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Development of ANJOYMC Program for Automatic Generation of Monte Carlo Cross Section Libraries

(몬테칼로 계산용 단면적 라이브러리 생산 자동화 프로그램 ANJOYMC 개발)

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제 출 문

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본 보고서를 “몬테칼로 코드용 단면적 라이브러리 생산 자동화 프로그램 ANJOYMC 개발”에 대한 기술보고서로 제출합니다.

2007년 3월

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요 약 문

미국의 Los Alamos 국립연구소에서 개발한 NJOY 코드는 ENDF/B 양식의 평가핵자료를 처리하여 MCNP 와 McCARD 등의 몬테칼로 코드에 사용되는 ACE 양식의 라이브러리를 생산한다. 수백종에 달하는 핵종과 온도에 따라 NJOY 입력을 준비하여 라이브러리를 생산하는 과정은 상당한 시간을 필요로 할 뿐만 아니라 사용자의 에러를 유발할 여지가 있다. 이러한 문제를 해결하기 위하여 간단한 사용자의 입력으로 NJOY 입력을 자동으로 생산하여 줄 뿐만 아니라 배치파일을 만들어 라이브러리를 생산하는 모든 과정을 자동으로 수행하는 프로그램인 ANJOYMC 를 개발하였다.

ANJOYMC 프로그램은 WINDOWS 와 LINUX 를 OS 로 하는 PC 에서 구동하도록 Fortran90 을 이용하여 개발되었다. 간단한 사용자 입력으로 짧은 시간안에 사용자의 에러 없이 ACE 양식의 라이브러리를 생산할 수 있다.

Abstract

The NJOY code developed at Los Alamos National Laboratory is to generate the cross section libraries in ACE format for the Monte Carlo codes such as MCNP and McCARD by processing the evaluated nuclear data in ENDF/B format. It takes long time to prepare all the NJOY input files for hundreds of nuclides with various temperatures, and there can be some errors in the input files. In order to solve these problems, ANJOYMC program has been developed. By using a simple user input deck, this program is not only to generate all the NJOY input files automatically, but also to generate a batch file to perform all the NJOY calculations.

The ANJOYMC program is written in Fortran90 and can be executed under the WINDOWS and LINUX operating systems in Personal Computer. Cross setion libraries in ACE format can be generated in a short time and without an error by using a simple user input deck.

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1. Introduction

The NJOY[1] proram was developed at Los Alamos National Laboratory which is to generate the cross section libraries for the Monte Carlo codes such as MCNP[2] and McCARD. This program can process the evaluated nuclear data in ENDF/B[3] format. The NJOY program is composed of modules such as MODER, RECONR, BROADR, UNRESR, GROUPR, ACER and others.

It takes long time to prepare all the NJOY input files for hundreds of nuclides with various temperatures, and there can be some errors in preparing NJOY input files. In order to solve these problems, ANJOYMC program has been developed. By using a simple user input deck, this program is not only to generate all the NJOY input files automatically, but also to generate a batch file to perform all the NJOY calculations. ANJOY program prepares all the input data for the modules required to generate cross section libraries in ACE format. The ANJOYMC program is written in Fortran90 and can be executed under the WINDOWS and LINUX operating systems in Personal Computer. Cross setion libraries in ACE format can be generated in a short time and without an error by using a simple user input deck.

2. Program Description

The overall procedure of the ANJOYMC program is shown in Figure 2.1. This program includes the following functions:

(a) Generate NJOY input files for neutron cross sections and thermal scattering data
(b) Generate directory for each nuclide
(c) Geneate a batch file to run all the NJOY input files
(d) Assemble all the cross section libraries and xsdir files

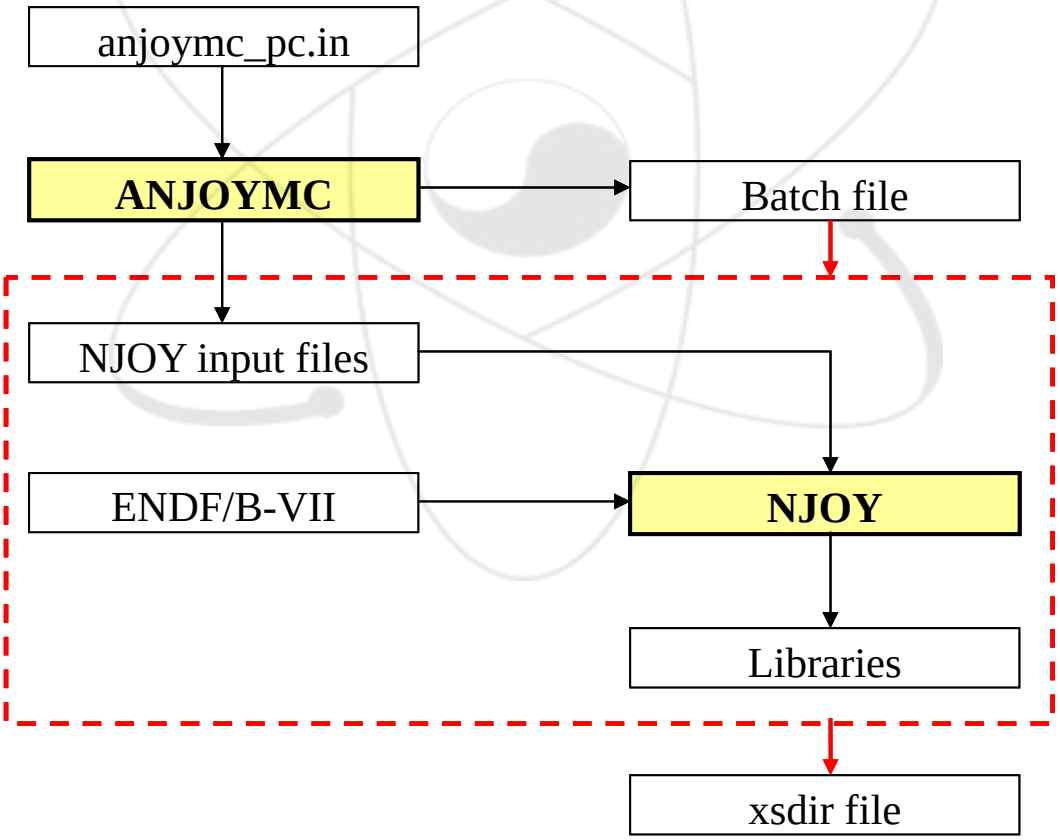

Figure 2.1 Flow chart of the ANJOYMC calculation

3. ANJOYMC Input Structure

3.1 How to Use

The ANJOYMC program includes a default input deck as follows:

anjoymc_pc.in: Default user input file (PC)
anjoymc_linux.in: Default user input file (Linux)

When using a default input, user can execute the execution file of the ANJOYMC code. Filename of the batch file to be generated is ‘runnjoym.bat’. If user runs this batch file, all the NJOY calculations will be performed. After completion of the NJOY calculations, all the libraries are moved into a directory ‘acer_out’ and ‘xsdir’ file will be generated.

3.2 Input Card Description

This Section is to describe the input cards in detail. For the explanation convenience, the following abbreviations are used.

(1) The Abbreviations for comment or default value

Abbreviation	Description
(C)	Comment
(D)	Default Value

(2) The Abbreviations for the Variable Formats:

Abbreviation	Variable Format
I	Integer
R	Real
A	Character
L	Logical

```
%TIT : DIEMNSION FOR MEMORY ALLOCATION
  [TITLE]
```

```
  ------------------------------------------------------------------------
   TITLE      (A12)  TITLE CARD
                     (C) This card is meaningless.


%DIM : DIEMNSION FOR MEMORY ALLOCATION
  [MXLIB1,MXN1]
  [MXLIB2,MXN2]
  ------------------------------------------------------------------------
   MXLIB1     (I)    THE NUMBER OF ENDF LIBRARIES
   MXN1       (I)    THE NUMBER OF NUCLIDES FOR NORMAL CROSS SECTIONS
   MXLIB2     (I)    THE NUMBER OF ENDF THERMAL SCATTERING LIBRARIES
   MXN2       (I)    THE NUMBER OF NUCLIDES FOR THERMAL SCATTERING LIBRARY
                     (C) The maximum number of evaluated nuclear data files are 10.


%OPT : OPTION
  [TOLERANCE]
  ------------------------------------------------------------------------
   TOLERANCE  (R)    TOLERANCE IN DATA
                     (C) This tolerance will be used in the modules of RECONR, BROADR,
                         and THERMR.


%LIB : ENDF/B LIBRARIES
  [I, LIBENDF1(I)] (I=1,MXLIB1)
  [I, LIBENDF2(I)] (I=1,MXLIB2)
  ------------------------------------------------------------------------
   I          (I)    ORDERING NUMBER
   LIBENDF1   (A25)  FILENAME FOR ENDF/B LIBRARY
   LIBENDF2   (A25)  FILENAME FOR ENDF/B THERMAL SCATTERING LIBRARY


%EXE : EXECUTION FILES
  [I, EXEFILE(1)]
  [I, EXEFILE(2)]
  ------------------------------------------------------------------------
   I          (I)    ORDERING NUMBER
   EXEFILE(1) (A25)  NJOY EXECUTION FILE
   EXEFILE(2) (A25)  CHECKSUM EXECUTION FILE


%NUC : NEUTRON CROSS SECTION LIBRARIES
  [I, NUCLX1(I), NUCLY1(I), (NDAT1(I,J),J=1,4), (TEMP1(I,K),K=1,NDAT1(I,3))]
  ------------------------------------------------------------------------
   I          (I)    ORDERING NUMBER
   NUCLX1(I)  (A10)  NUCLIDE
   NUCLY1(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME
   NDAT1(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF
                     J=2 : NUCLIDE ID NUMBER
                     J=3 : THE NUMBER OF TEMPERATURES
```

```
   TEMP1(I,K) (R)    TEMPERATURE IN KELVIN


%TSC : THERMAL SCATTERING LIBRARIES
  [I, NUCLX2(I), NUCLY2(I), (NDAT2(I,J),J=1,4), (TEMP2(I,K),K=1,NDAT2(I,4))]
  ------------------------------------------------------------------------
   I          (I)    NUCLIDE ORDERING NUMBER
   NUCLX2(I)  (A10)  NUCLIDE
   NUCLY2(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME
   NDAT2(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF
                     J=2 : NUCLIDE MATS NUMBER IN THERMAL SCATTERING LIBRARY
                     J=3 : NUCLIDE ID NUMBER
                     J=4 : # OF TEMPERATURE
   TEMP2(I,K) (R) TEMPERATURE IN KELVIN
```

3.3 Program ANJOYMC

Program ‘ANJOYMC’ has been developed to generate the nuclidewise NJOY input files for the cross section libraries to be used in the Monte Carlo calculations and the batch file automatically according to the main control deck. Program sources for WINDOWS and LINUX are shown in Appendices A and B, respectively . This program makes directory for each nuclide and NJOY input files in each directory, and prepares the batch file to run all the NJOY input files. The following is the underlined things in preparing NJOY input files for the cross section libraries to be used in the Monte Carlo calculations.

[MODER]

MAT number : from the main control deck

Others : Common to all nuclides

[RECONR]

MAT number : from the main control deck

Others : Common to all nuclides

[BROADR]

MAT number : from the main control deck

Temperature : from the main control deck

Others : Common to all nuclides

[UNRESR]

MAT number : from the main control deck
Temperature : from the main control deck
Background cross sections : 1.0E+15
Others : Common to all nuclides

[HEATR]
MAT number : from the main control deck

[PURR]
MAT number : from the main control deck
Temperature : from the main control deck
NBIN=20
NLADR=64
Background cross sections : 1.0E+15
Others : Common to all nuclides

[ACER]
Suffix : Number of temperature in order
MAT number : from the main control deck
Temperatures : from the main control deck

The following is the underlined things in preparing NJOY input files for the MCNP thermal scattering libraries.

[MODER]
MAT number : from the main control deck
Others : Common to all nuclides

[RECONR]
MAT number : from the main control deck
Others : Common to all nuclides

[BROADR]
MAT number : from the main control deck
Temperature : from the main control deck
Others : Common to all nuclides

[THERMR]

MAT number : from the main control deck

Temperatures : from the main control deck

Elastic option : Refer to Table 3.1

[ACER]

Suffix : Number of temperature in order

MAT number : from the main control deck

MTE : from Table 3.1

Temperatures : from the main control deck

Table 3.1 Elastic option for the thermal scattering library

MATS	Nuclide	ICOH	MTREF	MTE	NATOM	IELAS
31	Graphite	1	229	230	1	0
26	Be	2	231	232	1	0
27	BeO	3	233	234	1	0
37	Polyethylene	11	223	234	2	1
7	H(ZrH)	12	225	226	1	1
58	Zr(ZrH)	13	235	236	1	1
1	H(H2O)	0	222	-	2	-
11	D(D2O)	0	228	-	2	-

4. Sample Calculation

Sample calculation has been performed to generate cross section and thermal scattering libraries. Table 4.1 provides an ANJOYMC sample input for WINDOWS to generate cross section libraries for 20 nuclides at two temperatures, and thermal scattering libraries for 2 nuclides at three temperatures. Figure 4.1 shows all the directories generated by the ANJOYMC program. One directory is assigned to each nuclide. Directory ‘1_1001’ is for nuclide ‘ 1-H- 1 ’. Since there are two temperatures for ' 1-H - 1 ', two NJOY input files are generated. As shown in Figure 4.1 these NJOY files are included in the directory ‘1_1001’. Table 4.2 shows a part of ‘runnjoym.bat’ file which is a batch file to run all the NJOY input files.

After the completion of the NJOY calculations, ‘xsdir’ file is generated to be used in Monte Carlo calculations. Sample of ‘xsdir’ file is shown in Table 4.3. In this file ‘filename’ should be replaced manually with the library filenames to be found in the directory ‘acer_out’. All the cross section and thermal scattering libraries generated in each nuclide directory are moved to the directory ‘acer_out’.

Table 4.1 Sample ANJOYMC input file for WINDOWS

```
%TIT
  ENDF/B-VII_R0
%DIM
  1   20                                                    !ENDF N LIBRARY
  1    2
%OPT
  0.001                                                     ! Data Tolerance
%LIB
  1  '..\..\endf\n-endfb7.0'                                  !ENDF/B-VII R0
  1  '..\..\endf\tsl_endfb7.0'                                !ENDF/B-VII thermal scattering data
%EXE
  1  '..\..\bin\njoy.exe'                                     !NJOY execution
  2  '..\..\bin\sum.exe'                                      !Sum execution
%NUC
   1  '  1-H -  1 '    125     1   2  300  400
   2  '  1-H -  2 '    128     1   2  300  400
   3  '  1-H -  3 '    131     1   2  300  400
   4  '  2-He-  3 '    225     1   2  300  400
   5  '  2-He-  4 '    228     1   2  300  400
   6  '  3-Li-  6 '    325     1   2  300  400
   7  '  3-Li-  7 '    328     1   2  300  400
   8  '  4-Be-  7 '    419     1   2  300  400
   9  '  4-Be-  9 '    425     1   2  300  400
  10  '  5-B - 10 '    525     1   2  300  400
  11  '  5-B - 11 '    528     1   2  300  400
  12  '  6-C -  0 '    600     1   2  300  400
  13  '  7-N - 14 '    725     1   2  300  400
  14  '  7-N - 15 '    728     1   2  300  400
  15  '  8-O - 16 '    825     1   2  300  400
  16  '  8-O - 17 '    828     1   2  300  400
  17  '  9-F - 19 '    925     1   2  300  400
  18  ' 11-Na- 22 '   1122     1   2  300  400
  19  ' 11-Na- 23 '   1125     1   2  300  400
  20  ' 12-Mg- 24 '   1225     1   2  300  400
%TSC
   1  '  h_h2o    '    125     1  1  3    293.6 350  400
   2  '  graphite '    600    31  1  3    296   400  500
```

Table 4.2 Part of ‘runnjoym.bat’ file for WINDOWS

```
REM ========================================
REM  BATCH FILE FOR MULTIPLE NJOY RUN
REM ========================================
..\..\bin\sum.exe        ..\endf\n-endfb7.0
..\..\bin\sum.exe        ..\endf\tsl_endfb7.0

REM ============================================
REM   1    1-H -  1       125  300.0 K
REM ============================================
cd   1_1001
del  tape* output
copy ..\..\endf\n-endfb7.0     tape20
copy ..\..\endf\tsl_endfb7.0   tape29
..\..\bin\njoy.exe          <  1001.in1t
move output out_1001.in1t
move tape70 t70_1001.in1t
move tape71 xsd_1001.in1t
..\..\bin\sum.exe         t70_1001.in1t
..\..\bin\sum.exe         xsd_1001.in1t
type xsd_1001.in1t            >> ..\xsdir
move t70_* ..\acer_out\
move xsd_* ..\xsdir_out\
del  tape* output
cd ..

REM ============================================
REM   1    1-H -  1       125  400.0 K
REM ============================================
cd   1_1001
del  tape* output
copy ..\..\endf\n-endfb7.0     tape20
copy ..\..\endf\tsl_endfb7.0   tape29
..\..\bin\njoy.exe          <  1001.in2t
move output out_1001.in2t
move tape70 t70_1001.in2t
move tape71 xsd_1001.in2t
..\..\bin\sum.exe         t70_1001.in2t
..\..\bin\sum.exe         xsd_1001.in2t
type xsd_1001.in2t            >> ..\xsdir
move t70_* ..\acer_out\
move xsd_* ..\xsdir_out\
del  tape* output
cd ..
```

Table 4.3 Part of ‘xsdir’ file

```
 1001.01c    0.999167 filename route 1   1    7424     0     0 2.585E-08
 1001.02c    0.999167 filename route 1   1    7424     0     0 3.447E-08
 1002.01c    1.996800 filename route 1   1    9234     0     0 2.585E-08
 1002.02c    1.996800 filename route 1   1    9288     0     0 3.447E-08
 1003.01c    2.989596 filename route 1   1   10985     0     0 2.585E-08
 1003.02c    2.989596 filename route 1   1   11030     0     0 3.447E-08
 2003.01c    2.989032 filename route 1   1    6883     0     0 2.585E-08
 2003.02c    2.989032 filename route 1   1    6883     0     0 3.447E-08
 2004.01c    3.968219 filename route 1   1    5207     0     0 2.585E-08
 2004.02c    3.968219 filename route 1   1    5237     0     0 3.447E-08
 3006.01c    5.963400 filename route 1   1   32943     0     0 2.585E-08
 3006.02c    5.963400 filename route 1   1   32921     0     0 3.447E-08
 3007.01c    6.955732 filename route 1   1   18583     0     0 2.585E-08
 3007.02c    6.955732 filename route 1   1   18583     0     0 3.447E-08
 4007.01c    6.954500 filename route 1   1   28940     0     0 2.585E-08
 4007.02c    6.954500 filename route 1   1   29006     0     0 3.447E-08
 4009.01c    8.934780 filename route 1   1  579033     0     0 2.585E-08
 4009.02c    8.934780 filename route 1   1  579047     0     0 3.447E-08
 5010.01c    9.926921 filename route 1   1   50550     0     0 2.585E-08
 5010.02c    9.926921 filename route 1   1   50550     0     0 3.447E-08
 5011.01c   10.914700 filename route 1   1  143617     0     0 2.585E-08
 5011.02c   10.914700 filename route 1   1  143673     0     0 3.447E-08
 6000.01c   11.898000 filename route 1   1   77164     0     0 2.585E-08
 6000.02c   11.898000 filename route 1   1   77164     0     0 3.447E-08
 7014.01c   13.882780 filename route 1   1  139362     0     0 2.585E-08
 7014.02c   13.882780 filename route 1   1  139366     0     0 3.447E-08
 7015.01c   14.871000 filename route 1   1   30439     0     0 2.585E-08
 7015.02c   14.871000 filename route 1   1   30474     0     0 3.447E-08
 8016.01c   15.857510 filename route 1   1  402131     0     0 2.585E-08
 8016.02c   15.857510 filename route 1   1  402191     0     0 3.447E-08
 8017.01c   16.853100 filename route 1   1    6862     0     0 2.585E-08
 8017.02c   16.853100 filename route 1   1    6862     0     0 3.447E-08
 9019.01c   18.835000 filename route 1   1  126997     0     0 2.585E-08
 9019.02c   18.835000 filename route 1   1  127053     0     0 3.447E-08
11022.01c   21.805500 filename route 1   1   15576     0     0 2.585E-08 ptable
11022.02c   21.805500 filename route 1   1   15368     0     0 3.447E-08 ptable
11023.01c   22.792000 filename route 1   1   67273     0     0 2.585E-08
11023.02c   22.792000 filename route 1   1   67119     0     0 3.447E-08
12024.01c   23.779000 filename route 1   1   46189     0     0 2.585E-08
12024.02c   23.779000 filename route 1   1   46189     0     0 3.447E-08
```

Table 4.4 Sample NJOY input for cross section library generated by ANJOYMC

```
-- KAERI   ENDF/B-VII NJOY PROCESSING:   1-H -  1 ( 125)
moder  / Tape20(A) -> Tape21(B)
1 -21
'ENDF/B-VI R8   1-H -  1 ' /
20  125
0 /
reconr / XS Resconstruction Tape22(B)
-21 -22
'PENDF FOR  1-H -  1  FROM   ENDF/B-VII ' /
 125 2 /
   0.00100 / Reconstruction 0.1%
'  ENDF/B-VII FOR MCNP   1-H -  1 ' /
'PROCESSED BY NJOY-99.90 ' /
0 /
broadr / Doppler Broadening Tape23(B)
-21 -22 -23
 125  1 0 1 /
   0.00100 / Reconstruction 0.1%
  300.0 /
0 /
unresr / Unresolved XS Tape24(B)
-21 -23 -24
 125   1  1  1
  300.0 /
 1.0E+15 /
0 /
heatr / Kerma & Damage Tape25(B)
-21 -24 -25 /
 125 /
purr / Probalility table Tape26(B)
-21 -25 -26
 125   1  1 20 64 /
  300.0 /
 1.0E+15 /
0 /
acer  / Tape70(A)
-21 -26 0 50 51
  1  0  1  0.01 /
'  ENDF/B-VII FOR MCNP   1-H -  1 ( 300.0K)' /
 125   300.0 /
/
/
acer
0 50 0 70 71
7 1 1 -1 /
'  ENDF/B-VII FOR MCNP   1-H -  1 ( 300.0K)' /
stop
```

Table 4.5 Sample NJOY input for thermal scattering library generated by ANJOYMC

```
-- KAERI   ENDF/B-VII NJOY PROCESSING:   h_h2o    ( 125)
moder  / Tape20(A) -> Tape21(B)
1 -21
'  ENDF/B-VII   h_h2o    ' /
20  125
0 /
moder  / Tape29(A) -> Tape23(B)
29 -23
reconr / XS Resconstruction Tape22(B)
-21 -24
'PENDF FOR  h_h2o     FROM   ENDF/B-VII ' /
 125 2 /
   0.00100 / Reconstruction 0.1%
'  ENDF/B-VII FOR MCNP   h_h2o    ' /
'PROCESSED BY NJOY-99.90 ' /
0 /
broadr / Doppler Broadening Tape23(B)
-21 -24 -22
 125  1  /
   0.00100 / Reconstruction 0.1%
  293.6 /
0 /
thermr / Thermal Scattering XS
-23 -22 -24
  1  125  8  1  4  0  2 222  1
  293.6
   0.00100  4.0
acer  / Tape70(A)
-21 -24 0 70 71
  2  1  1  0.01 /
'ENDF/B-VI R8 FOR MCNP   h_h2o    ( 293.6K)' /
 125   293.6         /
     1 /
 222 /
stop
```

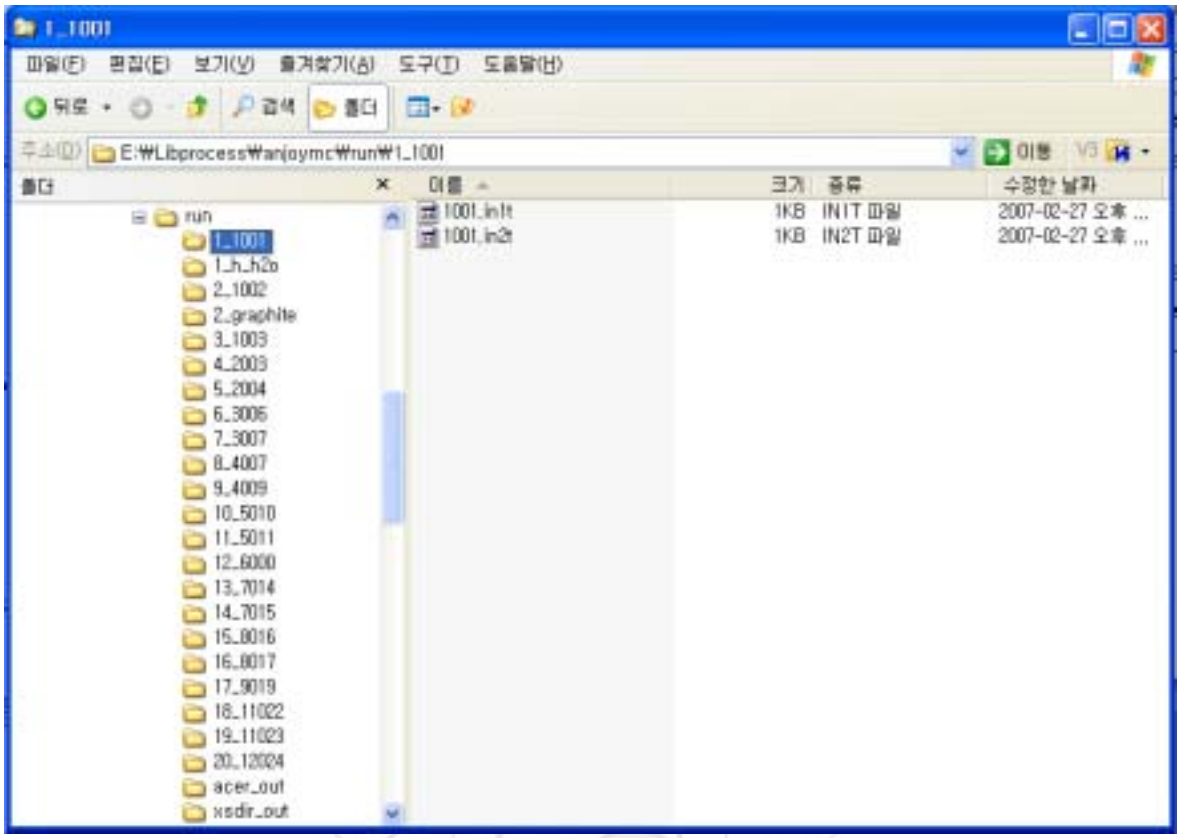

Figure 4.1 Directories and NJOY input files generated by ANJOYMC

5. Conclusions

The ANJOYMC program has been newly developed. With the aid of this program, cross section libraires for the Monte Carlo codes can be generated automatically and quickly. This program also reduces the possible human errors in preparing too many NJOY input files.

References

1. R. E. McFarlane, D. W. Muir, “The NJOY Nuclear Data Processing System Version 91,” LA-12740-M (1994)

2. J. F. Breismeister, et al., “MCNP – A General Monte Carlo N-Particle Transport Code, Version 4B,” LA-12625-M (1997)

3. V. McLane, “ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6,” BNL-NCS-44945-01/04, National Nuclear Data Center, Brookhaven National Laboratory (2001)

Appendix A. Program source of ANJOYMC for WINDOWS

```
      PROGRAM ANJOYMC_PC
!     ================================================================================
!     PROGRAM     : ANJOYMC_PC                                                       +
!                   (AUTOMATIC NJOY INPUT PREPARATION FOR MONTE CARLO CALCULATION)   +
!     FUNCTION    : AUTOMATIC PREPARATION FOR THE NJOY INPUT FILES AND BATCH FILE    +
!                   TO GENERATE ACE LIBRARY FILES FOR MONTE CARLO CODES               +
!     AUTHOR      : KANG-SEOG KIM                                                    +
!     DATE        : FEBRUARY 15, 2007                                                +
!     REMARKS     : NONE                                                             +
!     ================================================================================
      REAL,ALLOCATABLE :: TEMP1(:,:),TEMP2(:,:)
      INTEGER,ALLOCATABLE :: NDAT1(:,:),NDAT2(:,:),NUM(:)
      CHARACTER(11),ALLOCATABLE :: NUCLX1(:),NUCLX2(:)
      CHARACTER(6),ALLOCATABLE :: NUCLY1(:),NUCLY2(:)
      CHARACTER(20),ALLOCATABLE :: DIRNAME1(:),DIRNAME2(:),INPFILE1(:,:),            &
                                   INPFILE2(:,:),INPALL1(:),INPALL2(:)
      CHARACTER(2) AELEM(100)
!
      CHARACTER(1) SS1,BLANK
      CHARACTER(4) SS4
      CHARACTER(12) TITLE
      CHARACTER(25) LIBENDF1(10),LIBENDF2(10),EXEFILE(2)
      CHARACTER(13) AA,SS13
      CHARACTER(14) AA2,SS14
      CHARACTER(20) SS20,SS20A,DD,DD2,DELBLANK
      CHARACTER(50) BB,CC
!
      CHARACTER(1) S1
      CHARACTER(11) NIDXX
      CHARACTER(12) EE
      CHARACTER(13) SS13A
      CHARACTER(300) SSL
!
      PARAMETER (BLANK=' ')
!
      DATA AELEM/'h ','he','li','be','b ','c ','n ','o ','f ','ne',                  &
                 'na','mg','al','si','p ','s ','cl','ar','k ','ca',                  &
                 'sc','ti','v ','cr','mn','fe','co','ni','cu','zn',                  &
                 'ga','ge','as','se','br','kr','rb','sr','y ','zr',                  &
                 'nb','mo','tc','ru','rh','pd','ag','cd','in','sn',                  &
                 'sb','te','i ','xe','cs','ba','la','ce','pr','nd',                  &
                 'pm','sm','eu','gd','tb','dy','ho','er','tm','yb',                  &
                 'lu','hf','ta','w ','re','os','ir','pt','au','hg',                  &
                 'tl','pb','bi','po','at','rn','fr','ra','ac','th',                  &
                 'pa','u ','np','pu','am','cm','bk','cf','es','fm' /
!
      OPEN(1,FILE='anjoymc_pc.in',STATUS='OLD')          !MAIN CONTROL DECK
      OPEN(2,FILE='anjoymc.out',STATUS='UNKNOWN')        !OUTPUT FILE
      OPEN(3,FILE='runnjoym.bat',STATUS='UNKNOWN')       !BATCH FILE TO RUN NJOY
!
!     -------------------------------------------------------------------------------
!     [DESCRIPTION FOR THE MAIN CONTROL DECK]                                        +
!                                                                                    +
!     %TIT : DIEMNSION FOR MEMORY ALLOCATION                                         +
!       [TITLE]                                                                      +
!        TITLE      (A12)  TITLE CARD                                               +
!                                                                                    +
!     %DIM : DIEMNSION FOR MEMORY ALLOCATION                                         +
!       [MXLIB1,MXN1]                                                                +
!       [MXLIB2,MXN2]                                                                +
!        MXLIB1     (I)    THE NUMBER OF ENDF LIBRARIES                             +
```

```
!       MXN1       (I)    THE NUMBER OF NUCLIDES FOR NORMAL CROSS SECTIONS          +
!       MXLIB2     (I)    THE NUMBER OF ENDF THERMAL SCATTERING LIBRARIES           +
!       MXN2       (I)    THE NUMBER OF NUCLIDES FOR THERMAL SCATTERING LIBRARY     +
!                                                                                   +
!     %OPT : OPTION                                                                 +
!       [TOLERANCE]                                                                 +
!        TOLERANCE  (R)    TOLERANCE IN DATA                                        +
!                                                                                   +
!     %LIB : ENDF/B LIBRARIES                                                       +
!       [I, LIBENDF1(I)] (I=1,MXLIB1)                                               +
!       [I, LIBENDF2(I)] (I=1,MXLIB2)                                               +
!        I          (I)    ORDERING NUMBER                                         +
!        LIBENDF1   (A25)  FILENAME FOR ENDF/B LIBRARY                             +
!        LIBENDF2   (A25)  FILENAME FOR ENDF/B THERMAL SCATTERING LIBRARY          +
!                                                                                   +
!     %EXE : EXECUTION FILES                                                        +
!       [I, EXEFILE(1)]                                                             +
!       [I, EXEFILE(2)]                                                             +
!        I          (I)    ORDERING NUMBER                                         +
!        EXEFILE(1) (A25)  NJOY EXECUTION FILE                                     +
!        EXEFILE(2) (A25)  CHECKSUM EXECUTION FILE                                 +
!                                                                                   +
!     %NUC                                                                          +
!       [I, NUCLX1(I), NUCLY1(I), (NDAT1(I,J),J=1,4), (TEMP1(I,K),K=1,NDAT1(I,3))]  +
!        I          (I)    ORDERING NUMBER                                         +
!        NUCLX1(I)  (A10)  NUCLIDE                                                 +
!        NUCLY1(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME       +
!        NDAT1(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF                        +
!                          J=2 : NUCLIDE ID NUMBER                                 +
!                          J=3 : THE NUMBER OF TEMPERATURES                        +
!        TEMP1(I,K) (R)    TEMPERATURE IN KELVIN                                   +
!                                                                                   +
!     %TSC                                                                          +
!       [I, NUCLX2(I), NUCLY2(I), (NDAT2(I,J),J=1,4), (TEMP2(I,K),K=1,NDAT2(I,4))]  +
!        I          (I)    NUCLIDE ORDERING NUMBER                                 +
!        NUCLX2(I)  (A10)  NUCLIDE                                                 +
!        NUCLY2(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME       +
!        NDAT2(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF                        +
!                          J=2 : NUCLIDE MATS NUMBER IN THERMAL SCATTERING LIBRARY  +
!                          J=3 : NUCLIDE ID NUMBER                                 +
!                          J=4 : # OF TEMPERATURE                                  +
!        TEMP2(I,K) (R) TEMPERATURE IN KELVIN                                      +
!     -------------------------------------------------------------------------------
!
!     [%TIT]
      READ(1,*) SS4
      IF (SS4.NE.'%TIT') CALL ERROR('%TIT IS MISSING')
      READ(1,'(A12)') TITLE
!
!     [%DIM]
      READ(1,*) SS4
      IF (SS4.NE.'%DIM') CALL ERROR('%DIM IS MISSING')
      READ(1,*) MXLIB1,MXN1
      READ(1,*) MXLIB2,MXN2
      ALLOCATE(NDAT1(MXN1,3),NDAT2(MXN2,4),TEMP1(MXN1,20),TEMP2(MXN2,20),NUM(11),     &
               NUCLX1(MXN1),NUCLY1(MXN1),NUCLX2(MXN2),NUCLY2(MXN2),DIRNAME1(MXN1),    &
               DIRNAME2(MXN2),INPFILE1(MXN1,20),INPFILE2(MXN2,20),INPALL1(MXN1),      &
               INPALL2(MXN2))
!
!     [%OPT]
      READ(1,*) SS4
      IF (SS4.NE.'%OPT') CALL ERROR('%OPT IS MISSING')
      READ(1,*) TOLERANCE
!
```

```
!     [%LIB]
      READ(1,*) SS4
      IF (SS4.NE.'%LIB') CALL ERROR('%LIB IS MISSING')
      DO I=1,MXLIB1
        READ(1,*) IL1,LIBENDF1(I)
      ENDDO
      DO I=1,MXLIB2
        READ(1,*) IL1,LIBENDF2(I)
      ENDDO
!
!     [%EXE]
      READ(1,*) SS4
      IF (SS4.NE.'%EXE') CALL ERROR('%EXE IS MISSING')
      READ(1,*) IL3,EXEFILE(1)
      READ(1,*) IL4,EXEFILE(2)
!
!     [%NUC]
      READ(1,*) SS4
      IF (SS4.NE.'%NUC') CALL ERROR('%NUC IS MISSING')
      DO I=1,MXN1
        READ(1,*) IX,NUCLX1(I),(NDAT1(I,J),J=1,3),(TEMP1(I,K),K=1,NDAT1(I,3))
        IF (IX.NE.I) CALL ERROR('ORDERUNG NUMBER IS WRONG IN %NUC')
      ENDDO
!
!     [%TSC]
      READ(1,*) SS4
      IF (SS4.NE.'%TSC') CALL ERROR('%TSC IS MISSING')
      DO I=1,MXN2
        READ(1,*) IX,NUCLX2(I),(NDAT2(I,J),J=1,4),(TEMP2(I,K),K=1,NDAT2(I,4))
        IF (IX.NE.I) CALL ERROR('ORDERUNG NUMBER IS WRONG IN %TSC')
      ENDDO
!
!     [INITIALIZATION]
      DIRNAME1=' '
      DIRNAME2=' '
      INPFILE1=' '
      INPFILE2=' '
!
!     ============================================================================
!     INPUT FILENAME & DIRECTORY NAME
!     ============================================================================
      DO J1=1,MXN1
        READ(NUCLX1(J1),'(I3,4X,I3,A1)') NID1,NID2,SS1
        IF (SS1.EQ.'M') SS1='m'
        NID=NID1*1000+NID2
        DO IT=1,NDAT1(J1,3)
          SS20=' '
          WRITE(SS20,'(I6,A1,".in",I2,"t")') NID,SS1,IT
          INPFILE1(J1,IT)=DELBLANK(SS20)
        ENDDO
      ENDDO
      DO J1=1,MXN2
        DO IT=1,NDAT2(J1,4)
          SS20=' '
          WRITE(SS20,'(A11,".in",I2,"t")') NUCLX2(J1),IT
          INPFILE2(J1,IT)=DELBLANK(SS20)
          WRITE(2,*) INPFILE2(J1,IT)
        ENDDO
      ENDDO
!
!     [MAKE NUCLIDEWISE DIRECTORY & MOVE NJOY INPUT FILES]
!     +NEUTRON XS
      DO J1=1,MXN1
        READ(NUCLX1(J1),'(I3,4X,I3,A1)') NID1,NID2,SS1
```

```
        IF (SS1.EQ.'M'.OR.SS1.EQ.'m') THEN
          SS1='m'
        ELSE
          SS1=' '
        ENDIF
        NID=NID1*1000+NID2
        SS20=' '
        AA=' '
        WRITE(SS20,'(I3,"_",I6,A1)') J1,NID,SS1
        DIRNAME1(J1)=DELBLANK(SS20)
        SS20=' '
        WRITE(SS20,'(I6,A1,".in*")') NID,SS1
        INPALL1(J1)=DELBLANK(SS20)
      ENDDO
!
!     +THERMAL SCATTERING XS
      DO J1=1,MXN2
        SS20=' '
        WRITE(SS20,'(I3,"_",A11)') J1,NUCLX2(J1)
        DIRNAME2(J1)=DELBLANK(SS20)
        SS20=' '
        WRITE(SS20,'(A11,".in*")') NUCLX2(J1)
        INPALL2(J1)=DELBLANK(SS20)
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PREPARATION FOR NEUTRON CROSS SECTION
!     ================================================================================
      S1="'"
      DO J1=1,MXN1
        DO IT=1,NDAT1(J1,3)
          J2=IT*1000+J1
          AA=INPFILE1(J1,IT)
          OPEN (J2,FILE=AA,STATUS='UNKNOWN')
!
          MAT=NDAT1(J1,1)        !MAT no.
          NTEMP=1                !# of temperature
          NIDXX=NUCLX1(J1)       !Nuclide name
!
!         [TITLE] ---------------------------------------
          WRITE(J2,'("-- KAERI ",A12," NJOY PROCESSING: ",A11,"(",I4,")")') TITLE,NIDXX,MAT
!
!         [MODER] ---------------------------------------
          WRITE(J2,'("moder  / Tape20(A) -> Tape21(B)")')
          WRITE(J2,'("1 -21")')
          WRITE(J2,'(A1,"ENDF/B-VI R8 ",A11,A1," /")') S1,NIDXX,S1
          WRITE(J2,'("20",1X,I4)') MAT
          WRITE(J2,'("0 /")')
!
!         [RECONR] ---------------------------------------
          WRITE(J2,'("reconr / XS Resconstruction Tape22(B)")')
          WRITE(J2,'("-21 -22")')
          WRITE(J2,'(A1,"PENDF FOR",A11," FROM ",A12,1X,A1," /")') S1,NIDXX,TITLE,S1
          WRITE(J2,'(I4," 2 /")') MAT
          ERR=TOLERANCE
          WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') ERR
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,A1," /")') S1,TITLE,NIDXX,S1
          WRITE(J2,'(A1,"PROCESSED BY NJOY-99.90 ",A1," /")') S1,S1
          WRITE(J2,'("0 /")')
!
!         [BROADR] ---------------------------------------
          WRITE(J2,'("broadr / Doppler Broadening Tape23(B)")')
          WRITE(J2,'("-21 -22 -23")')
          WRITE(J2,'(I4,1X,I2,1X,"0 1 /")') MAT,NTEMP
```

```
          WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') TOLERANCE
!          WRITE(J2,'(" 0.001 /")')
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'("0 /")')
!
!         [UNRESR] --------------------------------------
          WRITE(J2,'("unresr / Unresolved XS Tape24(B)")')
          WRITE(J2,'("-21 -23 -24")')
          NSIGZ=1
          IPRINT=1
          SIGZ=1.0E+15
          WRITE(J2,'(I4,1X,3I3)') MAT,NTEMP,NSIGZ,IPRINT
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'(1PE8.1," /")') SIGZ
          WRITE(J2,'("0 /")')
!
!         [HEATR] --------------------------------------
          WRITE(J2,'("heatr / Kerma & Damage Tape25(B)")')
          WRITE(J2,'("-21 -24 -25 /")')
          WRITE(J2,'(I4," /")') MAT
!
!         [PURR] ---------------------------------------
          WRITE(J2,'("purr / Probalility table Tape26(B)")')
          WRITE(J2,'("-21 -25 -26")')
          NSIGZ=1
          NBIN=20
          NLADR=64
          SIGZ=1.0E+15
          WRITE(J2,'(I4,1X,4I3," /")') MAT,NTEMP,NSIGZ,NBIN,NLADR
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'(1PE8.1," /")') SIGZ
          WRITE(J2,'("0 /")')
!
!         [ACER] ---------------------------------------
          WRITE(J2,'("acer  / Tape70(A)")')
          WRITE(J2,'("-21 -26 0 50 51 ")')
          IOPT=1
          IPRINT=0
          NTYPE=1
          SUFF=FLOAT(IT)/100
          WRITE(J2,'(3I3,2X,F4.2," /")') IOPT,IPRINT,NTYPE,SUFF
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                           S1,TITLE,NIDXX,TEMP1(J1,IT),S1
          WRITE(J2,'(I4,2X,F6.1," /")') MAT,TEMP1(J1,IT)
          WRITE(J2,'("/")')
          WRITE(J2,'("/")')
          WRITE(J2,'("acer")')
          WRITE(J2,'("0 50 0 70 71 ")')
          WRITE(J2,'("7 1 1 -1 /")')
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                           S1,TITLE,NIDXX,TEMP1(J1,IT),S1
!
!         [END]
          WRITE(J2,'("stop")')
!
          CLOSE(J2)
        ENDDO
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PREPARATION FOR NEUTRON THERMAL SCATTERING
!       NDAT2(I,J)  : I=1,MXN2; J=1..4
!     ================================================================================
      DO J1=1,MXN2
```

```
      DO IT=1,NDAT2(J1,4)
!
        DD=INPFILE2(J1,IT)
        J2=IT*1000+J1
        OPEN (J2,FILE=DD,STATUS='UNKNOWN')
!
        MAT=NDAT2(J1,1)      !MAT no.
        MATS=NDAT2(J1,2)     !Thermal scattering MAT no.
        NTEMP=1              !# of temperature
        NIDXX=NUCLX2(J1)   !Nuclide name
!
!       [TITLE] ---------------------------------------
        WRITE(J2,'("-- KAERI ",A12," NJOY PROCESSING: ",A11,"(",I4,")")') TITLE,NIDXX,MAT
!
!       [MODER] ---------------------------------------
        WRITE(J2,'("moder  / Tape20(A) -> Tape21(B)")')
        WRITE(J2,'("1 -21")')
        WRITE(J2,'(A1,A12,1X,A11,A1," /")') S1,TITLE,NIDXX,S1
        WRITE(J2,'("20",1X,I4)') MAT
        WRITE(J2,'("0 /")')
!
!       [MODER] ---------------------------------------
        WRITE(J2,'("moder  / Tape29(A) -> Tape23(B)")')
        WRITE(J2,'("29 -23")')
!
!       [RECONR] --------------------------------------
        WRITE(J2,'("reconr / XS Resconstruction Tape22(B)")')
        WRITE(J2,'("-21 -24")')
        WRITE(J2,'(A1,"PENDF FOR",A11," FROM ",A12,1X,A1," /")') S1,NIDXX,TITLE,S1
        WRITE(J2,'(I4," 2 /")') MAT
        ERR=TOLERANCE
        WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') ERR
        WRITE(J2,'(A1,A12," FOR MCNP ",A11,A1," /")') S1,TITLE,NIDXX,S1
        WRITE(J2,'(A1,"PROCESSED BY NJOY-99.90 ",A1," /")') S1,S1
        WRITE(J2,'("0 /")')
!
!       [BROADR] --------------------------------------
        WRITE(J2,'("broadr / Doppler Broadening Tape23(B)")')
        WRITE(J2,'("-21 -24 -22")')
        WRITE(J2,'(I4,1X,I2,1X," /")') MAT,NTEMP
        WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') TOLERANCE
!        WRITE(J2,'("0.001 /")')
        WRITE(J2,'(F7.1," /")') TEMP2(J1,IT)
        WRITE(J2,'("0 /")')
!
!       [THERMR] --------------------------------------
        WRITE(J2,'("thermr / Thermal Scattering XS ")')
        WRITE(J2,'("-23 -22 -24")')
        NBIN=8
        IINC=4
        ICOH=0
        IF (MATS.EQ.31) ICOH=1      !Graphite
        IF (MATS.EQ.26) ICOH=2      !Be
        IF (MATS.EQ.27) ICOH=3      !BeO
        IF (MATS.EQ.37) ICOH=11     !Polyethylene
        IF (MATS.EQ.7)  ICOH=12     !H(ZrH)
        IF (MATS.EQ.58) ICOH=13     !Zr(ZrH)
        NATOM=1
        IF (MATS.EQ.1.OR.MATS.EQ.11.OR.MATS.EQ.37) NATOM=2
        IF (MATS.EQ.1)  MTREF=222   !H(H2O)
        IF (MATS.EQ.11) MTREF=228   !D(D2O)
        IF (MATS.EQ.26) MTREF=231   !Be metal  (MTE=232) coherent
        IF (MATS.EQ.31) MTREF=229   !Graphite  (MTE=230) coherent
        IF (MATS.EQ.58) MTREF=235   !Zr(ZrH)   (MTE=236) incoherent
```

```
          IF (MATS.EQ.7)  MTREF=225   !H(ZrH)     (MTE=226) incoherent
          IF (MATS.EQ.27) MTREF=233   !BeO        (MTE=234) coherent
          IF (MATS.EQ.37) MTREF=223   !H(CH2)     (MTE=224) incoherent
          IPRINT=1
          WRITE(J2,'(I3,I5,5I3,I4,I3)') MATS,MAT,NBIN,NTEMP,IINC,ICOH,NATOM,MTREF,IPRINT
          WRITE(J2,'(F7.1)') TEMP2(J1,IT)
          !WRITE(J2,'(" 0.001  4.0 ")')
          WRITE(J2,'(1F10.5,"  4.0 ")') TOLERANCE
!
!         [ACER] ---------------------------------------
          WRITE(J2,'("acer  / Tape70(A)")')
          WRITE(J2,'("-21 -24 0 70 71 ")')
          IOPT=2
          IPRINT=1
          NTYPE=1
          SUFF=FLOAT(IT)/100
          MTI=MTREF
          NBINT=16
          WRITE(J2,'(3I3,2X,F4.2," /")') IOPT,IPRINT,NTYPE,SUFF
          WRITE(J2,'(A1,"ENDF/B-VI R8 FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                           S1,NIDXX,TEMP2(J1,IT),S1
          WRITE(J2,'(I4,2X,F6.1,2X,A6," /")') MAT,TEMP2(J1,IT),NUCLY2(J1)
          WRITE(J2,'(I6," /")') NDAT2(J1,3)
          IF (MATS.EQ.7.OR.MATS.EQ.26.OR.MATS.EQ.27.OR.MATS.EQ.31.OR.MATS.EQ.37.OR.MATS.EQ.58) THEN
            IF (MATS.EQ.26) THEN
                  MTE=232; IELAS=0
            ELSEIF (MATS.EQ.31) THEN
                  MTE=230; IELAS=0
            ELSEIF (MATS.EQ.58) THEN
                  MTE=236; IELAS=1
            ELSEIF (MATS.EQ.7) THEN
                  MTE=226; IELAS=1
            ELSEIF (MATS.EQ.27) THEN
                  MTE=234; IELAS=0
            ELSEIF (MATS.EQ.37) THEN
                  MTE=224; IELAS=1
            ENDIF
            WRITE(J2,'(4I4," /")') MTI,NBINT,MTE,IELAS
                  ELSE
            WRITE(J2,'(I4," /")') MTI
          ENDIF
!
!         [END]
          WRITE(J2,'("stop")')
!
          CLOSE(J2)
        ENDDO
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PROCESSING
!     ================================================================================
!     [MAKE NUCLIDEWISE DIRECTORY & MOVE NJOY INPUT FILES]
!     +NEUTRON XS
      DO J1=1,MXN1
        AA=DIRNAME1(J1)
        AA2=INPALL1(J1)
        BB=' '
        CC=' '
        WRITE(BB,'("mkdir ",2X,A13)') AA
        WRITE(CC,'("move ",2X,A14,2X,A13)') AA2,AA
        I=SYSTEM(BB)
        I=SYSTEM(CC)
      ENDDO
```

```
!
!     +THERMAL SCATTERING XS
      DO J1=1,MXN2
        DD=DIRNAME2(J1)
        DD2=INPALL2(J1)
        BB=' '
        CC=' '
        WRITE(BB,'("mkdir ",2X,A20)') DD
        WRITE(CC,'("move ",2X,A20,2X,A20)') DD2,DD
        I=SYSTEM(BB)
        I=SYSTEM(CC)
      ENDDO
!
!     ================================================================================
!     PREPARE BATCH FILE TO RUN NJOY FOR ALL NUCLIDES
!     ================================================================================
!
!     [Prepare batch file to run NJOY for all nuclides]
      WRITE(3,'("REM ========================================")')
      WRITE(3,'("REM  BATCH FILE FOR MULTIPLE NJOY RUN ")')
      WRITE(3,'("REM ========================================")')
      DO I=1,MXLIB1
        WRITE(3,'(2A25)') EXEFILE(2),LIBENDF1(I)
      ENDDO
      DO I=1,MXLIB2
        WRITE(3,'(2A25)') EXEFILE(2),LIBENDF2(I)
      ENDDO
      WRITE(3,*)
!
      I=SYSTEM('mkdir acer_out')
      I=SYSTEM('mkdir xsdir_out')
!
      DO I=1,MXN1
        DO IT=1,NDAT1(I,3)
          WRITE(3,'("REM ========================================")')
          WRITE(3,'("REM ",I3,2X,A11,3X,I6,1X,F6.1," K")') I,NUCLX1(I),NDAT1(I,1),TEMP1(I,IT)
          WRITE(3,'("REM ========================================")')
          WRITE(3,'("cd   ",A20)') DIRNAME1(I)
          WRITE(3,'("del  tape* output")')
          WRITE(3,'("copy ",A25," tape20")') LIBENDF1(NDAT1(I,2))
          WRITE(3,'("copy ",A25," tape29")') LIBENDF2(1)
          WRITE(3,'(A25,"   <  ",A20)') EXEFILE(1),INPFILE1(I,IT)
          WRITE(3,'("move output",1X,"out_",A20)') INPFILE1(I,IT)
          WRITE(3,'("move tape70",1X,"t70_",A20)') INPFILE1(I,IT)
          WRITE(3,'("move tape71",1X,"xsd_",A20)') INPFILE1(I,IT)
          WRITE(3,'(A25,1X,"t70_",A20)') EXEFILE(2),INPFILE1(I,IT)
          WRITE(3,'(A25,1X,"xsd_",A20)') EXEFILE(2),INPFILE1(I,IT)
          WRITE(3,'("type ","xsd_",A20," >> ..\xsdir")') INPFILE1(I,IT)
          WRITE(3,'("move t70_* ..\acer_out\")')
          WRITE(3,'("move xsd_* ..\xsdir_out\")')
          WRITE(3,'("del  tape* output")')
          WRITE(3,'("cd .. ")')
          WRITE(3,*)
        ENDDO
      ENDDO
!
      DO I=1,MXN2
        DO IT=1,NDAT2(I,4)
          WRITE(3,'("REM ========================================")')
          WRITE(3,'("REM ",I3,2X,A11,3X,I6,1X,F6.1," K")') I,NUCLX2(I),NDAT2(I,1),TEMP2(I,IT)
          WRITE(3,'("REM ========================================")')
          WRITE(3,'("cd   ",A20)') DIRNAME2(I)
          WRITE(3,'("del  tape* output")')
          WRITE(3,'("copy ",A25," tape20")') LIBENDF1(1)
```

```
          WRITE(3,'("copy ",A25," tape29")') LIBENDF2(NDAT2(I,3))
          WRITE(3,'(A25,"   <  ",A20)') EXEFILE(1),INPFILE2(I,IT)
          WRITE(3,'("move output",1X,"out_",A20)') INPFILE2(I,IT)
          WRITE(3,'("move tape70",1X,"t70_",A20)') INPFILE2(I,IT)
          WRITE(3,'("move tape71",1X,"xsd_",A20)') INPFILE2(I,IT)
          WRITE(3,'(A25,1X,"t70_",A20)') EXEFILE(2),INPFILE2(I,IT)
          WRITE(3,'(A25,1X,"xsd_",A20)') EXEFILE(2),INPFILE2(I,IT)
          WRITE(3,'("type ","xsd_",A20," >> ..\xsdir")') INPFILE2(I,IT)
          WRITE(3,'("move t70_* ..\acer_out\")')
          WRITE(3,'("move xsd_* ..\xsdir_out\")')
          WRITE(3,'("del  tape* output")')
          WRITE(3,'("cd .. ")')
          WRITE(3,*)
        ENDDO
      ENDDO
!
      CLOSE(3)
!
      STOP
      END


      SUBROUTINE ERROR(SSWX)
!     ================================================================================
!     FUNCTION    : PRINT OUT ERROR MESSAGE                                         +
!     ================================================================================
      CHARACTER(*) SSWX
!
      WRITE(6,'(A)') SSWX
!
      STOP
      END


      CHARACTER(20) FUNCTION DELBLANK(SS20C)
!     ================================================================================
!     FUNCTION    : DELETE BLANKS                                                   +
!     ================================================================================
      CHARACTER(20) SS20C,SS20D
      CHARACTER(1) BLNK
      PARAMETER(BLNK=' ')
!
      SS20D=' '
      IX=0
      DO L=1,20
        IF (SS20C(L:L).NE.BLNK) THEN
          IX=IX+1
          SS20D(IX:IX)=SS20C(L:L)
        ENDIF
      ENDDO
      DELBLANK=SS20D
!
      RETURN
      END
```

Appendix B. Program source of ANJOYMC for LINUX

```
      PROGRAM ANJOYMC_LINUX
!     ================================================================================
!     PROGRAM     : ANJOYMC_LINUX                                                    +
!                   (AUTOMATIC NJOY INPUT PREPARATION FOR MONTE CARLO CALCULATION)   +
!     FUNCTION    : AUTOMATIC PREPARATION FOR THE NJOY INPUT FILES AND BATCH FILE    +
!                   TO GENERATE ACE LIBRARY FILES FOR MONTE CARLO CODES               +
!     AUTHOR      : KANG-SEOG KIM                                                    +
!     DATE        : FEBRUARY 15, 2007                                                +
!     REMARKS     : NONE                                                             +
!     ================================================================================
      REAL,ALLOCATABLE :: TEMP1(:,:),TEMP2(:,:)
      INTEGER,ALLOCATABLE :: NDAT1(:,:),NDAT2(:,:),NUM(:)
      CHARACTER(11),ALLOCATABLE :: NUCLX1(:),NUCLX2(:)
      CHARACTER(6),ALLOCATABLE :: NUCLY1(:),NUCLY2(:)
      CHARACTER(20),ALLOCATABLE :: DIRNAME1(:),DIRNAME2(:),INPFILE1(:,:),            &
                                   INPFILE2(:,:),INPALL1(:),INPALL2(:)
      CHARACTER(2) AELEM(100)
!
      CHARACTER(1) SS1,BLANK
      CHARACTER(4) SS4
      CHARACTER(12) TITLE
      CHARACTER(25) LIBENDF1(10),LIBENDF2(10),EXEFILE(2)
      CHARACTER(13) AA,SS13
      CHARACTER(14) AA2,SS14
      CHARACTER(20) SS20,SS20A,DD,DD2,DELBLANK
      CHARACTER(50) BB,CC
!
      CHARACTER(1) S1
      CHARACTER(11) NIDXX
      CHARACTER(12) EE
      CHARACTER(13) SS13A
      CHARACTER(300) SSL
!
      PARAMETER (BLANK=' ')
!
      DATA AELEM/'h ','he','li','be','b ','c ','n ','o ','f ','ne',                  &
                 'na','mg','al','si','p ','s ','cl','ar','k ','ca',                  &
                 'sc','ti','v ','cr','mn','fe','co','ni','cu','zn',                  &
                 'ga','ge','as','se','br','kr','rb','sr','y ','zr',                  &
                 'nb','mo','tc','ru','rh','pd','ag','cd','in','sn',                  &
                 'sb','te','i ','xe','cs','ba','la','ce','pr','nd',                  &
                 'pm','sm','eu','gd','tb','dy','ho','er','tm','yb',                  &
                 'lu','hf','ta','w ','re','os','ir','pt','au','hg',                  &
                 'tl','pb','bi','po','at','rn','fr','ra','ac','th',                  &
                 'pa','u ','np','pu','am','cm','bk','cf','es','fm' /
!
      OPEN(1,FILE='anjoymc_linux.in',STATUS='OLD')         !MAIN CONTROL DECK
      OPEN(2,FILE='anjoymc.out',STATUS='UNKNOWN')        !OUTPUT FILE
      OPEN(3,FILE='runnjoym.bat',STATUS='UNKNOWN')       !BATCH FILE TO RUN NJOY
!
!     -------------------------------------------------------------------------------
!     [DESCRIPTION FOR THE MAIN CONTROL DECK]                                        +
!                                                                                    +
!     %TIT : DIEMNSION FOR MEMORY ALLOCATION                                         +
!       [TITLE]                                                                      +
!        TITLE      (A12)  TITLE CARD                                               +
!                                                                                    +
!     %DIM : DIEMNSION FOR MEMORY ALLOCATION                                         +
!       [MXLIB1,MXN1]                                                                +
!       [MXLIB2,MXN2]                                                                +
!        MXLIB1     (I)    THE NUMBER OF ENDF LIBRARIES                             +
```

```
!       MXN1       (I)    THE NUMBER OF NUCLIDES FOR NORMAL CROSS SECTIONS          +
!       MXLIB2     (I)    THE NUMBER OF ENDF THERMAL SCATTERING LIBRARIES           +
!       MXN2       (I)    THE NUMBER OF NUCLIDES FOR THERMAL SCATTERING LIBRARY     +
!                                                                                   +
!     %OPT : OPTION                                                                 +
!       [TOLERANCE]                                                                 +
!        TOLERANCE  (R)    TOLERANCE IN DATA                                        +
!                                                                                   +
!     %LIB : ENDF/B LIBRARIES                                                       +
!       [I, LIBENDF1(I)] (I=1,MXLIB1)                                               +
!       [I, LIBENDF2(I)] (I=1,MXLIB2)                                               +
!        I          (I)    ORDERING NUMBER                                         +
!        LIBENDF1   (A25)  FILENAME FOR ENDF/B LIBRARY                             +
!        LIBENDF2   (A25)  FILENAME FOR ENDF/B THERMAL SCATTERING LIBRARY          +
!                                                                                   +
!     %EXE : EXECUTION FILES                                                        +
!       [I, EXEFILE(1)]                                                             +
!       [I, EXEFILE(2)]                                                             +
!        I          (I)    ORDERING NUMBER                                         +
!        EXEFILE(1) (A25)  NJOY EXECUTION FILE                                     +
!        EXEFILE(2) (A25)  CHECKSUM EXECUTION FILE                                 +
!                                                                                   +
!     %NUC                                                                          +
!       [I, NUCLX1(I), NUCLY1(I), (NDAT1(I,J),J=1,4), (TEMP1(I,K),K=1,NDAT1(I,3))]  +
!        I          (I)    ORDERING NUMBER                                         +
!        NUCLX1(I)  (A10)  NUCLIDE                                                 +
!        NUCLY1(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME       +
!        NDAT1(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF                        +
!                          J=2 : NUCLIDE ID NUMBER                                 +
!                          J=3 : THE NUMBER OF TEMPERATURES                        +
!        TEMP1(I,K) (R)    TEMPERATURE IN KELVIN                                   +
!                                                                                   +
!     %TSC                                                                          +
!       [I, NUCLX2(I), NUCLY2(I), (NDAT2(I,J),J=1,4), (TEMP2(I,K),K=1,NDAT2(I,4))]  +
!        I          (I)    NUCLIDE ORDERING NUMBER                                 +
!        NUCLX2(I)  (A10)  NUCLIDE                                                 +
!        NUCLY2(I)  (A6)   NUCLIDE NAME TO BE USED AS A PREFIX IN A FILENAME       +
!        NDAT2(I,J) (I)    J=1 : NUCLIDE MAT NUMBER IN ENDF                        +
!                          J=2 : NUCLIDE MATS NUMBER IN THERMAL SCATTERING LIBRARY  +
!                          J=3 : NUCLIDE ID NUMBER                                 +
!                          J=4 : # OF TEMPERATURE                                  +
!        TEMP2(I,K) (R) TEMPERATURE IN KELVIN                                      +
!     -------------------------------------------------------------------------------
!
!     [%TIT]
      READ(1,*) SS4
      IF (SS4.NE.'%TIT') CALL ERROR('%TIT IS MISSING')
      READ(1,'(A12)') TITLE
!
!     [%DIM]
      READ(1,*) SS4
      IF (SS4.NE.'%DIM') CALL ERROR('%DIM IS MISSING')
      READ(1,*) MXLIB1,MXN1
      READ(1,*) MXLIB2,MXN2
      ALLOCATE(NDAT1(MXN1,3),NDAT2(MXN2,4),TEMP1(MXN1,20),TEMP2(MXN2,20),NUM(11),     &
               NUCLX1(MXN1),NUCLY1(MXN1),NUCLX2(MXN2),NUCLY2(MXN2),DIRNAME1(MXN1),    &
               DIRNAME2(MXN2),INPFILE1(MXN1,20),INPFILE2(MXN2,20),INPALL1(MXN1),      &
               INPALL2(MXN2))
!
!     [%OPT]
      READ(1,*) SS4
      IF (SS4.NE.'%OPT') CALL ERROR('%OPT IS MISSING')
      READ(1,*) TOLERANCE
!
```

```
!     [%LIB]
      READ(1,*) SS4
      IF (SS4.NE.'%LIB') CALL ERROR('%LIB IS MISSING')
      DO I=1,MXLIB1
        READ(1,*) IL1,LIBENDF1(I)
      ENDDO
      DO I=1,MXLIB2
        READ(1,*) IL1,LIBENDF2(I)
      ENDDO
!
!     [%EXE]
      READ(1,*) SS4
      IF (SS4.NE.'%EXE') CALL ERROR('%EXE IS MISSING')
      READ(1,*) IL3,EXEFILE(1)
      READ(1,*) IL4,EXEFILE(2)
!
!     [%NUC]
      READ(1,*) SS4
      IF (SS4.NE.'%NUC') CALL ERROR('%NUC IS MISSING')
      DO I=1,MXN1
        READ(1,*) IX,NUCLX1(I),(NDAT1(I,J),J=1,3),(TEMP1(I,K),K=1,NDAT1(I,3))
        IF (IX.NE.I) CALL ERROR('ORDERUNG NUMBER IS WRONG IN %NUC')
      ENDDO
!
!     [%TSC]
      READ(1,*) SS4
      IF (SS4.NE.'%TSC') CALL ERROR('%TSC IS MISSING')
      DO I=1,MXN2
        READ(1,*) IX,NUCLX2(I),(NDAT2(I,J),J=1,4),(TEMP2(I,K),K=1,NDAT2(I,4))
        IF (IX.NE.I) CALL ERROR('ORDERUNG NUMBER IS WRONG IN %TSC')
      ENDDO
!
!     [INITIALIZATION]
      DIRNAME1=' '
      DIRNAME2=' '
      INPFILE1=' '
      INPFILE2=' '
!
!     ============================================================================
!     INPUT FILENAME & DIRECTORY NAME
!     ============================================================================
      DO J1=1,MXN1
        READ(NUCLX1(J1),'(I3,4X,I3,A1)') NID1,NID2,SS1
        IF (SS1.EQ.'M') SS1='m'
        NID=NID1*1000+NID2
        DO IT=1,NDAT1(J1,3)
          SS20=' '
          WRITE(SS20,'(I6,A1,".in",I2,"t")') NID,SS1,IT
          INPFILE1(J1,IT)=DELBLANK(SS20)
        ENDDO
      ENDDO
      DO J1=1,MXN2
        DO IT=1,NDAT2(J1,4)
          SS20=' '
          WRITE(SS20,'(A11,".in",I2,"t")') NUCLX2(J1),IT
          INPFILE2(J1,IT)=DELBLANK(SS20)
          WRITE(2,*) INPFILE2(J1,IT)
        ENDDO
      ENDDO
!
!     [MAKE NUCLIDEWISE DIRECTORY & MOVE NJOY INPUT FILES]
!     +NEUTRON XS
      DO J1=1,MXN1
        READ(NUCLX1(J1),'(I3,4X,I3,A1)') NID1,NID2,SS1
```

```
        IF (SS1.EQ.'M'.OR.SS1.EQ.'m') THEN
          SS1='m'
        ELSE
          SS1=' '
        ENDIF
        NID=NID1*1000+NID2
        SS20=' '
        AA=' '
        WRITE(SS20,'(I3,"_",I6,A1)') J1,NID,SS1
        DIRNAME1(J1)=DELBLANK(SS20)
        SS20=' '
        WRITE(SS20,'(I6,A1,".in*")') NID,SS1
        INPALL1(J1)=DELBLANK(SS20)
      ENDDO
!
!     +THERMAL SCATTERING XS
      DO J1=1,MXN2
        SS20=' '
        WRITE(SS20,'(I3,"_",A11)') J1,NUCLX2(J1)
        DIRNAME2(J1)=DELBLANK(SS20)
        SS20=' '
        WRITE(SS20,'(A11,".in*")') NUCLX2(J1)
        INPALL2(J1)=DELBLANK(SS20)
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PREPARATION FOR NEUTRON CROSS SECTION
!     ================================================================================
      S1="'"
      DO J1=1,MXN1
        DO IT=1,NDAT1(J1,3)
          J2=IT*1000+J1
          AA=INPFILE1(J1,IT)
          OPEN (J2,FILE=AA,STATUS='UNKNOWN')
!
          MAT=NDAT1(J1,1)        !MAT no.
          NTEMP=1                !# of temperature
          NIDXX=NUCLX1(J1)       !Nuclide name
!
!         [TITLE] ---------------------------------------
          WRITE(J2,'("-- KAERI ",A12," NJOY PROCESSING: ",A11,"(",I4,")")') TITLE,NIDXX,MAT
!
!         [MODER] ---------------------------------------
          WRITE(J2,'("moder  / Tape20(A) -> Tape21(B)")')
          WRITE(J2,'("1 -21")')
          WRITE(J2,'(A1,"ENDF/B-VI R8 ",A11,A1," /")') S1,NIDXX,S1
          WRITE(J2,'("20",1X,I4)') MAT
          WRITE(J2,'("0 /")')
!
!         [RECONR] ---------------------------------------
          WRITE(J2,'("reconr / XS Resconstruction Tape22(B)")')
          WRITE(J2,'("-21 -22")')
          WRITE(J2,'(A1,"PENDF FOR",A11," FROM ",A12,1X,A1," /")') S1,NIDXX,TITLE,S1
          WRITE(J2,'(I4," 2 /")') MAT
          ERR=TOLERANCE
          WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') ERR
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,A1," /")') S1,TITLE,NIDXX,S1
          WRITE(J2,'(A1,"PROCESSED BY NJOY-99.90 ",A1," /")') S1,S1
          WRITE(J2,'("0 /")')
!
!         [BROADR] ---------------------------------------
          WRITE(J2,'("broadr / Doppler Broadening Tape23(B)")')
          WRITE(J2,'("-21 -22 -23")')
          WRITE(J2,'(I4,1X,I2,1X,"0 1 /")') MAT,NTEMP
```

```
          WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') TOLERANCE
!          WRITE(J2,'(" 0.001 /")')
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'("0 /")')
!
!         [UNRESR] --------------------------------------
          WRITE(J2,'("unresr / Unresolved XS Tape24(B)")')
          WRITE(J2,'("-21 -23 -24")')
          NSIGZ=1
          IPRINT=1
          SIGZ=1.0E+15
          WRITE(J2,'(I4,1X,3I3)') MAT,NTEMP,NSIGZ,IPRINT
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'(1PE8.1," /")') SIGZ
          WRITE(J2,'("0 /")')
!
!         [HEATR] --------------------------------------
          WRITE(J2,'("heatr / Kerma & Damage Tape25(B)")')
          WRITE(J2,'("-21 -24 -25 /")')
          WRITE(J2,'(I4," /")') MAT
!
!         [PURR] ---------------------------------------
          WRITE(J2,'("purr / Probalility table Tape26(B)")')
          WRITE(J2,'("-21 -25 -26")')
          NSIGZ=1
          NBIN=20
          NLADR=64
          SIGZ=1.0E+15
          WRITE(J2,'(I4,1X,4I3," /")') MAT,NTEMP,NSIGZ,NBIN,NLADR
          WRITE(J2,'(F7.1," /")') TEMP1(J1,IT)
          WRITE(J2,'(1PE8.1," /")') SIGZ
          WRITE(J2,'("0 /")')
!
!         [ACER] ---------------------------------------
          WRITE(J2,'("acer  / Tape70(A)")')
          WRITE(J2,'("-21 -26 0 50 51 ")')
          IOPT=1
          IPRINT=0
          NTYPE=1
          SUFF=FLOAT(IT)/100
          WRITE(J2,'(3I3,2X,F4.2," /")') IOPT,IPRINT,NTYPE,SUFF
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                           S1,TITLE,NIDXX,TEMP1(J1,IT),S1
          WRITE(J2,'(I4,2X,F6.1," /")') MAT,TEMP1(J1,IT)
          WRITE(J2,'("/")')
          WRITE(J2,'("/")')
          WRITE(J2,'("acer")')
          WRITE(J2,'("0 50 0 70 71 ")')
          WRITE(J2,'("7 1 1 -1 /")')
          WRITE(J2,'(A1,A12," FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                           S1,TITLE,NIDXX,TEMP1(J1,IT),S1
!
!         [END]
          WRITE(J2,'("stop")')
!
          CLOSE(J2)
        ENDDO
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PREPARATION FOR NEUTRON THERMAL SCATTERING
!       NDAT2(I,J)  : I=1,MXN2; J=1..4
!     ================================================================================
      DO J1=1,MXN2
```

```
      DO IT=1,NDAT2(J1,4)
!
        DD=INPFILE2(J1,IT)
        J2=IT*1000+J1
        OPEN (J2,FILE=DD,STATUS='UNKNOWN')
!
        MAT=NDAT2(J1,1)      !MAT no.
        MATS=NDAT2(J1,2)     !Thermal scattering MAT no.
        NTEMP=1              !# of temperature
        NIDXX=NUCLX2(J1)   !Nuclide name
!
!       [TITLE] ---------------------------------------
        WRITE(J2,'("-- KAERI ",A12," NJOY PROCESSING: ",A11,"(",I4,")")') TITLE,NIDXX,MAT
!
!       [MODER] ---------------------------------------
        WRITE(J2,'("moder  / Tape20(A) -> Tape21(B)")')
        WRITE(J2,'("1 -21")')
        WRITE(J2,'(A1,A12,1X,A11,A1," /")') S1,TITLE,NIDXX,S1
        WRITE(J2,'("20",1X,I4)') MAT
        WRITE(J2,'("0 /")')
!
!       [MODER] ---------------------------------------
        WRITE(J2,'("moder  / Tape29(A) -> Tape23(B)")')
        WRITE(J2,'("29 -23")')
!
!       [RECONR] --------------------------------------
        WRITE(J2,'("reconr / XS Resconstruction Tape22(B)")')
        WRITE(J2,'("-21 -24")')
        WRITE(J2,'(A1,"PENDF FOR",A11," FROM ",A12,1X,A1," /")') S1,NIDXX,TITLE,S1
        WRITE(J2,'(I4," 2 /")') MAT
        ERR=TOLERANCE
        WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') ERR
        WRITE(J2,'(A1,A12," FOR MCNP ",A11,A1," /")') S1,TITLE,NIDXX,S1
        WRITE(J2,'(A1,"PROCESSED BY NJOY-99.90 ",A1," /")') S1,S1
        WRITE(J2,'("0 /")')
!
!       [BROADR] --------------------------------------
        WRITE(J2,'("broadr / Doppler Broadening Tape23(B)")')
        WRITE(J2,'("-21 -24 -22")')
        WRITE(J2,'(I4,1X,I2,1X," /")') MAT,NTEMP
        WRITE(J2,'(1F10.5," / Reconstruction 0.1% ")') TOLERANCE
!        WRITE(J2,'("0.001 /")')
        WRITE(J2,'(F7.1," /")') TEMP2(J1,IT)
        WRITE(J2,'("0 /")')
!
!       [THERMR] --------------------------------------
        WRITE(J2,'("thermr / Thermal Scattering XS ")')
        WRITE(J2,'("-23 -22 -24")')
        NBIN=8
        IINC=4
        ICOH=0
        IF (MATS.EQ.31) ICOH=1      !Graphite
        IF (MATS.EQ.26) ICOH=2      !Be
        IF (MATS.EQ.27) ICOH=3      !BeO
        IF (MATS.EQ.37) ICOH=11     !Polyethylene
        IF (MATS.EQ.7)  ICOH=12     !H(ZrH)
        IF (MATS.EQ.58) ICOH=13     !Zr(ZrH)
        NATOM=1
        IF (MATS.EQ.1.OR.MATS.EQ.11.OR.MATS.EQ.37) NATOM=2
        IF (MATS.EQ.1)  MTREF=222   !H(H2O)
        IF (MATS.EQ.11) MTREF=228   !D(D2O)
        IF (MATS.EQ.26) MTREF=231   !Be metal  (MTE=232) coherent
        IF (MATS.EQ.31) MTREF=229   !Graphite  (MTE=230) coherent
        IF (MATS.EQ.58) MTREF=235   !Zr(ZrH)   (MTE=236) incoherent
```

```
          IF (MATS.EQ.7)  MTREF=225   !H(ZrH)     (MTE=226) incoherent
          IF (MATS.EQ.27) MTREF=233   !BeO        (MTE=234) coherent
          IF (MATS.EQ.37) MTREF=223   !H(CH2)     (MTE=224) incoherent
          IPRINT=1
          WRITE(J2,'(I3,I5,5I3,I4,I3)') MATS,MAT,NBIN,NTEMP,IINC,ICOH,NATOM,MTREF,IPRINT
          WRITE(J2,'(F7.1)') TEMP2(J1,IT)
          !WRITE(J2,'(" 0.001  4.0 ")')
          WRITE(J2,'(1F10.5,"  4.0 ")') TOLERANCE
!
!         [ACER] ---------------------------------------
          WRITE(J2,'("acer  / Tape70(A)")')
          WRITE(J2,'("-21 -24 0 70 71 ")')
          IOPT=2
          IPRINT=1
          NTYPE=1
          SUFF=FLOAT(IT)/100
          MTI=MTREF
          NBINT=16
          WRITE(J2,'(3I3,2X,F4.2," /")') IOPT,IPRINT,NTYPE,SUFF
          WRITE(J2,'(A1,"ENDF/B-VI R8 FOR MCNP ",A11,"(",F6.1,"K)",A1," /")')         &
                          S1,NIDXX,TEMP2(J1,IT),S1
          WRITE(J2,'(I4,2X,F6.1,2X,A6," /")') MAT,TEMP2(J1,IT),NUCLY2(J1)
          WRITE(J2,'(I6," /")') NDAT2(J1,3)
          IF (MATS.EQ.7.OR.MATS.EQ.26.OR.MATS.EQ.27.OR.MATS.EQ.31.OR.MATS.EQ.37.OR.MATS.EQ.58) THEN
            IF (MATS.EQ.26) THEN
                  MTE=232; IELAS=0
            ELSEIF (MATS.EQ.31) THEN
                  MTE=230; IELAS=0
            ELSEIF (MATS.EQ.58) THEN
                  MTE=236; IELAS=1
            ELSEIF (MATS.EQ.7) THEN
                  MTE=226; IELAS=1
            ELSEIF (MATS.EQ.27) THEN
                  MTE=234; IELAS=0
            ELSEIF (MATS.EQ.37) THEN
                  MTE=224; IELAS=1
            ENDIF
            WRITE(J2,'(4I4," /")') MTI,NBINT,MTE,IELAS
                  ELSE
            WRITE(J2,'(I4," /")') MTI
          ENDIF
!
!         [END]
          WRITE(J2,'("stop")')
!
          CLOSE(J2)
        ENDDO
      ENDDO
!
!     ================================================================================
!     NJOY INPUT PROCESSING
!     ================================================================================
!     [MAKE NUCLIDEWISE DIRECTORY & MOVE NJOY INPUT FILES]
!     +NEUTRON XS
      DO J1=1,MXN1
        AA=DIRNAME1(J1)
        AA2=INPALL1(J1)
        BB=' '
        CC=' '
        WRITE(BB,'("mkdir ",2X,A13)') AA
        WRITE(CC,'("mv ",2X,A14,2X,A13)') AA2,AA
        I=SYSTEM(BB)
        I=SYSTEM(CC)
      ENDDO
```

```
!
!     +THERMAL SCATTERING XS
      DO J1=1,MXN2
        DD=DIRNAME2(J1)
        DD2=INPALL2(J1)
        BB=' '
        CC=' '
        WRITE(BB,'("mkdir ",2X,A20)') DD
        WRITE(CC,'("mv ",2X,A20,2X,A20)') DD2,DD
        I=SYSTEM(BB)
        I=SYSTEM(CC)
      ENDDO
!
!     ============================================================================
!     PREPARE BATCH FILE TO RUN NJOY FOR ALL NUCLIDES
!     ============================================================================
!
!     [Prepare batch file to run NJOY for all nuclides]
      WRITE(3,'("# ========================================")')
      WRITE(3,'("#  BATCH FILE FOR MULTIPLE NJOY RUN ")')
      WRITE(3,'("# ========================================")')
      DO I=1,MXLIB1
        WRITE(3,'(2A25)') EXEFILE(2),LIBENDF1(I)
      ENDDO
      DO I=1,MXLIB2
        WRITE(3,'(2A25)') EXEFILE(2),LIBENDF2(I)
      ENDDO
      WRITE(3,*)
!
      I=SYSTEM('mkdir acer_out')
      I=SYSTEM('mkdir xsdir_out')
!
      DO I=1,MXN1
        DO IT=1,NDAT1(I,3)
          WRITE(3,'("# ========================================")')
          WRITE(3,'("# ",I3,2X,A11,3X,I6,1X,F6.1," K")') I,NUCLX1(I),NDAT1(I,1),TEMP1(I,IT)
          WRITE(3,'("# ========================================")')
          WRITE(3,'("cd   ",A20)') DIRNAME1(I)
          WRITE(3,'("rm -rf tape* output")')
          WRITE(3,'("cp ",A25," tape20")') LIBENDF1(NDAT1(I,2))
          WRITE(3,'("cp ",A25," tape29")') LIBENDF2(1)
          WRITE(3,'(A25,"   <  ",A20)') EXEFILE(1),INPFILE1(I,IT)
          WRITE(3,'("mv output",1X,"out_",A20)') INPFILE1(I,IT)
          WRITE(3,'("mv tape70",1X,"t70_",A20)') INPFILE1(I,IT)
          WRITE(3,'("mv tape71",1X,"xsd_",A20)') INPFILE1(I,IT)
          WRITE(3,'(A25,1X,"t70_",A20)') EXEFILE(2),INPFILE1(I,IT)
          WRITE(3,'(A25,1X,"xsd_",A20)') EXEFILE(2),INPFILE1(I,IT)
          WRITE(3,'("cat ","xsd_",A20," >> ../xsdir")') INPFILE1(I,IT)
          WRITE(3,'("mv t70_* ../acer_out/")')
          WRITE(3,'("mv xsd_* ../xsdir_out/")')
          WRITE(3,'("rm -rf  tape* output temp*")')
          WRITE(3,'("cd .. ")')
          WRITE(3,*)
        ENDDO
      ENDDO
!
      DO I=1,MXN2
        DO IT=1,NDAT2(I,4)
          WRITE(3,'("# ========================================")')
          WRITE(3,'("# ",I3,2X,A11,3X,I6,1X,F6.1," K")') I,NUCLX2(I),NDAT2(I,1),TEMP2(I,IT)
          WRITE(3,'("# ========================================")')
          WRITE(3,'("cd   ",A20)') DIRNAME2(I)
          WRITE(3,'("rm -rf  tape* output")')
          WRITE(3,'("cp ",A25," tape20")') LIBENDF1(1)
```

```
          WRITE(3,'("cp ",A25," tape29")') LIBENDF2(NDAT2(I,3))
          WRITE(3,'(A25,"   <  ",A20)') EXEFILE(1),INPFILE2(I,IT)
          WRITE(3,'("mv output",1X,"out_",A20)') INPFILE2(I,IT)
          WRITE(3,'("mv tape70",1X,"t70_",A20)') INPFILE2(I,IT)
          WRITE(3,'("mv tape71",1X,"xsd_",A20)') INPFILE2(I,IT)
          WRITE(3,'(A25,1X,"t70_",A20)') EXEFILE(2),INPFILE2(I,IT)
          WRITE(3,'(A25,1X,"xsd_",A20)') EXEFILE(2),INPFILE2(I,IT)
          WRITE(3,'("cat ","xsd_",A20," >> ../xsdir")') INPFILE2(I,IT)
          WRITE(3,'("mv t70_* ../acer_out/")')
          WRITE(3,'("mv xsd_* ../xsdir_out/")')
          WRITE(3,'("rm -rf  tape* output temp*")')
          WRITE(3,'("cd .. ")')
          WRITE(3,*)
        ENDDO
      ENDDO
!
      CLOSE(3)
!
      STOP
      END


      SUBROUTINE ERROR(SSWX)
!     ================================================================================
!     FUNCTION    : PRINT OUT ERROR MESSAGE                                         +
!     ================================================================================
      CHARACTER(*) SSWX
!
      WRITE(6,'(A)') SSWX
!
      STOP
      END


      CHARACTER(20) FUNCTION DELBLANK(SS20C)
!     ================================================================================
!     FUNCTION    : DELETE BLANKS                                                   +
!     ================================================================================
      CHARACTER(20) SS20C,SS20D
      CHARACTER(1) BLNK
      PARAMETER(BLNK=' ')
!
      SS20D=' '
      IX=0
      DO L=1,20
        IF (SS20C(L:L).NE.BLNK) THEN
          IX=IX+1
          SS20D(IX:IX)=SS20C(L:L)
        ENDIF
      ENDDO
      DELBLANK=SS20D
!
      RETURN
      END
```

서 지 정 보 양 식			
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몬테칼로 코드용 단면적 라이브러리 생산 자동화 프로그램 ANJOYMC 개발	
연구책임자 및 부서명 (AR,TR일 경우 주저자)	김강석 (원자로공학연구부)
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초 록

미국의 Los Alamos 국립연구소에서 개발한 NJOY 코드는 ENDF/B 양식의 평가핵자료를 처리하여 MCNP와 McCARD 등의 몬테칼로 코드에 사용되는 ACE 양식의 라이브러리를 생산한다. 수백종에 달하는 핵종과 온도에 따라 NJOY 입력을 준비하여 라이브러리를 생산하는 과정은 상당한 시간을 필요로 할 뿐만 아니라 사용자의 에러를 유발할 여지가 있다. 이러한 문제를 해결하기 위하여 간단한 사용자의 입력으로 NJOY 입력을 자동으로 생산하여 줄 뿐만 아니라 배치파일을 만들어 라이브러리를 생산하는 모든 과정을 자동으로 수행하는 프로그램인 ANJOYMC를 개발하였다.

ANJOYMC 프로그램은 WINDOWS 와 LINUX 를 OS 로 하는 PC 에서 구동하도록 Fortran90 을 이용하여 개발되었다. 간단한 사용자 입력으로 짧은 시간안에 사용자의 에러 없이 ACE 양식의 라이브러리를 생산할 수 있다.

주제명키워드

ANJOYMC, ENDF/B, 몬테칼로, 라이브러리

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Abstract

The NJOY code developed at Los Alamos National Laboratory is to generate the cross section libraries in ACE format for the Monte Carlo codes such as MCNP and McCARD by processing the evaluated nuclear data in ENDF/B format. It takes long time to prepare all the NJOY input files for hundreds of nuclides with various temperatures, and there can be some errors in the input files. In order to solve these problems, ANJOYMC program has been developed. By using a simple user input deck, this program is not only to generate all the NJOY input files automatically, but also to generate a batch file to perform all the NJOY calculations.

The ANJOYMC program is written in Fortran90 and can be executed under the WINDOWS and LINUX operating systems in Personal Computer. Cross setion libraries in ACE format can be generated in a short time and without an error by using a simple user input deck.

Subject Keyword

ANJOYMC, ENDF/B, Monte Carlo, Library