
| line | NZAM(1)+2: | THZAID(2) NMIX(2) NZAM(2) |
| line | NZAM(1)+3: | IZAM(1,2) |
| line | NZAM(1)+4: | IZAM(2,2) |
| | | ... |
| | | IZAM(j,2) |
| | | ... |
| line | NZAM(1)+NZAM(2)+2: | IZAM(NZAM(2),2) |
| | | ... |
| | | ... |
| line | NZAM(1)+...+NZAM(i-1)+i: | THZAID(i) NMIX(i) NZAM(i) |
| line | NZAM(1)+...+NZAM(i-1)+i+1: | IZAM(1,i) |
| line | NZAM(1)+...+NZAM(i-1)+i+2: | IZAM(2,i) |
| | | ... |
| | | IZAM(j,i) |
| | | ... |
| line | NZAM(1)+...+NZAM(i-1)+NZAM(i)+i: | IZAM(NZAM(i),i) |
| | | ... |
| | | ... |
| where i=1,2,3, ... NMATH and | | |
| THZAID(i): Thermal ZAID for material MAT(i), up to a maximum of 6 characters (Examples: lwtr, hwtr, H_ZrH, grph0) | | |
| NMIX(i): Number of atom types mixed in the TSL of material MAT(i) (Default: 1) | | |
| NZAM(i): Number of moderator materials for which the TSL of material MAT(i) is applicable (up to a maximum of 16) | | |
| IZAM(j,i): ZA=1000*Z+A value of moderator material j for which the TSL of material MAT(i) is applicable. | | |
| The first line of each NMATH set contains the values of THZAID(i), NMIX(i) and NZAM(i) for material MAT(i). The following NZAM(i) lines contain the ZA value of each moderator material(one by line) | | |

The keywords can be entered in any order. The keyword END plays the role of case terminator. If a keyword is missing, its default value is applied. Therefore, it is only necessary to include the keywords that change defaults. Several cases can be stacked in the *acemaker.inp* file by appending after the current END a new title line and new input options, finishing with a new END keyword. ACEMAKER will stop after the last END. Examples of the ACEMAKER input files are given in Figs 3 and 4 for IACE=0 (fast).

FIG. 3: Example of *acemaker.inp* (*IACE=0*)

```
ACEMAKER title
ACE      0
ENDF    \fendl32\endf\fendlen.dat
MAT      1
        125
TEMP     2
        293.6
        400.0
TOL      0.005
YMIN     1.0e-30
DXMU     0.01
SUFF     .01
PTAB     1
PNDF     0
MON      0
KEEP     0
MCNP     0
END
```

Figure 3 presents a fast continuous energy calculation. The data for H-1 (MAT-125) is retrieved from the `\fendl32\endf\fendlen.dat` evaluated nuclear data library. Two temperatures will be processed: 293.6 and 400.0 K. The fractional tolerance for linearization and the maximum cosine interval are set to 0.005 and 0.01 respectively. PTAB is set to 1, but ACEMAKER manages cases like this, where there are no unresolved resonance data. Therefore, no probability tables will be produced. Minimal results will be printed and all intermediate files deleted.

ACEMAKER generates a fast ACE-formatted file for each material and each temperature. The name of each file follows the pattern `ZAzzzaaa.XXc.acef`, where `zzzaaa` is the ZA number printed in a field of six positions and filled with zeroes in place of spaces. It is in agreement with GROUPIE-2019 conventions. The suffix `.XX` (`.XXX`) is equal to the one entered as input for the first temperature and it is increased in `.01` (`MCNPX=0`) or `.001` (`MCNPX=1`) steps for each additional temperature (`NTEMP>1`). In the example above, ACEMAKER generates two ACE-formatted files:

- 1.) `ZA001001.01c.acef` for H-1 at 293.6 K with `ZAID = 1001.01c`
- 2.) `ZA001001.02c.acef` for H-1 at 400.0 K with `ZAID = 1001.02c`

Additionally, ACEMAKER produces a directory file named `ZAzzzaaaa.XXc.xsd` for each ACE-formatted file containing the relevant information for the XSDIR file of MCNP.

The files `ZAzzzaaa.XXc.lst` and `acemaker.log` are also saved. The first file compiles all the listing outputs from all modules called by the driver code. The file `acemaker.log` contains the processing messages.

FIG. 4: Example of multiple cases (*acemaker.inp*)

```
Case 1 title
ENDF   FENDLEN.DAT
MAT    3
      5728
      725
      825
SUFF   .32
END
Case 2 title
ENDF   \ENDF-B-VIII.0\n-001_H_001.endf
TEMP   2
      293.6
      600.0
SUFF   .80
END
Case 3 title
ENDF   \ENDF\ENDFBVIII.endf
MAT    2
      9228
      9237
TEMP   2
      293.6
      600.0
SUFF   .80
END
```

Figure 4 shows three cases stacked on the same *acemaker.inp* file applying some default options. In case 1, evaluated data will be retrieved from FENDLEN.DAT for three materials with MAT number 5728(La-139), 725(N-14) and 825(O-16). The ZAID identifier for each material on the ACE formatted file will have the suffix .32c. Default values apply to the rest of input options. The ACE-formatted files ZA057139.32c.acef for La-139, ZA007014.32c.acef for N-14 and ZA008016.32c.acef for O-16 are generated.

In case 2, evaluated nuclear data are read from \ENDF-B-VIII.0\n001_H_001.endf for H-1, using by default NMAT=0, results in the first material in the ENDF tape being processed. Two temperatures are requested, therefore two ACE-formatted files will be generated: one at 293.6 K and the other at 600.0 K. The ZAID numbers will be 1001.80c and 1001.81c. Default values are used for the rest of input options. The files ZA001001.80c.acef and ZA001001.81c.acef are prepared for H-1.

In case 3, evaluated nuclear data are retrieved for U-235 (9228) and U-238 (9237) from tape \ENDF\ENDFBVIII.endf. Two temperatures are requested for each material. The main ZAID suffix is .80. Default values are taken for the rest of input options. Four ACE-formatted files are generated:

- 1.) ZA092235.80c (ZAID=92235.80c) at 293.6K for U-235 (MAT=9228)
- 2.) ZA092235.81c (ZAID=92235.81c) at 600.0K for U-235 (MAT=9228)
- 3.) ZA092238.80c (ZAID=92238.80c) at 293.6K for U-238 (MAT=9237)
- 4.) ZA092238.81c (ZAID=92238.81c) at 600.0K for U-238 (MAT=9237)

The options IMON=1 and IKEEP=1 are useful for checking intermediate results or debugging a module crash. Option IPNDF=1 is convenient to save the PENDF tape used to produce the ACE-formatted file.

If *acemaker.inp* is not found on the working directory, then ACEMAKER will try all default options: process first material from ENDF tape ENDFB.IN at 293.6 K using default tolerances and trigger values for linearization and reconstruction of the data to produce a fast ACE-formatted file.

Figures 5 and 6 show some input examples for generating a thermal ACE-formatted file (IACE=1). For the thermal option ACE 1 (IACE=1) it is compulsory to enter the keywords: ACE, MAT and THDAT. The rest of the options could get the default values.

FIG. 5: Input example for IACE=1 (thermal)

```

H bound in H2O
ACE      1
ENDF    \ENDF-B-VIII.0\tsl\tsl-HinH2O.endf
MAT      1
        1
TEMP     1
        293.6
MON      2
NBIN     64
ETHM     4.0
TOL      0.001
EPS      0.003
THDAT    1
        H_H2O 1 1
        1001
SUFF     .00
MCNP     0
END

```

FIG. 6: Thermal (IACE=1) multiple materials

```
ZrH(H in ZrH and Zr in ZrH are contained on tsl-ZrH.endf)
ACE      1
ENDF    \ENDF-B-VIII.0\tsl\tsl-ZrH.endf
MAT      2
        7
        58
TEMP     1
        296.0
MON      2
NBIN     64
ETHM     4.0
TOL      0.001
EPS      0.003
THDAT    2
        H_ZrH  1  1
        1001
        Zr_ZrH 1  3
        40000
        40090
        40091
SUFF     .00
MCNP     0
END
```

In the previous examples for IACE=1 (thermal), the following files are generated:

- H_H2O.00t.acef at 293.6 K (thermal ACE-formatted file)
- H_H2O.00t.xsd (thermal directory file for xsdir)
- H_H2O.00t.plt (input options files for PLOTTAB, see IMON=2)
- H_H2O.00t.cur (curve file for PLOTTAB, see IMON=2)
- H_H2O.00t.log (DOTSL log file)
- H_H2O.00t.lst (DOTSL output file)
- H_ZrH.00t.acef at 296.0 K
- H_ZrH.00t.xsd
- H_ZrH.00t.plt
- H_ZrH.00t.cur
- H_ZrH.00t.log
- H_ZrH.00t.lst
- Zr_ZrH.00t.acef at 296.0 K
- Zr_ZrH.00t.xsd
- Zr_ZrH.00t.plt
- Zr_ZrH.00t.cur
- Zr_ZrH.00t.log
- Zr_ZrH.00t.lst

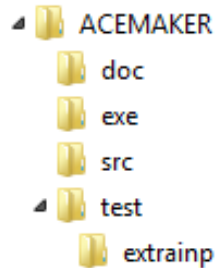
The modules SIXLIN, DOACE, DOTSL and ACEMAKER are well commented and they include the last-minute description of the input options and updates as comment lines.

8. Availability

The ACEMAKER package is distributed by the IAEA Nuclear Data Section on request. It is also freely available at <https://github.com/IAEA-NDS/ACEMAKER/releases>

A compressed file is supplied. After decompression on the root directory of the user, the following directory structure is created.

FIG. 5: ACEMAKER package directory structure



The subdirectory `\ACEMAKER\doc` eventually includes some documentation on ACEMAKER. The subdirectory `\ACEMAKER\exe\` contains the executables for the PREPRO-2019-1 and ACEMAKER-2.0 code packages. The executables were generated using the FORTRAN compiler LAHEY 7.8 for WINDOWS. The subdirectory `\ACEMAKER\test\` stores the test cases inputs (*testfast.inp* and *testtsl.inp*) and their output files. The inner subdirectory `\ACEMAKER\test\extrainp` includes extra-examples inputs for ACEMAKER. The subdirectory `\ACEMAKER\src\` contains the FORTRAN source codes *sixlin.f*, *doce.f*, *dotsl* and *acemaker.f*. Additionally, two batch files are supplied for compiling and linking the FORTRAN sources using LAHEY FORTRAN 7.8 and GFORTRAN.

For LINUX systems the ACEMAKER-2.0 source codes (*sixlin.f*, *doace.f*, *dotsl.f*, *acemaker.f*) should be compiled using the corresponding version of FORTRAN compiler. Furthermore, the LINUX version of PREPRO-2019-1 executables must be used.

As mentioned above, it is possible to prepare the configuration file *acemaker.cfg* on the working directory, which should include the PREPRO-2019-1 and ACEMAKER-2.0 full-paths for executables.

To run ACEMAKER, the user only must invoke the ACEMAKER executable from the system prompt on his/her working directory. The input file *acemaker.inp* and eventually the configuration file *acemaker.cfg* should exist on the working directory. Some batch examples to run ACEMAKER and to plot TSL data are provided on the `\ACEMAKER\test\` directory.

Appendix A shows some snapshots on how to run ACEMAKER from the system prompt and Appendix B presents some plots from PLOTTAB using the data files generated by DOTSL.

9. Final comments and recommendations

The package code ACEMAKER 2.0 has been developed as a complement to the PREPRO-2019-1 code systems for preparing continuous-energy ACE-formatted data files for

neutron transport calculations using MCNP. The code package is freely available at the 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 benchmarks.

Further development of the ACEMAKER system will include capabilities for processing photonuclear, charge particle production, damage and heating data.

10. References

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Appendix A

FIG. A.1: Running ACEMAKER

```
Command Prompt
C:\Users\dldaldama>:
D:\>cd example
D:\example>dir
Volume in drive D is Data
Volume Serial Number is C8DB-0A71

Directory of D:\example

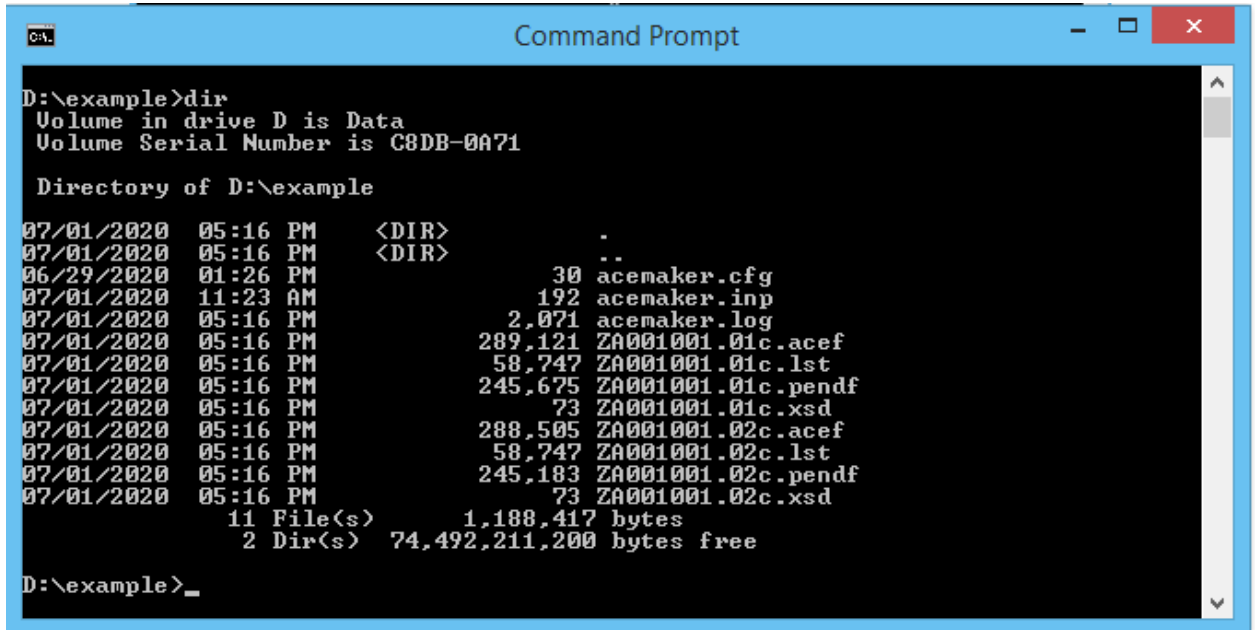
07/01/2020  05:15 PM    <DIR>          .
07/01/2020  05:15 PM    <DIR>          ..
06/29/2020  01:26 PM                30 acemaker.cfg
07/01/2020  11:23 AM                192 acemaker.inp
                2 File(s)                222 bytes
                2 Dir(s)  74,493,411,328 bytes free

D:\example>\ACEMAKER\exe\acemaker.exe
=====
ACEMAKER log file  2020/07/01 17:16:27:19
=====
Read filepaths will be used:
PREPRO  filepath: \ACEMAKER\exe\
ACEMAKER filepath: \ACEMAKER\exe\

MAT= 125
=====
17:16:27:22 2020/07/01 \ACEMAKER\exe\merger
17:16:27:66 2020/07/01 \ACEMAKER\exe\linear
17:16:27:69 2020/07/01 \ACEMAKER\exe\recent
17:16:27:70 2020/07/01 \ACEMAKER\exe\legend
17:16:27:75 2020/07/01 \ACEMAKER\exe\spectra
17:16:27:77 2020/07/01 \ACEMAKER\exe\sixlin
MAT= 125 TEMP= 2.9360D+02
17:16:31:05 2020/07/01 \ACEMAKER\exe\sigma1
17:16:31:52 2020/07/01 \ACEMAKER\exe\fixup
17:16:32:70 2020/07/01 \ACEMAKER\exe\groupie
** Warning: No unresolved probability tables
17:16:32:84 2020/07/01 \ACEMAKER\exe\dictin
17:16:32:87 2020/07/01 \ACEMAKER\exe\doace
ACE-file: ZA001001.01c.acef saved for MAT= 125 TEMP= 2.9360D+02
MAT= 125 TEMP= 4.0000D+02
17:16:32:95 2020/07/01 \ACEMAKER\exe\sigma1
17:16:33:44 2020/07/01 \ACEMAKER\exe\fixup
17:16:38:11 2020/07/01 \ACEMAKER\exe\groupie
** Warning: No unresolved probability tables
17:16:38:23 2020/07/01 \ACEMAKER\exe\dictin
17:16:38:27 2020/07/01 \ACEMAKER\exe\doace
ACE-file: ZA001001.02c.acef saved for MAT= 125 TEMP= 4.0000D+02
=====
End of ACEMAKER log file 2020/07/01 17:16:38:33
=====

D:\example>
```


FIG. A.2: Example of the files created by running ACEMAKER



```
Command Prompt
D:\example>dir
Volume in drive D is Data
Volume Serial Number is C8DB-0A71

Directory of D:\example

07/01/2020  05:16 PM    <DIR>          .
07/01/2020  05:16 PM    <DIR>          ..
06/29/2020  01:26 PM                30 acemaker.cfg
07/01/2020  11:23 AM                192 acemaker.inp
07/01/2020  05:16 PM                2,071 acemaker.log
07/01/2020  05:16 PM           289,121 ZA001001.01c.acef
07/01/2020  05:16 PM            58,747 ZA001001.01c.lst
07/01/2020  05:16 PM           245,675 ZA001001.01c.pendf
07/01/2020  05:16 PM                73 ZA001001.01c.xsd
07/01/2020  05:16 PM           288,505 ZA001001.02c.acef
07/01/2020  05:16 PM            58,747 ZA001001.02c.lst
07/01/2020  05:16 PM           245,183 ZA001001.02c.pendf
07/01/2020  05:16 PM                73 ZA001001.02c.xsd
          11 File(s)          1,188,417 bytes
           2 Dir(s)  74,492,211,200 bytes free

D:\example>_
```

Appendix B

