Appendix C.   TEST PROBLEMS

The NJOY test problems have two purposes: first, they provide readily available examples for the user on how to run the code, and second, they provide Quality Assurance (QA) verification that the code has been installed correctly on the user's computer system. The current test problem suite is inadequate for the second purpose, and we hope to expand it significantly.

1.   Test Problem 1

This problem demonstrates how to prepare data for natural carbon as given on the ENDF/B-V "Standards Tape." This evaluation is freely available without restrictions (which is not true of all of ENDF/B-V).

The input cards for NJOY are listed below in the form of a UNIX shell script. We normally run this script in a subdirectory called `TEST`, and the first few cards copy the ENDF general-purpose and thermal data from their normal locations in the next higher directory into the test subdirectory. Note that the data files are assigned the local names `TAPE20` and `TAPE26`. The `CAT` line starts a "here" file, which continues down to the `EOF` line near the end of the input. The NJOY code is then run using this new input file, and the output file and PENDF file are saved in the names `OUT1` and `PEND1` for later comparisons with previous runs.

The following input file is given using uppercase characters. On many systems, lowercase will be used instead. The user will have to determine if an uppercase or lowercase method was used when NJOY was installed.

```
ECHO 'GETTING ENDF TAPE 511'
CP ../T511 TAPE20
ECHO 'GETTING THERMAL TAPE 322'
CP ../T322 TAPE26
ECHO 'RUNNING NJOY'
CAT>INPUT <<EOF
 0
 5
 *MODER*
 20 -21
 *RECONR*
 -21 -22
 *PENDF TAPE FOR C-NAT FROM ENDF/B TAPE 511*/
 1306 3/
 .005 0. 7/
 *6-C-NAT FROM TAPE 511*/
 *PROCESSED BY THE NJOY NUCLEAR DATA PROCESSING SYSTEM*/
 *SEE ORIGINAL ENDF/B-V TAPE FOR DETAILS OF EVALUATION*/
 0/
```

```
*BROADR*
-22 -23
1306 1/
.005/
300.
0/
*HEATR*
-21 -23 -22
1306 1/
444
*THERMR*
26 -22 -24
1065 1306 8 1 1 0 1 221 0
300.
.05 1.2
*THERMR*
26 -24 -23
1065 1306 8 1 4 1 1 229 0
300.
.05 1.2
*GROUPR*
-21 -23 0 -24
1306 3 3 3 3 1 1 1
*CARBON IN GRAPHITE*/
300
1.E10
3 1 *TOTAL*/
3 2 *ELASTIC*/
3 4 *INELASTIC*/
3 51 *DISCRETE INELASTIC*/
3 -68 *CONTINUED*/
3 91 *CONTINUUM INELASTIC*/
3 102 *N,G*/
3 103 *(N,P)*/
3 104 *(N,D)*/
3 107 *(N,A)*/
3 203 *TOTAL H PRODUCTION*/
3 204 *TOTAL H2 PRODUCTION*/
3 207 *TOTAL HE4 PRODUCTION*/
3 221 *FREE THERMAL SCATTERING*/
3 229 *GRAPHITE INELASTIC THERMAL SCATTERING*/
3 230 *GRAPHITE ELASTIC THERMAL SCATTERING*/
3 251 *MUBAR*/
3 252 *XI*/
3 253 *GAMMA*/
3 301 *TOTAL HEAT PRODUCTION*/
3 444 *TOTAL DAMAGE ENERGY PRODUCTION*/
6 2 *ELASTIC*/
6 51 *DISCRETE INELASTIC*/
6 -68 *CONTINUED*/
6 91 *CONTINUUM INELASTIC*/
6 221 *FREE THERMAL SCATTERING*/
6 229 *GRAPHITE INELASTIC THERMAL SCATTERING*/
```

```
 6 230 *GRAPHITE ELASTIC THERMAL SCATTERING*/
 17 51 *INELASTIC GAMMA PRODUCTION*/
 16 102 *CAPTURE GAMMA PRODUCTION*/
 0/
 0/
 *MODER*
 -23 25
 *STOP*
EOF
../XNJOY<INPUT
ECHO 'SAVING OUTPUT FILES'
CP OUTPUT OUT1
CP TAPE25 PEND1
```

The first step is to run the MODER module to convert the ASCII ENDF file to binary mode. Using binary mode will often cut the cost of running NJOY jobs by a factor of two. RECONR is then used to linearize and unionize the cross sections (no resonance reconstruction is needed for carbon). A tolerance of 0.5% was requested for this linearization, and 7 significant figures will be used for all energy grid values. The BROADR module is used to Doppler-broaden the carbon cross sections to 300 K. It is recommended that the same thinning and reconstruction tolerances be used in BROADR as are used in RECONR.

This NJOY run supplements the original ENDF data with computed values for heating, radiation damage, and thermal scattering. The call to the HEATR module requests MT444 to get the damage cross section; heating (MT301) is automatically provided. The first of the two THERMR runs generates thermal scattering data for a carbon free gas at 300 K (MT221). The second THERMR run generates data for graphite (MT229). The "4" on the input card directs the module to use the $S(\alpha, \beta)$ data from MT1065 on `TAPE26` in order to compute the inelastic scattering cross section and scattering matrix, and the following "1" directs it to compute the coherent elastic scattering cross section using built-in parameters for graphite.

When the second THERMR run has finished, `TAPE23` contains the complete PENDF tape needed by GROUPR. Multigroup neutron reaction and photon production cross sections are computed using the Los Alamos 30-group structure for neutrons, the Los Alamos 12-group structure for photons, and the CLAW weight function. The scattering order is P_3. Note that the long-input form is used to specify the list of reactions to be processed. Most users now prefer the automatic input option. The user has to carefully look at the reactions available on the ENDF tape and to consider the additional reactions added by HEATR and THERMR. Note especially the inclusion of several gas production reactions from the ENDF tape, the thermal reactions MT221 and MT229 from the PENDF tape, and MT301 and MT444 as generated by HEATR from the PENDF tape. The output is easy to read, but remember that groups are given in the order of increasing energy.

The thermal scattering reactions must also be requested in the scattering matrix section (MFD=6). MT230 was automatically generated by THERMR at MT229+1 when coherent elastic scattering for graphite was requested.

Photon production matrices are requested in the lines with `MFD=17` and `MFD=16`. Actually, the use of "17" to denote data given in MF13 on the ENDF tape is no longer required by GROUPR.

As a last step, this problem runs MODER once more to convert the binary PENDF tape to ASCII mode.

2. Test Problem 2

The second problem supplements the first by adding resonance reconstruction and output formatting. The ENDF/B-IV material Pu-238 (MAT1050) was originally chosen for this problem because it was freely available and its execution time was fairly small.

```
ECHO 'GETTING ENDF TAPE 404'
CP ../T404 TAPE20
ECHO 'RUNNING NJOY'
CAT>INPUT <<EOF
 0
 4
 *MODER*
 20 -21
 *RECONR*
 -21 -22
 *PENDF TAPE FOR PU-238 FROM ENDF/B-IV TAPE 404*/
 1050 3/
 .005 0. 7/
 *94-PU-238 FROM ENDF/B TAPE T404*/
 *PROCESSED BY THE NJOY NUCLEAR DATA PROCESSING SYSTEM*/
 *SEE ORIGINAL ENDF/B-IV TAPE FOR DETAILS OF EVALUATION*/
 0/
 *BROADR*
 -22 -23
 1050 3 0 1 0 /
 .005/
 300. 900. 2100.
 0/
 *UNRESR*
 -21 -23 -22
 1050 3 7 1
 300 900 2100
```

```
 1.E10 1.E5 1.E4 1000. 100. 10. 1
 0/
 *GROUPR*
 -21 -22 0 -25
 1050 5 0 4 3 3 7 1
 *94-PU-238*/
 300. 900. 2100.
 1.E10 1.E5 1.E4 1000. 100. 10. 1
 .1 0.025 0.8208E06 1.4E06
 3 1 *TOTAL*/
 3 2 *ELASTIC*/
 3 16 *N2N*/
 3 17 *N3N*/
 3 18 *FISSION*/
 3 102 *CAPTURE*/
 3 251 *MUBAR*/
 3 252 *XI*/
 3 253 *GAMMA*/
 3 259 *1/V*/
 6 2 *ELASTIC*/
 6 16 *N2N*/
 6 17 *N,3N*/
 6 18 *FISSION*/
 6 51 *DISCRETE INELASTIC*/
 6 -59 *CONTINUED*/
 6 91 *CONTINUUM INELASTIC*/
 0/
 3 1 *TOTAL*/
 3 2 *ELASTIC*/
 3 18 *FISSION*/
 3 102 *CAPTURE*/
 6 2 *ELASTIC*/
 0/
 3 1 *TOTAL*/
 3 2 *ELASTIC*/
 3 18 *FISSION*/
 3 102 *CAPTURE*/
 6 2 *ELASTIC*/
 0/
 0/
 *CCCCR*
 -25 21 22 0
 1 1 *T2LANL NJOY*/
 *CCCCR TESTS FOR NJOY87*/
 50 0 1 4 1
 *PU238* *PU238* *ENDFB4* * 1050 * 1050 10.89
 1 0 50 -1
 0 2.3821E02 3.3003E-11 1.7461E-12 0. 1.E10 0.0
 3 6
 300 900 2100
 1.E5 1.E4 1000. 100. 10. 1
 *STOP*
EOF
```

```
../XNJOY<INPUT
ECHO 'SAVING OUTPUT FILES'
CP OUTPUT OUT2
```

The RECONR input is identical to the one in Problem 1, but reading the listing file will demonstrate that RECONR added about 2700 points to the original grid in the resonance region. After a little thinning, it ended up with about 2800 resonance energy points at 0 K for .5 % reconstruction. The data from RECONR was then passed to BROADR for preparation of cross sections at 300, 900, and 2100 K. An examination of the output listing shows that some thinning was possible because of the smoothing effect of Doppler broadening; the zero degree grid of 3241 points changed to 2341 points at 2100 degrees.

One of the new features of this run is the call to UNRESR. The user will normally notice that unresolved-resonance parameters are available for a material by reading the introductory information on the ENDF tape, but UNRESR will return gracefully if no unresolved data are present in the evaluation. The long output from UNRESR gives a table of the self-shielded cross sections by reaction (vertical) and sigma-zero value (horizontal) for each point of the unresolved-range energy grid. The reactions are flux-weighted total, elastic, fission, capture, and current-weighted total reading from the top down. Heating, damage, and thermal cross sections were omitted for this particular problem. Therefore, the final PENDF tape is on `TAPE22`, the output from UNRESR.

The GROUPR run shown here adds several new features over the one given for problem 1. First, multiple temperatures and sigma-zero values are specified in order to get tables of self-shielded cross sections for the total, elastic, fission, and capture reactions. It is desirable to use the same sigma-zero grid in GROUPR that was used in UNRESR, although GROUPR will attempt to interpolate if the grids are different. Note that a section of GROUPR input is given for 300 K with complete coverage of all the reactions, and additional sections are given for the two higher temperatures with only the self-shielded reactions included. An examination of the output listing will show that self-shielded cross sections are given for the low-energy reactions (total, elastic, fission, capture), with group index reading down and sigma-zero value reading across.

Another new feature of this input is the computation of the fission matrix (`MFD=6`, `MTD=18`). More complicated input may be necessary for other materials. Examination of the output listing will show that GROUPR discovered that the fission spectrum shape was constant over the entire energy range; therefore, it only put out a spectrum and a fission-neutron production cross section.

When the GROUPR run is complete, the final GENDF tape will be found on TAPE25. This file is used as input to the CCCCR module to produce ISOTXS and BRKOXS files for Pu-238.

3. Test Problem 3

This problem demonstrates the use of GAMINR to prepare photon interaction (or photoatomic) cross sections. It also demonstrates DTFR, including plotting, and MATXSR. For the sake of continuity, this test problem uses a rather old version of the photon interaction files called DLC7E. The MF23 and MF27 parts of these data are written on two separate files. Later libraries have everything on a single tape.

```
ECHO 'GETTING PHOTOATOMIC TAPE GAM23'
CP ../GAM23 TAPE30
ECHO 'GETTING PHOTOATOMIC TAPE GAM27'
CP ../GAM27 TAPE32
ECHO 'RUNNING NJOY'
CAT>INPUT <<EOF
 0
 4
 *RECONR*
 30 31
 *PENDF TAPE FOR PHOTON INTERACTION CROSS SECTIONS FROM DLC7E*/
 1 1 0
 .001/
 *1-HYDROGEN*/
 92 1 0
 .001/
 *92-URANIUM*/
 0/
 *GAMINR*
 32 31 0 33
 1 3 3 4 1
 *12 GROUP PHOTON INTERACTION LIBRARY*/
 -1 0/
 92
 -1 0/
 0/
 *DTFR*
 33 34 31
 1 1 0
 5 12 4 5 16 1 0
 *PHEAT*
 1 621 1
 0/
 *H* 1 1 0./
 *U* 92 1 0./
 0/
 *MATXSR*
```

```
 0 33 35/
 1 *T2LANL NJOY*/
 1 1 1 2
 *12-GROUP PHOTON INTERACTION LIBRARY*/
 *G*
 12
 *GSCAT*/
 1
 1
 *H* 1 1
 *U* 92 92
 *STOP*
EOF
../XNJOY<INPUT
ECHO 'SAVING OUTPUT AND PLOT FILES'
CP OUTPUT OUT3
CP PLOT PLOT3
```

This run starts with an application of the RECONR module to linearize and unionize the File 23 cross sections. Of course, there is no resonance reconstruction required here. This RECONR run demonstrates the use of a material loop; both hydrogen and uranium are processed in one run. GAMINR is then used to prepare the multigroup photon interaction cross sections, including heating; this run also uses a multimaterial loop. The Los Alamos 12-group photon structure is used. The GENDF tape (TAPE33) is processed into two completely different library formats. First, DTFR is called. This is a rather old output module, but it is still useful for some purposes. For one thing, it automatically produces plots of the multigroup data overlayed with the PENDF data. Examples of the plots are given in the DTFR chapter of this manual. The MATXS output is more useful, because it can be used in a much more flexible way by the TRANSX code.

4. Test Problem 4

This problem illustrates several aspects of the calculation of covariances (uncertainties) of multigroup data using ERRORR. The first ERRORR problem produces, on unit 23, a file of multigroup cross section covariances (MFCOV=23) for all reactions present (IREAD=0) in File 33 for ^{235}U. The group structure employed is identical to the energy grid selected by the evaluator (IGN=19); however, no covariances are produced for cross sections below 1 eV or above 1 keV. The second ERRORR run adds to the above results a second data set containing multigroup $\overline{\nu}$ covariances. Note that the use of MFCOV=31 dictates that a GENDF file be produced (NGOUT=24) prior to the start of ERRORR. In the $\overline{\nu}$ run, a user-defined group structure is employed (IGN=1).

```
ECHO 'GETTING ENDF TAPE 511'
```

```
CP ../T511 TAPE20
ECHO 'RUNNING NJOY...'
CAT>INPUT <<EOF
 0
 5
 *MODER*
 20 -21
 *RECONR*
 -21 -22
 *U-235 10% PENDF FOR ERRORR TEST PROBLEM FROM T511*/
 1395 0 0
 .10/
 0/
 *ERRORR*
 -21 -22 0 23 0/
 1395 19 1 1
 3 0 0
 0 33
 1
 1.E0 1.E3
 *GROUPR*
 -21 -22 0 24
 1395 3 0 3 0 1 1 1
 *U-235 MULTIGROUP NUBAR CALCULATION*/
 0.
 1.E10
 3 452 *TOTAL NUBAR*/
 0/
 0/
 *ERRORR*
 -21 0 24 25 23/
 1395 1 1 1
 0 31
 7
 1.E0 1.E1 1.E2 1.E3 1.E4 1.E5 1.E6 1.E7
 *STOP*
EOF
../XNJOY<INPUT
ECHO 'SAVING OUTPUT'
CP OUTPUT OUT4
```

5. Test Problem 5

This short problem produces multigroup covariances for ^{12}C, again using IGN=19, but here all cross sections from 1E-5 to 2E7 are treated. The COVR module reads the binary output file from ERRORR and produces publication-quality plots of all reactions for which covariance data exist. This simple problem setup could be used with only a few simple changes for any nuclide, in order to take a quick look at the contents of the covariance files. For applications where the resonance region is of interest, it is necessary to replace the second MODER step with a resonance reconstruction step using RECONR, as in the previous example.

```
ECHO 'GETTING ENDF TAPE 511'
CP ../T511 TAPE30
ECHO 'RUNNING NJOY...'
CAT>INPUT <<EOF
 0
 5
 MODER
 30 -31
 MODER
 -31 -32
 ERRORR
 -31 -32 0 -33/
 1306 19 1/
 2 0 0
 0 33
 1
 1E-5 2E7/
 COVR
 -33/
 /
 /
 1306/
 STOP
EOF
../XNJOY<INPUT
ECHO 'SAVING OUTPUT AND PLOT'
CP OUTPUT OUT5
CP PLOT PLOT5
```

6. Test Problem 6

This test problem demonstrates and tests a number of different kinds of plots using data from ENDF/B-V Tape 511 (the "Standards Tape"). The graphs produced and a detailed discussion of the input cards will be found in the PLOTR chapter of this manual.

```
ECHO 'GETTING ENDF TAPE 511'
CP ../T511 TAPE30
ECHO 'RUNNING NJOY'
CAT>INPUT <<EOF
 0
 5
 PLOTR
 /
 1/
 *ENDF/B-V CARBON*/
 *T<OTAL> C<ROSS> S<ECTION>*/
 4/
 1E3 2E7/
```

```
/
.5 10/
/
5 30 1306 3 1/
/
1/
*ENDF/B-V CARBON*/
*<(N,#A<) WITH FAKE DATA*/
1 0 2 1 1.4E7 .32/
/
/
/
/
5 30 1306 3 107/
/
*ENDF/B-V MAT1306*/
2/
0/
-1 0/
*S<MITH> & S<MITH> 1914*/
0/
1.1E7 .08 .05 .05/
1.2E7 .10 .05 .05/
1.3E7 .09 .04 .04/
1.4E7 .08 .03 .03/
-1/
3/
0/
-1 2/
*B<LACK> & B<LUE> 2008*/
0/
1.15E7 .07 .02 0. .2E6 0./
1.25E7 .11 .02 0. .2E6 0./
1.35E7 .08 .015 0. .2E6 0./
1.45E7 .075 .01 0. .2E6 0./
-1/
1/
*ENDF/B-V CARBON*/
*E<LASTIC> MF4*/
-4/
/
/
/
/
5 30 1306 4 2/
/
1/
*ENDF/B-V L<I>-6*/
*<(N,2N)#A <NEUTRON DISTRIBUTION*/
-1/
/
/
0 12E6 2E6/
```

```
 /
 5 30 1303 5 24/
 /
 1/
 *ENDF/B-V L<I>-6*/
 *<(N,2N)#A <NEUTRON SPECTRA VS >E*/
 4 0 2 2/
 10. 2.E7/
 /
 1E-11 1E-6/
 *C<ROSS> S<ECTION> (<BARNS/E>V)*/
 5 30 1303 5 24 0. 12/
 /
 *10 M<E>V*/
 1E3 2E-11 1E2/
 2/
 5 30 1303 5 24 0. 16/
 /
 *14 M<E>V*/
 1E4 2E-10 2E3/
 3/
 5 30 1303 5 24 0. 20/
 /
 *20 M<E>V*/
 1E5 2E-9 4E4/
 99/
 STOP
EOF
../XNJOY<INPUT
ECHO 'SAVING PLOT FILE'
CP PLOT PLOT6
```

7. Test Problem 7

This test problem demonstrates and tests the preparation of ACE-format libraries for the MCNP continuous-energy Monte Carlo code. The material selected for processing was U-235 from ENDF/B-V. Since this material is given on the "Standards Tape," there are no restrictions on its distribution.

```
ECHO 'GETTING ENDF TAPE 511'
CP ../T511 TAPE20
ECHO 'RUNNING NJOY...'
CAT>INPUT <<EOF
 0
 5
 *MODER*
 20 -21
 *RECONR*
 -21 -22
 *PENDF TAPE FOR U-235 FROM ENDF/B-V TAPE 511* /
 1395 3 /
```

```
 .005 /
 *92-U-235 FROM ENDF/B-V TAPE 511 * /
 *PROCESSED BY THE NJOY NUCLEAR DATA PROCESSING SYSTEM* /
 *SEE ORIGINAL ENDF/B-V TAPE FOR DETAILS OF EVALUATION* /
 0 /
 *BROADR*
 -22 -23
 1395 1 0 1 0 /
 .005 /
 300.
 0 /
 *HEATR*
 -21 -23 -24
 1395 /
 *GROUPR*
 -21 -24 0 -25
 1395 3 2 9 0 1 1 1 /
 *U-235 FROM TAPE 511* /
 300.
 1.0E10
 16 /
 0 /
 0 /
 *ACER*
 -21 -24 -25 26 27 /
 1/
 *NJOY TEST PROBLEM 7*/
 1395 300. /
 0.05 /
 /
 *STOP*
EOF
../XNJOY<INPUT
ECHO 'SAVING OUTPUT AND ACE FILES'
CP OUTPUT OUT7
CP TAPE26 ACE7
```

CONTENTS