NJOY99 Tutorial

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NJOY99 Tutorial

Introduction & General Information

- Workshop Outline
  - Introduction
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    - Thermal Kernels (MCNP .t files)
    - Covariances
  - User Feedback (throughout the presentation, not just at the end!)

NJOY99 Tutorial

Introduction & General Information

- What is NJOY?
  - A comprehensive ENDF/B processing program.
  - Consists of a number of “modules” that handle discrete processing tasks.
    - RECONR: convert an ENDF/B input tape into a “pendf” tape where all cross sections are linearly interpolable to within a user specified accuracy. This is a zero degree cross section reconstruction, and all cross sections use a unionized energy grid.
    - BROADR: doppler broaden a pendf tape to one or more user specified temperatures, maintaining a union grid and linear interpolation to within a user specified accuracy.
    - other modules, such as MODER, UNRESR, HEATR, THERMR, PURR, GASPR, ACER, GROUPR, LEAPR, ERRORR/ERRORJ, PLOTR and VIEWR will be discussed during this tutorial.
  - Primary developer is Bob MacFarlane.
    - Now retired, but remains active in ongoing development.

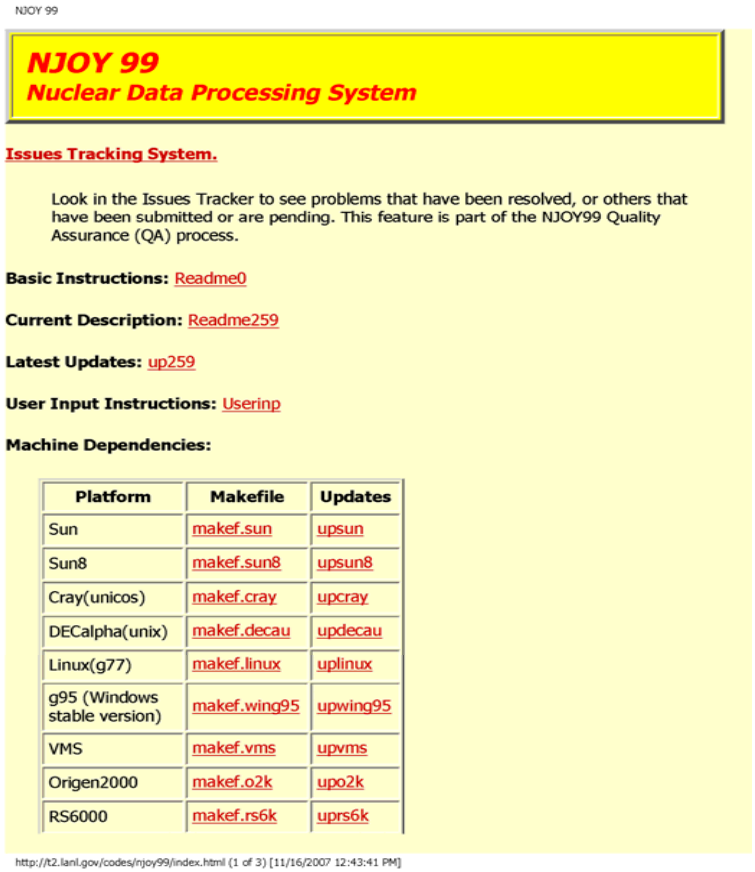
NJOY99 Tutorial

Introduction & General Information

- The NJOY99 code package may be obtained from ORNL's RSICC or from the OECD/NEA in Paris.
  - RSICC: http://www-rsicc.ornl.gov/
  - NEA: http://www.nea.fr/html/dbprog/
- This package includes the basic source code (src), an update utility code (upd), test problem i/o files (but see the "t2" web site for the latest info), machine-dependent code and sample makefiles.
  - updates to "src" are posted at http://t2.lanl.gov/codes/njoy99/.
  - upd merges these updates and "src" to produce a set of fortran source that the user compiles and links to create a new executable.

NJOY99 Tutorial

General Information – Web Sources



NJOY 99

NJOY 99
Nuclear Data Processing System

Issues Tracking System.

Look in the Issues Tracker to see problems that have been resolved, or others that have been submitted or are pending. This feature is part of the NJOY99 Quality Assurance (QA) process.

Basic Instructions: Readme0

Current Description: Readme259

Latest Updates: up259

User Input Instructions: Userinp

Machine Dependencies:

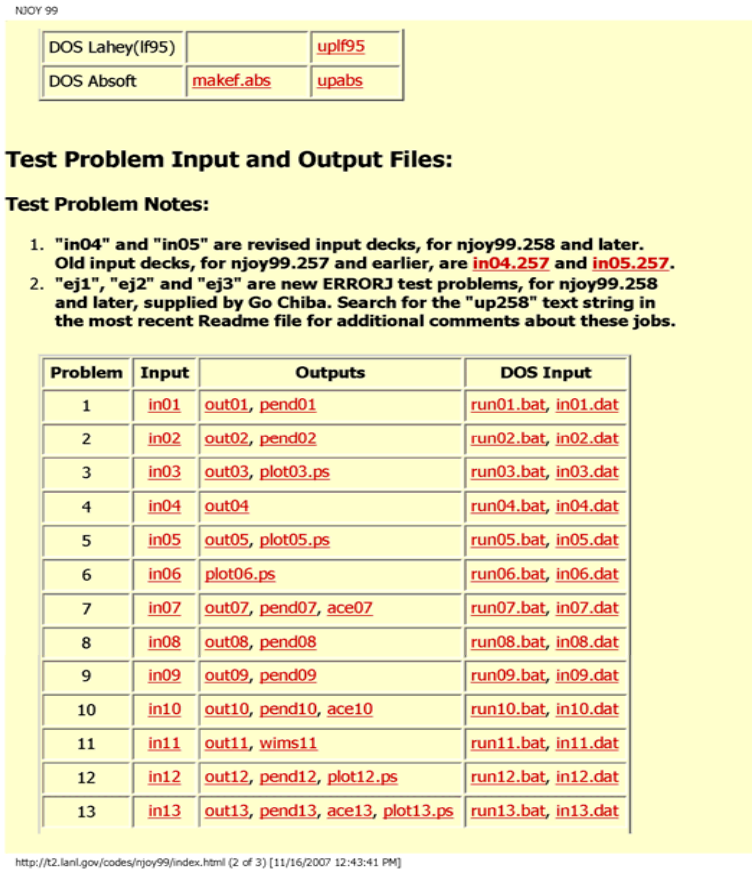
Platform	Makefile	Updates
Sun	makef.sun	upsun
Sun8	makef.sun8	upsun8
Cray(unicos)	makef.cray	upcray
DECalpha(unix)	makef.decau	updecau
Linux(g77)	makef.linux	uplinux
g95 (Windows stable version)	makef.wing95	upwing95
VMS	makef.vms	upvms
Origen2000	makef.o2k	upo2k
RS6000	makef.rs6k	uprs6k

http://t2.lanl.gov/codes/njoy99/index.html (1 of 3) [11/16/2007 12:43:41 PM]

- http://t2.lanl.gov/codes/njoy99/.
- Readme259: Latest information on code changes in this update.
- Userinp: Latest information on User Input Options (updated for up259).
- G95: Information for this Compiler option is new with the up259 release.

NJOY99 Tutorial

General Information – Web Sources



NJOY 99

DOS Lahey(lf95)		uplf95
DOS Absoft	makef.abs	upabs

Test Problem Input and Output Files:

Test Problem Notes:

1. **"in04" and "in05" are revised input decks, for njoy99.258 and later. Old input decks, for njoy99.257 and earlier, are in04.257 and in05.257.**
2. **"ej1", "ej2" and "ej3" are new ERRORJ test problems, for njoy99.258 and later, supplied by Go Chiba. Search for the "up258" text string in the most recent Readme file for additional comments about these jobs.**

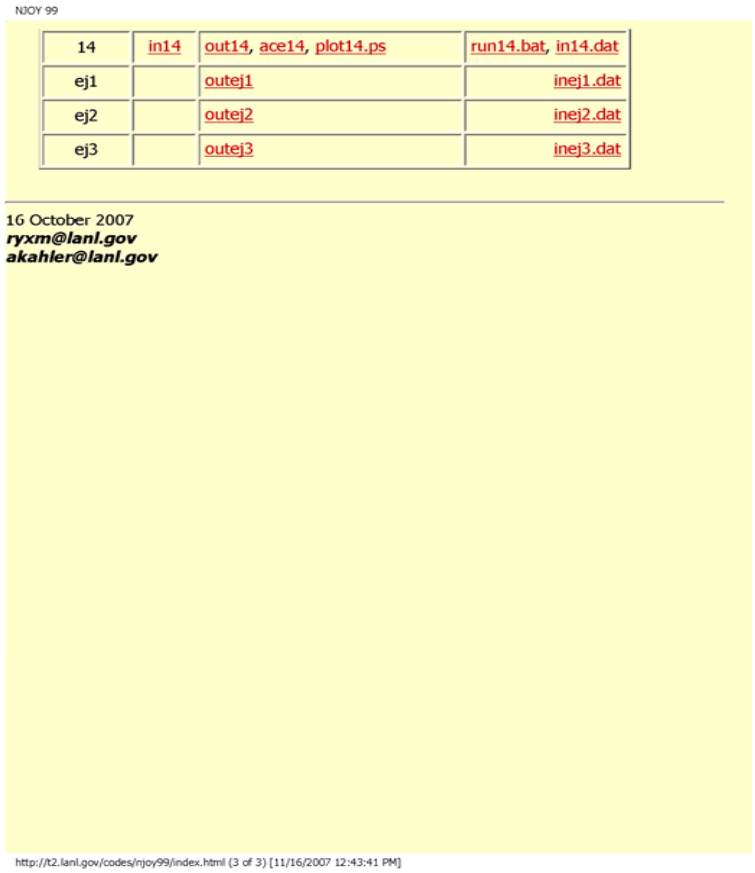
Problem	Input	Outputs	DOS Input
1	in01	out01, pend01	run01.bat, in01.dat
2	in02	out02, pend02	run02.bat, in02.dat
3	in03	out03, plot03.ps	run03.bat, in03.dat
4	in04	out04	run04.bat, in04.dat
5	in05	out05, plot05.ps	run05.bat, in05.dat
6	in06	plot06.ps	run06.bat, in06.dat
7	in07	out07, pend07, ace07	run07.bat, in07.dat
8	in08	out08, pend08	run08.bat, in08.dat
9	in09	out09, pend09	run09.bat, in09.dat
10	in10	out10, pend10, ace10	run10.bat, in10.dat
11	in11	out11, wims11	run11.bat, in11.dat
12	in12	out12, pend12, plot12.ps	run12.bat, in12.dat
13	in13	out13, pend13, ace13, plot13.ps	run13.bat, in13.dat

http://t2.lanl.gov/codes/njoy99/index.html (2 of 3) [11/16/2007 12:43:41 PM]

- Changes to the test problem suite:
  - in04 and in05 are revised to support ERRORJ input requirements.
  - these modified input files must be used for NJOY99.258 and later.
  - links to old versions of these input files remain for user's who choose not to include ERRORJ.

NJOY99 Tutorial

General Information – Web Sources



NJOY 99

14	in14	out14, ace14, plot14.ps	run14.bat, in14.dat
ej1		outej1	inej1.dat
ej2		outej2	inej2.dat
ej3		outej3	inej3.dat

16 October 2007
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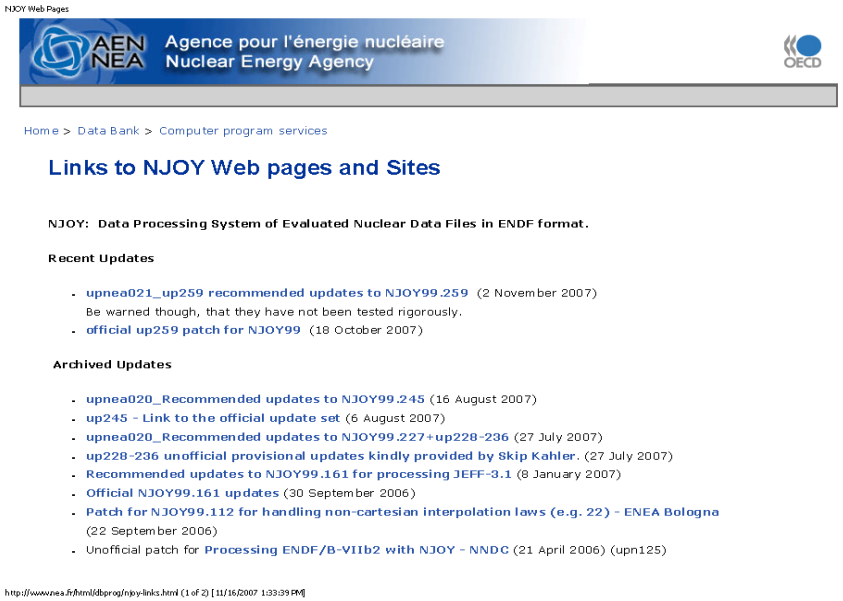
http://t2.lanl.gov/codes/njoy99/index.html (3 of 3) [11/16/2007 12:43:41 PM]

- New test problems (from Go Chiba) are provided to test ERRORJ.
  - Required input files include JENDL-3.3 ^{235,238}U and ^{239}Pu.
  - Long run time (for reconr/ broadr), but pointwise resonance region reconstruction will not be required for future test jobs unless modifications have been made to reconr and/or broadr.

NJOY99 Tutorial

General Information – Web Sources

- Additional NJOY information is available at http://www.nea.fr/html/dbprog/njoy-links.html:


NJOY Web Pages

Agence pour l'énergie nucléaire
Nuclear Energy Agency

Home > Data Bank > Computer program services

Links to NJOY Web pages and Sites

NJOY: Data Processing System of Evaluated Nuclear Data Files in ENDF format.

Recent Updates

- upnea021_up259 recommended updates to NJOY99.259 (2 November 2007)
  Be warned though, that they have not been tested rigorously.
- official up259 patch for NJOY99 (18 October 2007)

Archived Updates

- upnea020_Recommended updates to NJOY99.245 (16 August 2007)
- up245 - Link to the official update set (6 August 2007)
- upnea020_Recommended updates to NJOY99.227+up228-236 (27 July 2007)
- up228-236 unofficial provisional updates kindly provided by Skip Kahler. (27 July 2007)
- Recommended updates to NJOY99.161 for processing JEFF-3.1 (8 January 2007)
- Official NJOY99.161 updates (30 September 2006)
- Patch for NJOY99.112 for handling non-cartesian interpolation laws (e.g. 22) - ENEA Bologna (22 September 2006)
- Unofficial patch for Processing ENDF/B-VIIb2 with NJOY - NNDC (21 April 2006) (upn125)

http://www.nea.fr/html/dbprog/njoy-links.html (1 of 2) [11/16/2007 1:33:39 PM]


NJOY Web Pages

US Web pages

- NJOY official Web Site
- Understanding NJOY
- NJOY99 Issue Tracker
- NJOY Notebook (RSICC)

Data Bank Web pages

Workshops / Meetings

- NJOY-2007 User Group Meeting Registration, 26 November 2007
- NJOY-2006 User Group Meeting Proceedings, 20 November 2006
- NJOY-2005 Workshop and User Group Meeting Proceedings, 2 May 2005
- NJOY-2001 Workshop and User Group Meeting Proceedings 15 May 2001
- Proceedings NJOY91 & Themis Seminar 1992
- Proceedings of the Seminar on NJOY and THEMIS 1989

NJOY Notes and Forum

- NJOY Listserver Archive (NEA Data Bank) (March 2000 - present)
- NJOY User Notes Archive (1991-January 2000)

ENDF- 6 Formats Manual - Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII, Document ENDF-102 Report BNL-NCS-44945-05-Rev. Revised, June 2005

Last updated: 2 November 2007

http://www.nea.fr/html/dbprog/njoy-links.html (2 of 2) [11/16/2007 1:33:39 PM]

NJOY99 Tutorial

General Information – Updating & Compiling

- To create an NJOY99 executable file we need:
  - an executable version of njoy's update program, upd.
  - the original njoy source file, src
  - a upd input file, upn
    - "upn" is a text file containing:
      - commands to perform modifications to "src" (optional).
      - version control information (should always be included).
      - platform dependent code (should always be included).
        - "should always be included" is my opinion – not a upd requirement.
- The output from upd is a series of .f files which the User must compile and link to create the NJOY99 executable.
  - compiler and linker options will always be dependent upon the User's local environment, but possible options are provided on our t2 web site.

NJOY99 Tutorial

General Information – Updating & Compiling

- The “scr” file looks like:

```
*deck njoy
c
      program njoy
c
.
. ... comments and main program source code ...
.
      end
c
      subroutine ....
c
.
. ... comments and subroutine source code ...
.
      return
      end
*deck reconr
c
      subroutine reconr
c
c     ********************************************************************
c     *                                                                  *
c     * reconstruct pointwise cross sections                             *
c     *                                                                  *
.
. ... comments and subroutine source code ...
.
      return
      end
*deck broadr
c
      subroutine broadr
c
c     ********************************************************************
c     *                                                                  *
c     * doppler broaden and thin neutron point cross sections            *
c     *                                                                  *
.
. ... comments and subroutine source code ...
.
      return
      end
*deck unresr
*deck heatr
*deck thermr
*deck groupr
*deck gaminr
*deck errorr
*deck covr
*deck moder
*deck dtfr
*deck ccccr
*deck matxsr
*deck resxsr
*deck acer
*deck powr
*deck wimsr
*deck plotr
*deck viewr
*deck mixr
*deck purr
*deck leapr
*deck gaspr
c
      subroutine gaspr
c     ********************************************************************
c     *                                                                  *
c     * add gas production reactions (mt203-207) to the pendf tape.      *
.
. ... comments and subroutine source code ...
.
      return
      end
```

NJOY99 Tutorial

General Information – Updating & Compiling

- The “upn” file looks like:

```
*cpl all
*set sw
*/ (optional) comments about "ident up1".
*ident up1
*/ (optional) more comments
*/ example:  insert the following code after line # in module xxxxx.
*i xxxxx.#
     new source code
     more new source code
     ...
*/ example:  delete line # in module yyyyy.
*/          any text following this command will be inserted into
*/          "scr" at this point.
*d yyyyy.#
*d zzzzz.#
     replacement source code
     more code
     ...
*ident up2
*/ delete commands may span a range of lines and modules.
*/
*/ delete from line # to ## in module aaaaa.
*d aaaaa.#,##
*/
*/ delete from line # in module aaaaa through ## in module bbbbb.
*d aaaaa.#,bbbbb##


.
.
.


*ident vers
*/ update the version name and date
*/ to reflect the date of the latest modifications
*d njoy.8,9
c     *    version 99.259                                  *
c     *    16 Oct 2007                                     *
*d njoy.307
     data vers/'99.259  '/
*ident pc_ifort
*/ ---------------------------------------------
*/ machine-dependent changes to njoy99
*/ for pc with the Intel 9.x compiler and 32 bits
*/ be sure to use "*set sw"
*/ ---------------------------------------------
*d njoy.308,309
     data lab/'lanl t16'/
     data mx/'pc_ifort'/


.
.
.

*/ machine constants for slatec functions.
*/ provide code for either double or single precision.
*/ this is the double precision code:
*d njoy.5323,5334
*d njoy.5338,5746
c
c     for intel ifort (or any f90 and later compiler)
     dmach(1)=tiny(1.d0)
     dmach(2)=huge(1.d0)
     dmach(3)=2.d0**(-digits(1.d0))
     dmach(4)=2.d0**(1-digits(1.d0))
     dmach(5)=log10(2.d0)
*/ this is the single precision code:
*/ *d njoy.5798,5809
*/ *d njoy.5813,6139
*/ c
*/ c     for intel ifort (or any f90 and later compiler)
*/      rmach(1)=tiny(1.e0)
*/      rmach(2)=huge(1.e0)
*/      rmach(3)=2.e0**(-digits(1.e0))
*/      rmach(4)=2.e0**(1-digits(1.e0))
*/      rmach(5)=log10(2.e0)
```

NJOY99 Tutorial

General Information – Updating & Compiling

```
C:\Documents and Settings\Skip\NJOY\NJOY99>upd
 upd: vers: 2.0
 upd: src: 93325 cards   24 decks
 upd: upn: 21063 cards  261 idents
 upd: cpl: 98101 lines written
 upd: complete

C:\Documents and Settings\Skip\NJOY\NJOY99>nmake fc=g95

Microsoft (R) Program Maintenance Utility   Version 1.50
Copyright (c) Microsoft Corp 1988-94. All rights reserved.

Creating an executable using the gnu g95 compiler.
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c njoy.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c reconr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c broadr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c unresr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c heatr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c thermr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c groupr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c gaminr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c errorr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c covr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c moder.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c dtfr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c ccccr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c matxsr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c resxsr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c acer.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c powr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c wimsr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c plotr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c viewr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c mixr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c purr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c leapr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -c gaspr.f
        g95 -O0 -fsloppy-char -ftrace=full -fbounds-check -freal=nan -o njoy
njoy.o reconr.o broadr.o unresr.o heatr.o thermr.o  groupr.o gaminr.o errorr.o
covr.o moder.o dtfr.o ccccr.o  matxsr.o resxsr.o acer.o powr.o wimsr.o plotr.o
viewr.o  mixr.o purr.o leapr.o gaspr.o

C:\Documents and Settings\Skip\NJOY\NJOY99>
```

- Open a CMD window
- Run “upd” to create the new source code.
  - Input to upd is the base NJOY99 source code file, src and the update command file, upn.
- Compile and link to create the new executable.
  - MS Windows users can use “nmake”.
    - Available in the .NET environment or as a standalone download v1.5 from Microsoft (http://support.microsoft.com/kb/132084).

NJOY99 Tutorial

General Information – Test Problems

- A 17-Problem Test Suite is Available to (Partially!) Check NJOY99.
- 14 Problems Created by Bob MacFarlane Many Years Ago.
  - NJOY Input Decks, ENDF Input Decks and Selected Output Files are Available at http://t2.lanl.gov/codes/njoy99/index.html.
- 3 Problems Developed by Go Chiba for ERRORJ.
  - NJOY Input Decks and Selected Output Files are Available.
  - User Must Supply JENDL-3.3 ^{235,238}U and ^{239}Pu Nuclear Data Files.
- Differences in the Least Significant Digits may be observed when comparing results from different platforms or from executables with differing compiler options.

NJOY99 Tutorial

A Few Words About Evaluated Nuclear Data Files

- Evaluated Nuclear Data Files (ENDF) are fixed record (80 columns per line) text files.
- Character or numerical information appear in columns 1 to 66, control information appears in columns 67 to 80.
  - mostly six 11-column fields for real or integer data per record.
  - 67 – 70: up to 4 digits for the material number.
  - 71 – 72: one or two digits for the “file” number, MF.
  - 73 – 75: one to three digits for a “section” or “type” number, MT.
  - 76 – 80: up to five digits for sequence number.
  - ENDF/B data records include “CONT”, “LIST”, TAB1” and “TAB2” that define a single record, a list of real numbers, function data (e.g., E, f(E)), or a 2D function (e.g., E,T,f(E,T)).

NJOY99 Tutorial

A Few Words About Evaluated Nuclear Data Files

- Each evaluation contains a number of “files”, and each “file” contains a specific type of information:
  - MF = 1: mostly evaluator comments;
  - MF = 2: resonance parameter information;
  - MF = 3: pointwise cross sections (E, σ(E));
  - MF = 4: angular distribution data;
  - MF = 5: secondary energy distributions;
  - MF = 6: coupled energy-angle distribution data;
  - MF = 7: thermal kernel data
  - MF = 12 – 15: photon data, related to the corresponding neutron data from MF = 2 through 5.
  - …

NJOY99 Tutorial

A Few Words About Evaluated Nuclear Data Files

- Each “file” contains one or more “sections”, where each section is defined by an “MT” number.
  - Within a given file, section numbers appear in ascending order but are not contiguous.
    - MF = 1
      - MT = 451: Evaluator comments.
      - MT = 452: Total nu-bar (not present if this material does not fission).
    - MF = 2
      - MT = 151: Resolved and Unresolved Resonance parameter data
    - MF = 3
      - MT = 1, 2, …: MT1 is the total cross section, MT2 is elastic scattering, MT16 is (n,2n), MT18 is (n,fission), MT102 is (n,γ), …
    - Data in a given MT may depend upon the content of other MT’s.
    - The presence of a specific MF, MT pair may be mandatory, depending upon the sections that are present in an earlier MF.

NJOY99 Tutorial

A Few Words About Evaluated Nuclear Data Files

- CAUTION:
  - NJOY is not an ENDF checking code.
    - NJOY jobs may run to completion but not produce correct or meaningful results (GIGO).
  - If calculated results, and warning or error messages, seem strange or unrealistic it is likely due to bad or missing data from the input ENDF tape.
  - User suggestions for improvements are welcome ☺.
    - Unfunded improvements may not be implemented quickly ☹.

NJOY99 Tutorial

A Few Words About Evaluated Nuclear Data Files

- ENDF/B-VII.0 Data Files may be downloaded from the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL).
  - NNDC home page is http://www.nndc.bnl.gov/.
  - Download site is http://www.nndc.bnl.gov/exfor/endf00.htm.
- Many of the known deficiencies in ENDF/B-VII.0 files are summarized at
  http://www.nndc.bnl.gov/proceedings/2007csewgusndp/Tuesday/CSEWG/HermanDeficiencies.pdf
  - Users are encouraged to report errors to Mike Herman (mwherman@bnl.gov) and LANL (akahler@lanl.gov).

NJOY99 Tutorial

Examples of Specific NJOY Tasks

- Create MCNP/MCNPX continuous energy (.c) files.
- Create MCNP/MCNPX thermal kernel (.t) files.
- Process covariance data with ERRORJ.

NJOY99 Tutorial

Specific Applications – Creating MCNP .c Files

- A minimum NJOY job will include:
  - reconr/broadr/purr/acer
  - optionally, include moder to convert between ascii and binary files, extract data for one material from a tape with multiple materials, or make copies of a given tape.
  - optionally include plotr & viewr to generate User defined plots.
    - viewr's output is a postscript formatted file.
- A more complete job will include:
  - reconr/broadr/(unresr)/heatr/purr/thermr/gaspr/acer
- A second heatr or acer, coupled with viewr, job may be executed to generate a standard set of plots.

NJOY99 Tutorial
MODER

```
--
-- See comments at the start of moder.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nin, nout
--          nin = If  1 < abs(nin) < 20, this is an input option flag.  If abs(nin) ≥ 20 this is
--                an input tape number.
--                = 1 = input and output tapes are endf- (or pendf-) format.
--                = 2 = input and output tapes are gendf-format.
--                = 3 = input and output tapes are errorr-format.
--          nout = an output tape number.
-- Card 2:  tpid
--          text that defines the output tape "tape id" record.  Text is delimited with
--          ' and the record is terminated with /.
-- Card 3:  ninn, mat
--          ninn = an input tape number.
--          mat = id for the material data to be read from the input tape and written to the
--                output tape.  If the output tape already exists, these data are appended to
--                that tape.
--
-- Cards 2 and 3 are only needed when 1 < abs(nin) < 20.
-- Card 3 may be repeated to create an output tape with multiple materials,
-- terminate moder input with 0 /.
--
-- a sample input deck:
moder
 +20 -21 /   ← convert ascii tape20 to binary tape21.


-- another sample input deck:
moder
 +1 -21 /     ← option 1, create a binary output (tape21).
 'tape id label goes here.' /
 +20 125 /   ← extract material 125 from ascii tape20, write to binary tape21.
 0 /          ← terminate input.
```

- Convert between ascii and binary tape formats.
  - Makes for more efficient i/o, but not really needed in today's computing environments.
- Extract data for a given material from a tape with multiple materials.
  - May be needed (e.g. GASPR).
- Create a custom tape with specific materials.
- Make a copy of a given tape.

NJOY99 Tutorial
MODER

MODER Output for "sample input deck":

```
 moder...change the mode of an endf/b tape or njoy output tape    0.0s

 input unit (+ for coded, - for bb) ...          20
 output unit (+ for coded, - for bb) ..         -21
 tape id is blank

 using endf-6 format
                                                                  0.0s
 ********************************************************************
```

MODER Output for "another sample input deck":

```
 moder...change the mode of an endf/b tape or njoy output tape    0.0s

 put materials from various tapes on output tape -21

 tape id for nout
 ----------------
 tape id label goes here

 processing endf or pendf tape.

          nin          matd
          ---          ----
           20           125

 using endf-6 format
                                                                  0.0s
 ********************************************************************
```

- MODER Output
  - First Job
    - Output identifies i/o tape numbers, ascii/binary format and input file endf format.
  - Second Job
    - Output identifies the output tape number (with ascii/binary format implied by its sign), tape id label, input tape, material to extract and endf format for that material.
    - For multiple card 3 input, the input tape number, material number and data format are repeated.

NJOY99 Tutorial
RECONR

```
--
-- See comments at the start of reconr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, npend
--          integers that specify input and output tapes.
-- Card 2:  tlabel
--          text that defines the output tape "tape id" record.  Text is delimited with
--          ' and the record is terminated with /.
-- Card 3:  mat, ncards, ngrid
--          mat = material id to be read from the input tape.
--          ncards = # of user comment records to insert in mf1, mt451 of the output tape
--                   (default = 0).
--          ngrid = # of user energy grid points that are forced into the energy grid
--                  (default = 0).
-- Card 4:  err, tempr, errmax, errint
--          err = fractional reconstruction tolerance for the final energy grid.
--          tempr = reconstruction temperature (degreesKelvin, default = 0.0).
--          errmax = fractional reconstruction tolerance (default is 10*err).
--          errint = fractional reconstruction tolerance (default is err/20000).
-- Card 5:  text (repeat for "ncards" text records, not present if ncards=0)
--          text = user comment line to appear in mf1, mt451 of the output tape.
-- Card 6:  enode(i) (not present if ngrid=0)
--          user specified list of energy values, in eV and ascending order, that will appear
--          in the reconstructed energy grid.
--
-- Repeat cards 3, 4, 5 and 6.
-- Set mat = 0 to terminate reconr input.
--
reconr
-21 -22 /            ← tape21 must exist (for input), tape22 will be created.
 'User text, to serve as the tape_id record for tape22' /
 125 2 3 /
 0.001 0. 0.01 5.0e-8 /
 'user text – will be part of tape22 mf1, mt451 comment' /
 'more user text, since ncards on the second input card was 2' /
 0.1 1.0 10. /      ← Three numbers, since ngrid on card 2 was 3.
 0 /                ← Loop back to read another card 3, set mat=0 to terminate input.
```

- Create a pointwise endf (pendf) file.
  - Resolved resonance parameters are converted into a pointwise file 3 (E,σ(E)) TAB1 array.
- RECONR will create a unionized energy grid for all file 3 cross sections.
- Grid density depends upon satisfying a user specified linear-linear interpolation accuracy.

NJOY99 Tutorial
RECONR

```
reconr...reconstruct pointwise cross sections in pendf format    0.0s

unit for endf/b tape ..................        -21
unit for pendf tape ...................        -22

label for pendf tape
-----------------------------------------------------------------
User text, to serve as the tape_id record for tape22

tape label
-----------------------------------------------------------------
tape id label goes here


                                          storage  17/  100000

material to be processed ..............        125
reconstruction tolerance ..............      0.001
reconstruction temperature ............       0.00k
resonance-integral-check tolerance ....      0.010
max resonance-integral error ..........  5.000E-08

descriptive cards for pendf tape
-----------------------------------------------------------------
user text - will be part of tape22 mf1, mt451 comment
more user text, since ncards on the second input card was 2

no. users energy grid points .........          3
   1.00000E-01 1.00000E+00 1.00000E+01

processing mat  125 in endf-6 format
-----------------------------------------------------------------
  1-H -  1 LANL       EVAL-OCT05 G.M.Hale


mat has no resonance parameters

number of user and resonance nodes       =      3
points in initial unionized grid         =     96
points added by linearization            =    586                0.1s
number of points in final unionized grid =    682

                                         usage   26969/  100000
                                                            0.1s
*****************************************************************
```

- RECONR Output
  - identify i/o tape numbers
  - repeat user tape id text
  - print input tape id text
  - identify material number, pointwise reconstruction parameters
  - print user comments that go into mf1, mt451
  - identify extra energy points
  - evaluator information from the input tape
  - comment on resonance parameters
  - information on initial and final number of energy points.

NJOY99 Tutorial
RECONR

Partial RECONR output, for endf/b-vii.0 235U:

```
 material to be processed .............       9228
 reconstruction tolerance .............      0.010
 reconstruction temperature ...........       0.00k
 resonance-integral-check tolerance ...      0.100
 max resonance-integral error .........  5.000E-07
 . . .
processing mat 9228 in endf-6 format
 ---------------------------------------------------------------
  92-U -235 ORNL,LANL,+EVAL-SEP06 Young,Chadwick,Talou,Madland,Leal


 changed threshold from 1.219440E+07 to 1.219442E+07 for mt 17.

 ---message from lunion---xsec nonzero at threshold for mt= 37
                          adusted using jump in xsec

 changed threshold from 7.712958E+01 to 7.712959E+01 for mt 51.
 . . .
 changed threshold from 5.000000E+05 to 5.000002E+05 for mt 91.

 number of user and resonance nodes       =   9508
 points in initial unionized grid         =   9916
 points added by linearization            =     83                2.1s

              estimated maximum error due to
              resonance integral check (errmax,errint)

   upper     elastic  percent  capture  percent  fission  percent
   energy    integral  error   integral  error   integral  error
  1.00E-05
  1.00E-04    3.50E+01  0.000   8.15E+03  0.000   4.29E+04  0.000
  1.00E-03    3.50E+01  0.000   2.57E+03  0.000   1.36E+04  0.000
  1.00E-02    3.49E+01  0.000   8.01E+02  0.000   4.24E+03  0.000
  . . .
  5.00E+02    1.10E+01  0.001   6.82E+00  0.005   1.51E+01  0.003
  1.00E+03    8.28E+00  0.012   3.44E+00  0.123   7.62E+00  0.050
  2.00E+03    8.27E+00  0.069   2.54E+00  0.593   5.06E+00  0.363

 points added by resonance reconstruction = 84480
 points affected by resonance integral check = 13712
 final number of resonance points = 94057
 number of points in final unionized grid =  94479

                                          usage   56596/  100000
                                                    232.4s
 ***************************************************************
```

- Partial RECONR Output for ^{235}U:
  - Additional output includes
    - reaction threshold energy check.
    - warning when threshold xs is not equal to zero.
    - resonance reconstruction information.

NJOY99 Tutorial
BROADR

```
--
-- See comments at the start of broadr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output tape.
-- Card 2:  matl, ntemp2, istart, istrap, temp1
--          matl = material to be processed.
--          ntemp2 = number of final temperatures (.le. 10).
--          istart = 0/1 = restart option.
--                   0 = create a new output tape for these data.
--                   1 = copy existing data up to and including temp1 to nout, then append
--                       ntemp2 additional data sets to this output file.
--          istrap = 0/1 = bootstrap option.
--                   0 = compute the next temperature starting with the temp1 data set.
--                   1 = compute the next temperature starting with the most recently
--                       generated data set.
--          temp1 = temperature for data read from nin (0.0 degK).
-- Card 3:  errthn, thnmax, errmax, errint
--          errthn = fractional tolerance for thinning the final energy grid.
--          thnmax = maximum energy for broadening and thinning (1.e6).
--          errmax = fractional reconstruction tolerance.
--                   (default value is 10*errthn).
--          errint = fractional reconstruction tolerance.
--                   (default value is errthn/20000).
--          General guidance:  use the same values for errthn, errmax and errint in broadr
--                             as were used in reconr.
-- Card 4:  temp2(i)
--          temp2(i) = list of ntemp2 temperatures.  Temperatures are given in degrees
--                     Kelvin.  Temperatures must be in ascending order and temp2(1)
--                     must be greater than temp1.
--
-- Repeat cards 2, 3 and 4.
-- Set matl = 0 to terminate broadr input.
--
broadr
-21 -22 -23 /       ← tape21 and tape22 must exist (for input), tape23 will be created.
 9228 2 0 0 0.0 /
 0.001 1.0e6 0.01 5.0e-8 /
 293.6 500.0 /     ← Two numbers, since ntemp2 on card 2 was 2.
 0 /               ← Loop back to read another card 2, set matl=0 to terminate input.
```

- Doppler broaden cross sections to one or more (up to 10) user specified temperatures.
- BROADR will maintain a unionized energy grid for all cross sections.
- Grid density depends upon satisfying a user specified linear-linear interpolation accuracy.

NJOY99 Tutorial
BROADR

```
broadr...doppler broadening of endf/b data                          0.1s

unit for input endf tape .............        -21
unit for input pendf tape ............        -22
unit for output pendf tape ...........        -23
material to be processed .............        125
number of final temperatures .........          2
restart (0 no, 1 yes) ................          0
bootstrap (0 no, 1 yes) ..............          0
starting material temperature ........        0.0k
thinning tolerance ...................      0.001
max. energy ..........................  1.000E+06
errmax for thinning ..................  1.000E-02
errint for thinning ..................  5.000E-08
final temperatures ...................  2.936E+02
                                        5.000E+02

                                              storage  10/ 2000000

files are in endf-6 format

max energy for broadening and thinning =   1.00000E+06
                                                                    0.1s

broadened mat 125 from  0.0000E+00 to  2.9360E+02 k
        points in=   682  points out=   590
        mt   2 102

   thermal quantities at 293.6 K = 0.0253 eV
   -----------------------------------------
          thermal capture xsec:  3.3204E-01
      thermal capture integral:  2.9428E-01
    capture resonance integral:  1.4916E-01
   -----------------------------------------
                                                                    1.0s

broadened mat 125 from  0.0000E+00 to  5.0000E+02 k
        points in=   682  points out=   590
        mt   2 102
                                                                    2.0s
************************************************************************
```

- BROADR Output
  - User input (i/o tapes, material, final temperatures, recon-struction convergence criteria).
  - Number of points in the initial and final energy mesh.
  - Reaction mt numbers for cross sections that were broadened.
  - At room temperature, selected resonance integral information.

NJOY99 Tutorial
BROADR

```
broadr...doppler broadening of endf/b data                        232.4s

 unit for input endf tape .............        -21
 unit for input pendf tape ............        -22
 unit for output pendf tape ...........        -23
 material to be processed .............       9228
 number of final temperatures .........          1
 restart (0 no, 1 yes) ................          0
 bootstrap (0 no, 1 yes) ..............          0
 starting material temperature ........        0.0k
 thinning tolerance ...................      0.010
 max. energy ..........................  1.000E+06
 errmax for thinning ..................  1.000E-01
 errint for thinning ..................  5.000E-07
 final temperatures ...................  2.936E+02


                                          storage  10/ 2000000

 files are in endf-6 format

 max energy for broadening and thinning =   2.24998E+03
                                                   233.1s

 broadened mat9228 from  0.0000E+00 to  2.9360E+02 k
         points in= 94479  points out= 31075
         mt   2  18 102

    thermal quantities at 293.6 K = 0.0253 eV
    -----------------------------------------
           thermal fission xsec:  5.8529E+02
         thermal fission nubar:  2.4367E+00
           thermal capture xsec:  9.8754E+01
       thermal capture integral:  8.6755E+01
     capture resonance integral:  1.4057E+02
       thermal fission integral:  5.0662E+02
       thermal fission g-factor:  9.7672E-01
         thermal alpha integral:  1.6831E-01
           thermal eta integral:  2.0858E+00
            thermal k1 integral:  6.4110E+02
                  equivalent k1:  7.2341E+02
     fission resonance integral:  2.7619E+02
    -----------------------------------------
                                                   250.3s
 ************************************************************
```

- BROADR Output for ^{235}U:
  - Additional output includes
    - Maximum broadening energy defaults to maximum resolved resonance energy.
    - Room temperature summary includes fission related data.

NJOY99 Tutorial
PLOTR

```
--
-- See comments at the start of plotr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Cards 0 and 1 appear once.  Cards 2 through 13 are repeated for each curve, per
-- the rules that follow.
--
-- Card 0:  nplt, nplt0
--          nplt   = unit for output plot commands.
--          nplt0 = unit for input plot commands (default = 0).  User input that follows
--                  is appended to nplt0 when this value is non-zero.
--
-- Card 1:  lori, istyle, size, ipcol
--          lori = 0/1 = portrait/landscape orientation (7.5x10.0in, or vice-versa).
--          istyle = 1/2 = roman/swiss character style.
--          size = +/- = height in page units (inches)/fraction of subplot size (0.30).
--          ipcol = 0/1/2/3/4/5/6/7 = page color (white, Navajo white, blanched almond,
--                  antique white, very pale yellow, very pale rose, very pale green, very
--                  pale blue).
--
-- Card 2:  iplot, iwcol, factx, facty, xll, yll, ww, wh, wr
--          iplot =  99 = terminate plotr input;
--                   +1 = define new axes and use a new page for this plot;
--                   -1 = define new axes but use existing page for this plot;
--                   +n = n^th curve on existing axes and page;
--                   -n = start a new set of curves using the alternate y axis.
--          iwcol = window color (use Card #1 "ipcol" color codes, default = 0);
--          factx = 1.0 = energy multiplicative factor.
--          facty = 1.0 = cross section multiplicative factor.
--          xll,yll = lower left corner of plot.
--          ww,wh,wr = window width, height and rotation angle (defaults to one plot
--                     per page.
```

- Use PLOTR (feed output to VIEWR) to produce postscript formatted plots.
  - User can specify all plot attributes (NJOY/PLOTR defaults are available for most attributes).
  - Multiple curves per plot frame are permitted.

NJOY99 Tutorial
PLOTR

--
-- **Note: Cards 3 through 7 are only read if iplot = ±1.**
--
-- Card 3: t1 (may be blank)
-- Card 3a: t2 (may be blank)
-- t1 = first line of title (≤60 characters).
-- t2 = second line of title (≤60 characters).
--
-- Card 4: ***itype, jtype, igrid, ileg, xtag, ytag***
-- itype = 1/2/3/***4*** = primary axis scale (use < 0 for 3D plot).
-- 1 = linear x, linear y;
-- 2 = linear x, log y;
-- 3 = log x, linear y;
-- 4 = log x, log y
-- jtype = ***0***/1/2 = ***none***/linear/log scale for alternate y axis.
-- igrid = 0/1/2/3 = no grid lines nor tic marks/grid lines/internal tic marks/
-- external tic marks.
-- ileg = ***0***/1/2 = legend control.
-- 0 = no legend;
-- 1 = legend with upper left corner at xtag, ytag;
-- 2 = label each curve with a vector from the label to the curve.
-- xtag, ytag = x and y coordinates for upper left corner of legend (***default coordinates are upper left corner of the plot***).
--
-- Card 5: el, eh, xstep
-- el = lowest energy to be plotted;
-- eh = largest energy to be plotted;
-- xstep = x-axis step (linear scales only).
-- The user must define all or none of these quantities. ***The default is none***.
-- Xstep is ignored if the x-axis uses a log scale.
--
-- Card 5a: ***xlabl***
-- xlabl = x-axis label (≤60 characters, default = "Energy (eV)").

--
-- **Note: Cards 3 through 7 are only read if iplot = ±1.**
--
--
-- Card 6: yl, yh, ystep
-- yl = lowest value of y-axis;
-- yh = largest value of y-axis;
-- ystep = y-axis step (linear scales only).
-- The user must define all or none of these quantities. The default is none.
-- Ystep is ignored if the y-axis uses a log scale.
--
-- Card 6a: ***ylabl***
-- ylabl = y-axis label (≤60 characters, default = "Cross section (barns)"
-- regardless of the value of ntp (card #8, below)).
--
-- **Note: When requesting % difference or ratio plots (ntp=2 or 3 on card #8), the x and y axis limits (cards 5 and 6) must be explicitly defined.**
--
-- **Cards 7 and 7a only appear if jtype (card #4) is ≠ 0.**
-- Card 7: rbot, rtop rstep
-- rbot = lowest value of secondary y-axis or of z-axis;
-- rtop = largest value of secondary y-axis or of z-axis;
-- rstep = secondary y-axis or z-axis step (linear scales only).
-- The user must define all or none of these quantities. The default is none.
-- Rstep is ignored if the axis uses a log scale.
--
-- Card 7a: ***rlabl***
-- rlabl = axis label (≤60 characters, default = blank).
--

NJOY99 Tutorial
PLOTR

--
-- Card 8 must always be present.
--
-- Card 8: iverf, nin, matd, mfd, mtd, ***temper, nth, ntp, nkh***
-- iverf = endf tape version (or 0 if card 0 nplt0 ≠ 0. When iverf=0, the
-- remaining items on this card are ignored);
-- nin = input tape (nin2 ≠ nin for ntp > 1, see below);
-- matd, mfd, mtd = endf/b material, file and section data to be plotted.
-- If mtd=0, loop over all reactions for this mfd;
-- temper = temperature (***default = 0.0 degK***);
-- nth, ntp, nkh (***defaults = 1***) = special flags, defined below.
--
-- **nth, ntp and nkh definitions when mfd = 3 or 5:**
-- nth = number of subsection to be plotted;
-- ntp = ***1***/2/3
-- 1 = normal plot (default);
-- 2 = read a second "card #8" and plot the percent difference of the
-- second curve with respect to the first curve;
-- 3 = read a second "card #8" and plot the ratio of the second curve to
-- the first curve.
-- nkh = not used.
--
-- **nth, ntp and nkh definitions are available for endf mfd = 6 or 7 as well**
-- **as for gendf mfd = 3 or 6. These definitions are given in the comments**
-- **at the beginning of the plotr.f source code and are beyond the scope of**
-- **this tutorial.**
--
-- Card 9 is required for 2D plots.
-- Cards 10 and 10a may be required for 2D plots.
-- Card 11 is required for 3D plots.

--
-- Card 9 is required for 2D plots.
-- Cards 10 and 10a may be required for 2D plots.
-- Card 11 is required for 3D plots.
--
-- Card 9: ***icon, isym, idash, iccol, ithick, ishade***
-- icon = ***0***/-i/+i = symbol and point-to-point connection option.
-- 0 = points connected, no symbols;
-- -i = plot i^{th} points only;
-- +i = plot and connect i^{th} points.
-- isym = ***0***, 1, 2, …, 18 = code for plot symbol.
-- 0 = square;
-- 1 to 18 = see plotr.f source code comments.
-- idash = ***0***, 1, 2, 3, 4 = line texture.
-- 0 = solid line;
-- 1, 2, 3, 4 = dashed, chain-dashed, chain-dotted, dot
-- iccol = ***0***, 1, 2, …, 7 = curve color.
-- 0 = black;
-- 1, 2, …, 7 = red, green, blue, magenta, cyan, brown, purple.
-- ithick = 0, ***1***, 2, … = curve thickness.
-- 0 = invisible (use with shaded areas);
-- ishade = ***0***, 1 to 10, 11 to 20, 21 to 30, …, 71 to 80 = shade pattern & color.
-- 0 = none;
-- 1 to 10, … = see plotr.f source code comments.
--
-- Card 10 only appears if ileg (card #4) is ≠ 0.
-- Card 10: aleg = curve or legend title (≤60 characters).
--
-- Card 10a only appears if ileg (card #4) = 2.
-- Card 10a: xtag, ytag, xpoint
-- xtag = local x coordinate of curve title;
-- ytag = local y coordinate of curve title;
-- xpoint = local x coordinate of vector (if ≤0, omit the vector).
--

NJOY99 Tutorial
PLOTR / VIEWR

```
--
-- Card 11 is required for 3D plots.
-- Card 11:  xv, yv, zv, x3, y3, z3 = viewing and 3D box volume coordinates.
--           xv, yv, zv = 15.0, -15.0, 15.0 = absolute coordinates of view point;
--           x3, y3, z3 = 2.5, 6.5, 2.5 = absolute length of x, y and z axes.
--
-- Cards 12 and 13 are required when iverf (card #0) = 0.
-- Card 12:  nform = format code for input data
--           nform = 0 = free form input with optional error bars.
--
-- Card 13 format depends upon the value of nform (card #12).  At present zero is
-- the only legal value for nform.
-- Card 13:  xdata, ydata, yerr1, yerr2, xerr1, xerr2
--           xdata = dependent value (terminate input for this curve with a /);
--           ydata = independent value;
--           yerr1 = lower y value error bar limit (if zero, no y error bar defined);
--           yerr2 = upper y value error bar limit (if zero, yerr2 = yerr1);
--           xerr1 = lower x value error bar limit (if zero, no x error bar defined);
--           xerr2 = upper x value error bar limit (if zero, xerr2 = xerr1);
--
```

- VIEWR input is a single card, specifying an input tape and an output tape.
  - Output, tape51 in the example below, is a postscript formatted file.

```
--
-- See comments at the start of viewr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nin, nout
--          integers that specify the input and output tapes.  These are ascii tapes.
--
viewr
 41 51                    ← tape41 must exist, tape51 will be created.
```

NJOY99 Tutorial
MODER / RECONR / BROADR / PLOTR / VIEWR

- Can run sample jobs using these modules:
  - "Job1" folder for ENDF/B-VII.0 ^{1}H (mat = 125)
    - PENDF output from BROADR will contain mt=1,2 and 102.
  - "Job2" folder for ENDF/B-VII.0 ^{10}B (mat = 525).
    - PENDF output from BROADR will contain mt=1, 2, 4, 51 – 85, 102, 103, 104, 107, 113, 600 – 605 and 800 – 801.
  - Input decks for multiple PLOTR jobs are provided to demonstrate some of the plotting options.

NJOY99 Tutorial
UNRESR

```
--
-- See comments at the start of unresr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output tape.
-- Card 2:  matd, ntemp, nsig0, iprint
--          matd = material to be processed.
--          ntemp = number of final temperatures (≤ 10).
--          nsig0 = number of sigma-zero values (≤ 10).
--          iprint = 0/1 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
-- Card 3:  tempk(i)
--          tempk(i) = ntemp temperatures, including zero.  These data are in degrees
--                     Kelvin and must be in ascending order.
-- Card 4:  sigz(i)
--          sigz(i) = nsig0 sigma-zero values.  These data are given in descending order
--                    and should include 1.0e+10 (if infinitely dilute results are desired).
--
-- Repeat cards 2, 3 and 4.
--
-- Set matd = 0 to terminate unresr input.
--
unresr
 -21 -22 -23 /          ← tape21 and tape22 must exist (for input), tape23 will be created.
 9228 2 3 0 /
 0. 293.6 /             ← Two temperatures, since ntemp on card 2 was 2.
 1.e+10 1.e+4 1000. /   ← Three sigma zero values, since nsig0 on card 2 was 3.
 0 /                    ← Loop back to read another card 2, set matd=0 to terminate input.
```

- Convert URR parameters into average cross sections.
  - Save results as MF=2, MT=152 (not an official ENDF mt) for use by other NJOY modules.
- Assume URR parameters span the specified energy range.
- Overwrite infinitely dilute cross section data previously saved from RECONR.
  - Caution – calculated cross sections can be negative.
- ***This module no longer required.***

NJOY99 Tutorial
UNRESR

```
unresr...calculation of unresolved resonance cross sections     250.3s

                                          storage   8/   20000

 unit for input endf/b tape ...........       -21
 unit for input pendf tape ............       -23
 unit for output pendf tape ...........       -24

 temperatures ......................... 0.000E+00
                                       2.936E+02
 sigma zero values ...................  1.000E+10
                                       1.000E+04
                                       1.000E+03
 print option (0 min., 1 max.) ........         1

 mat = 9228    temp =  0.000E+00                                 250.3s
 energy =  2.2500E+03
   1.978E+01  1.977E+01  1.968E+01  ← Sig(total)  for each sigma-0.
   1.211E+01  1.210E+01  1.209E+01  ← Sig(elscat) for each sigma-0.
   5.636E+00  5.631E+00  5.586E+00  ← Sig(fiss)   for each sigma-0.
   2.036E+00  2.033E+00  2.001E+00  ← Sig(capt)   for each sigma-0.
   1.978E+01  1.976E+01  1.958E+01

 … (repeat for all urr region tabulated energies)

energy =  2.5000E+04
   1.427E+01  1.427E+01  1.427E+01
   1.133E+01  1.133E+01  1.133E+01
   2.185E+00  2.185E+00  2.183E+00
   7.590E-01  7.589E-01  7.580E-01
   1.427E+01  1.427E+01  1.427E+01
 generated cross sections at  14 points                          250.6s

… (repeat for next temperature)

 generated cross sections at  14 points                          250.8s

                                        usage    2940/   20000

                                                                250.8s
*********************************************************************
```

- UNRESR Output
  - Summarize user specified i/o units, temperatures and σ_0 values.
  - Edit total, elastic scattering, fission and capture cross sections at each input file energy with URR parameter data.
    - Data are calculated at each tabulated energy for each temperature and each σ_0 value.

NJOY99 Tutorial
HEATR

```
--
-- See comments at the start of heatr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout, nplot
--          integers that specify endf and pendf input tapes plus an output pendf tape and an
--          optional output plot tape (0=plot tape default) that can be processed by viewr.
-- Card 2:  matd, npk, nqa, ntemp, local, iprint, ed
--          matd = material to be processed.
--          npk = number of partial kermas desired, ≤ 7 when iprint=2 (0) .
--          nqa = number of user q values (0).
--          ntemp = number of temperatures to process (0 = all on input pendf tape).
--          local = 0/1 = gamma rays are transported/deposited locally.
--          iprint = 0/1/2 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
--                   2 = perform kinematic checks and create an output plot file.
--          ed = displacement energy for damage calculations (0 = use internal default).
--
-- Card 3 is only present if npk > 0.
-- Card 3:  mtk(i), i=1,npk
--          mtk(i) = list of partial kerma mt numbers, given as endf mt+300.  Total kerma,
--                   mt=301, is always calculated and should not be listed.
--          Special values include (bold, italic mt's were typically calculated when
--          LANL created the ENDF70 library):
--            302 = elastic (mt=2).
--            303 = non-elastic (all but mt=2).
--            304 = inelastic (sum mt=51 through mt=90).
--            318 = fission (mt18 or sum mt=19, 20, 21 and 38).
--            401 = disappearance (sum mt=102 through mt=120).
--            402 = capture (mt=102).
--            442 = total photon (eV-barns).
--            443 = total kinematic kerma (high limit).
--          Damage energy production values include:
--            444 = total.
--            445 = elastic (mt=2).
--            446 = inelastic (sum mt=51 through mt=90).
--            447 = disappearance (sum mt=102 through mt=120).
```

- Only process one material per set of input cards.
- Compute various heating and damage cross sections.
- Neutrons and photon reactions are treated.
  - If no photon data exist, local heating will be overestimated.
- Heating data typically requested when LANL created ENDF70 are highlighted.
- Input continued on the next slide.

NJOY99 Tutorial
HEATR

- Input cards 4, 5 and 6 are rarely needed when processing modern evaluations.

```
--
-- Cards 4, 5 and 6 are only present if nqa > 0.
-- Card 4:  mta(i), i=1,nqa
--          mta(i) = mt values corresponding to User specified reaction q-values.
-- Card 5:  qa(i), i=1,nqa
--          qa(i) = User specified q-values.
-- Card 6 is only present if one or more qa(i) values are .ge. 99.e+6 eV.
-- Card 6:  qbar
--          qbar = an ENDF tab1 record defining an energy-dependent q-value.
```

```
-- a sample input deck:
heatr
 -21 -24 -25 /              ← input tape21 & tape24 must exist, tape25 will be created.
 9228 5 0 0 0 1 /
 302 303 402 443 444 /      ← Five partial kermas, since npk on card 2 was 5.
```

```
-- another sample input deck (include request for kinematic checks and plot generation):
heatr
 -21 -24 -25 30 /                ← tape30 is a plot file (to be processed by viewr).
 9228 7 0 1 0 2 /                ← first temperature only, perform kinematic checks.
 302 303 304 318 402 443 444 /   ← Seven partial kermas, since npk on card 2 was 7.
```

NJOY99 Tutorial
HEATR

```
heatr...prompt kerma                                        250.3s

                                              storage  15/   25000

input endf/b unit .....................        -21
input pendf unit ......................        -23
output pendf unit .....................        -25
mat to be processed ...................       9228
no. temperatures (0=all) ..............          1
gamma heat (0 nonlocal, 1 local) ......          0
print option (0 min, 1 more, 2 chk) ...          0
damage displacement energy ............    default
partial kerma mt-s desired ............        303
                                               304
                                               318
                                               402
                                               443
                                               444

default damage energy = 25.0 ev

---message from hinit---mt19 has no spectrum
                        mt18 spectrum will be used.

q correction for delayed fission energy
  delayed gammas:      6.3300E+06
  delayed betas:       6.5000E+06
  total correction:    1.2830E+07

---message from hinit---mf6, mt 16 does not give recoil za=92234
                        one-particle recoil approx. used.
. . .
---message from hinit---mf6, mt 91 does not give recoil za=92235
                        one-particle recoil approx. used.
                                                 temp 1     251.2s

  generating recoil with one-particle approx.

---message from nheat---changed q from   1.9348E+08 to   1.8065E+08
                        for mt  18


  generating recoil with one-particle approx.
                                                 temp 1     255.0s

photon energy production check
             e      ev-barns           min           max
    1.0000E-05    2.4581E+11    5.5577E+12    5.3119E+12   ----
. . .
    2.0000E+07    2.6226E+07    3.5463E+08    3.2841E+08   ----

                                              usage   12622/   25000
                                                              258.6s
*******************************************************************
```

- HEATR output can be extensive.
  - Example of minimal output for ENDF/B-VII.0 ^{235}U is shown.

NJOY99 Tutorial
PURR

```
--
-- See comments at the start of purr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output pendf tape.
--
-- Card 2:  matd, ntemp, nsigz, nbin, nladr, iprint, nunx
--          matd = material to be processed.
--          ntemp = number of temperatures (.le. 10).
--          nsigz = number of sigma-0 values (.le. 10).
--          nbin = number of probability bins.
--          nladr = number of resonance ladders.
--          iprint = 0/1 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
--          nunx = number of energy points (0 = all).
--
-- Card 3:  tempk(i), i=1,ntemp
--          tempk(i) = list of temperatures in degrees Kelvin, given in ascending order
--                     and including zero.
--
-- Card 4:  sigz(i), i=1,nsigz.
--          sigz(i) = sigma-0 values, including infinity.  Given in descending order (with
--                    1.0**10 used to represent infinity).
--
--  Repeat cards 2, 3 and 4.
--
-- Set matd = 0 to terminate purr input.
--
--
purr
 -21 -25 -26 /          ← input tape21 & tape25 must exist, tape26 will be created.
 9228 1 1 4 2 /         ← One temperature, one sigma-0, 4 bins, 2 ladders.
 293.6 /                ← One temperature since ntemp on card 2 was 1.
 1.e+10 /               ← One sigma-0 value since nsigz on card 2 was 1.
 0 /                    ← Terminate purr input.
```

- Create URR probability tables for use in MCNP calculations.
  - PURR output saved as MF=2, MTs 152 & 153 for subsequent processing in ACER.
- User selects number of probability bins and number of resonance ladders per bin.
  - These variables will affect the calculated cross sections.
  - 20 bins, 32 to 64 ladders are typical input parameters.
- ***Process URR data with PURR rather than UNRESR.***

NJOY99 Tutorial
PURR

```
purr...probabalistic unresolved calculation          291.0s

                                    storage  24/  180000
 unit for input endf/b tape ...........        -21
 unit for input pendf tape ............        -25
 unit for output pendf tape ...........        -26
 temperatures .........................  2.936E+02
                                         5.000E+02
 sigma zero values ....................   infinity
                                         1.000E+06
                                         1.000E+03
 number of probability bins ...........          4
 number of resonance ladders ..........          2
 print option (0=min, 1=max) ..........          1
 no. of energy points (0=all) .........          0

 mat = 9228                                    291.0s

 competition starts at  1.3100E+04
   ur competes with mt 51
   ur competes with mt 52
 inelastic competition flag set to   4
 absorption competition flag set to   0
```

- PURR Output
  - List i/o tape units.
  - List user temperatures.
  - List σ_0 values.
  - List # of probability bins.
  - List # of resonance ladders.
  - List material number.
  - Identify if URR overlaps with other reactions.

NJOY99 Tutorial
PURR

```
e= 2.2500E+03   spot= 1.1700E+01   dbar= 1.6137E-01   sigx= 0.0000E+00
             total     elastic     fission     capture
     1  1.9603E+01  1.2086E+01  5.3780E+00  2.1390E+00   ← First of 2 bins.
     2  1.9402E+01  1.2059E+01  5.2951E+00  2.0475E+00   ← Second of 2 bins.
  bkgd  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  infd  1.9778E+01  1.2105E+01  5.6364E+00  2.0363E+00   ← Infinitely Dilute xs.
  aver  1.9502E+01  1.2073E+01  5.3366E+00  2.0932E+00   ← Average xs over bins.
  pcsd        0.52        0.11        0.78        2.19   ← % Difference from Dilute.
  nres        3664

 bondarenko cross sections by direct sampling
         temp      sig0    p0 total     elastic     fission     capture    p1 total
    2.936E+02 1.000E+10  1.9502E+01  1.2073E+01  5.3366E+00  2.0932E+00  1.9502E+01
    2.936E+02 1.000E+06  1.9502E+01  1.2073E+01  5.3366E+00  2.0932E+00  1.9502E+01
    2.936E+02 1.000E+03  1.9483E+01  1.2070E+01  5.3253E+00  2.0882E+00  1.9465E+01
    5.000E+02 1.000E+10  1.9494E+01  1.2067E+01  5.3433E+00  2.0838E+00  1.9494E+01
    5.000E+02 1.000E+06  1.9494E+01  1.2067E+01  5.3433E+00  2.0838E+00  1.9494E+01
    5.000E+02 1.000E+03  1.9482E+01  1.2066E+01  5.3359E+00  2.0806E+00  1.9470E+01

 probability table
 tmax  2.936E+02  1.477E+01  1.858E+01  2.580E+01  3.842E+01   ← XS(Tot) at bin bdry.
 prob  2.936E+02  1.077E-01  3.920E-01  4.044E-01  9.590E-02   ← Probability per bin.
 tot   2.936E+02  1.391E+01  1.667E+01  2.151E+01  2.890E+01
 els   2.936E+02  1.132E+01  1.171E+01  1.231E+01  1.339E+01
 fis   2.936E+02  1.923E+00  3.594E+00  6.622E+00  1.087E+01
 cap   2.936E+02  6.707E-01  1.366E+00  2.575E+00  4.635E+00
 tmax  5.000E+02  1.552E+01  1.896E+01  2.439E+01  3.338E+01   ← repeat for next T.
 prob  5.000E+02  1.120E-01  3.838E-01  4.110E-01  9.320E-02
 tot   5.000E+02  1.467E+01  1.721E+01  2.130E+01  2.672E+01
 els   5.000E+02  1.143E+01  1.175E+01  1.232E+01  1.301E+01
 fis   5.000E+02  2.380E+00  3.943E+00  6.472E+00  9.694E+00
 cap   5.000E+02  8.567E-01  1.517E+00  2.509E+00  4.020E+00

 bondarenko cross sections from probability table
         temp      sig0    p0 total     elastic     fission     capture    p1 total
    2.936E+02 1.000E+10  1.9502E+01  1.2073E+01  5.3366E+00  2.0932E+00  1.9502E+01
    2.936E+02 1.000E+06  1.9502E+01  1.2073E+01  5.3366E+00  2.0932E+00  1.9502E+01
    2.936E+02 1.000E+03  1.9486E+01  1.2070E+01  5.3268E+00  2.0890E+00  1.9470E+01
    5.000E+02 1.000E+10  1.9494E+01  1.2067E+01  5.3433E+00  2.0838E+00  1.9494E+01
    5.000E+02 1.000E+06  1.9494E+01  1.2067E+01  5.3433E+00  2.0838E+00  1.9494E+01
    5.000E+02 1.000E+03  1.9484E+01  1.2066E+01  5.3368E+00  2.0811E+00  1.9473E+01
```

- PURR Output (con't)
  - Tabulate cross section data at each urr energy from the input endf/b file.
  - Check for good agreement between bin average values and infinitely dilute values.
  - Check for positive cross sections.
    - Re-run with more bins or resonance ladders, if necessary.

NJOY99 Tutorial
THERMR

```
--
-- See comments at the start of thermr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output pendf tape.
--          nendf (may be 0 when iinc=1) contains mf7 data, nin contains pointwise
--          data from reconr, broadr, … for this isotope.
--
-- Card 2:  matde, matdp, nbin, ntemp, iinc, icoh, natom, mtref, iprint
--          matde = thermal material to be processed (from nendf input file), or zero.
--          matdp = pointwise material to be processed (from nin input file).
--          nbin = number of equi-probable angles.
--          ntemp = number of temperatures (1 ≤ ntemp ≤ 10).
--          iinc = inelastic options.
--               = 0 = none.
--               = 1 = compute as free gas.
--               = 4 = read S(α,β) and compute scattering matrix.
--          icoh = elastic options (only needed for endf/b-iii thermal input tapes).
--               =  0 = none.
--               =  1 = graphite.
--               =  2 = beryllium.
--               =  3 = beryllium-oxide.
--               = 11 = polyethylene.
--               = 12 = h-zrh.
--               = 13 = zr-zrh.
--          natom = number of principal atoms in the molecule.
--          mtref = mt value used for output inelastic data (221 ≤ mtref ≤ 250).
--          iprint = 0/1/2 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
--                   2 = maximum plus intermediate results send to standard output.
--
-- Card 3:  tempk(i), i=1,ntemp
--          tempk(i) = list of temperatures in degrees Kelvin, given in ascending order.
--
-- Card 4:  tol, emax
--          tol = cross section reconstruction tolerance.
--          emax = maximum energy for thermal treatment (reduced to 10 eV if input
--                 is greater).
--
```

- THERMR Input
  - Free gas scattering for any nuclide.
  - Thermal kernel processing for ENDF/B-III, ENDF/B-VI or LEAPR output with File 7 data.

NJOY99 Tutorial
THERMR

```
--
-- execute thermr for free gas inelastic scattering.
thermr
 0 -26 -27                    ← no thermal input tape, tape26 must exist, tape27 will be created.
 0 9228 16 1 1 0 1 221 2 /    ← Free gas calculation, calculated σs to be saved in mt=221.
 293.6 /                      ← One temperature, since ntemp on card 2 was 1.
 .005 10. /                   ← 0.1% σs reconstruction tolerance, calculated up to 10 eV.
```

Partial THERMR output for 235U free gas calculation:

```
thermr...compute thermal scattering cross sections and matrices      1022.9s

                                                  storage  10/  800000

 unit for endf/b tape .................          0
 unit for input pendf tape ............        -26
 unit for output pendf tape ...........        -27

 material to be processed (endf) ......          0
 material to be processed (pendf) .....       9228
 number of angle bins .................         16
 number of temperatures ...............          1
 inelastic option .....................          1  ← free gas.
 elastic option .......................          0
 number of principal atoms ............          1
 reference mt .........................        221  ← mt for scat output.
 print option (0 min, 1 max) ..........          2
 temperatures (kelvin) ................ 2.9360E+02
 tolerance ............................ 5.0000E-03
 max energy for thermal treatment ..... 1.0000E+01

 endf uses endf-5 format                           ← ignore.

 pendf uses endf-6 format
```

- THERMR Input & Output
  - Free gas calculation.
  - Not used by ACER when creating a type 1 (FAST) library.

NJOY99 Tutorial
THERMR

```
enow   1.0000E-05   xsec    3.818E+00   mubar   -1.023E-02
 mu interval:                 1/11      2/12       6/16       7        8        9       10
    0.00000E+00  0.0000E+00   0.0000    0.0000  .   0.0000   0.0000   0.0000   0.0000   0.0000
                              0.0000    0.0000  .   0.0000
    7.32420E-09  2.2842E+02  -0.9360   -0.8081  .  -0.3009  -0.1751  -0.0497   0.0754   0.1999
                              0.3241    0.4479  .   0.9390
    9.76560E-09  2.6377E+02  -0.9357   -0.8075  .  -0.2991  -0.1731  -0.0477   0.0773   0.2019
                              0.3259    0.4496  .   0.9392
    1.22070E-08  2.9491E+02  -0.9355   -0.8069  .  -0.2975  -0.1714  -0.0459   0.0791   0.2036
                              0.3275    0.4510  .   0.9394
    1.46484E-08  3.2306E+02  -0.9353   -0.8063  .  -0.2960  -0.1699  -0.0443   0.0807   0.2051
                              0.3290    0.4523  .   0.9395
    1.95312E-08  3.7305E+02  -0.9350   -0.8054  .  -0.2935  -0.1672  -0.0415   0.0835   0.2078
                              0.3315    0.4545  .   0.9400
    2.44140E-08  4.1710E+02  -0.9347   -0.8045  .  -0.2912  -0.1648  -0.0390   0.0860   0.2102
                              0.3338    0.4565  .   0.9403

    . . .

    6.84661E-03  1.3807E-03  -0.9740   -0.9201  .  -0.6688  -0.5942  -0.5132  -0.4244  -0.3262
                             -0.2160   -0.0902  .   0.7828
    7.46183E-03  3.3741E-04  -0.9749   -0.9228  .  -0.6792  -0.6066  -0.5276  -0.4410  -0.3448
                             -0.2366   -0.1126  .   0.7708
    1.23836E-02  4.4433E-09  -0.9790   -0.9357  .  -0.7363  -0.6768  -0.6111  -0.5369  -0.4515
                             -0.3557   -0.2464  .   0.6774
    2.22272E-02  0.0000E+00   0.0000    0.0000  .   0.0000   0.0000   0.0000   0.0000   0.0000
                              0.0000    0.0000  .   0.0000

 . . .

Repeat for next value of "enow", up to User specified "emax".
```

- THERMR Output (con't)
  - Input E → Output E plus angular distribution data

NJOY99 Tutorial
GASPR

```
--
-- See comments at the start of gaspr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output pendf tape.
--
--
-- Since there is no matn specified, the nendf and nin tapes should only contain data for
-- the material of interest.
--
--
-- Sample input deck:
gaspr
 -21 -27 -28                ← tape21 & tape27 must exist, tape28 will be created.
```

- Gas production (h, d, t, ^{3}He & α).
  - Include results from capture reactions and inelastic reactions, using LR breakup flags, to identify outgoing light particle.
- Input tapes should only contain data for one material.

NJOY99 Tutorial
GASPR

```
gaspr...add gas production cross sections                          0.7s

units:   -21   -25   -28

the gas production threshold is  1.0000E-05 ev

found   600 points

pendf mt  mt203  mt204  mt205  mt206  mt207
________  _____  _____  _____  _____  _____
      55    0.0    0.0    0.0    0.0    1.0 ← Multiplicity or yield.
      56    0.0    0.0    0.0    0.0    1.0
      58    0.0    0.0    0.0    0.0    1.0
      59    0.0    0.0    0.0    0.0    1.0
      60    0.0    0.0    0.0    0.0    1.0
      61    0.0    0.0    0.0    0.0    1.0
      62    0.0    1.0    0.0    0.0    2.0
      63    0.0    0.0    0.0    0.0    1.0
      64    0.0    1.0    0.0    0.0    2.0
      65    1.0    0.0    0.0    0.0    0.0
      66    0.0    0.0    0.0    0.0    1.0
      67    0.0    0.0    0.0    0.0    1.0
      68    0.0    1.0    0.0    0.0    2.0
      69    0.0    0.0    0.0    0.0    1.0
      70    0.0    1.0    0.0    0.0    2.0
      71    0.0    1.0    0.0    0.0    2.0
      72    0.0    0.0    0.0    0.0    1.0
      73    0.0    1.0    0.0    0.0    2.0
      74    0.0    1.0    0.0    0.0    2.0
      75    0.0    0.0    0.0    0.0    1.0
      76    0.0    1.0    0.0    0.0    2.0
      77    0.0    1.0    0.0    0.0    2.0
      78    1.0    0.0    0.0    0.0    0.0
      79    0.0    1.0    0.0    0.0    2.0
      80    0.0    1.0    0.0    0.0    2.0
      81    0.0    1.0    0.0    0.0    2.0
      82    0.0    0.0    0.0    0.0    1.0
      83    0.0    1.0    0.0    0.0    2.0
      84    0.0    1.0    0.0    0.0    2.0
      85    0.0    0.0    0.0    0.0    1.0
     103    1.0    0.0    0.0    0.0    0.0
     104    0.0    1.0    0.0    0.0    0.0
     107    0.0    0.0    0.0    0.0    1.0
     113    0.0    0.0    1.0    0.0    2.0

*** means that the yield is energy dependent

found 1 temperatures
                                                                   0.8s
************************************************************************
```

- GASPR Output
  - "pendf mt" are input cross sections that produce gas particles.
  - mt203 to mt207 are gas production cross sections
    - will be written (or will overwrite) to the output pendf tape.

NJOY99 Tutorial
ACER

```
--
-- See comments at the start of acer.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Cards 1 through 3 are always present.  Cards 4 and later depend upon one or
-- more of the options specified on the initial three cards.
--
-- Card 1:  nendf, npend, ngend, nace, ndir
--          nendf = endf input tape (may be zero if iopt = 7 or 8).
--          npend = pendf input tape, or a previously existing ace file if iopt = 7 or 8.
--          ngend = multigroup input tape, or an output plot file if iopt = 7 or 8.
--          nace = output ace tape.
--          ndir = output file with xsdir information for nace.
--
-- Card 2:  iopt, iprint, ntype, suff, nxtra
--          iopt = acer output file designator (+iopt for mcnp, -iopt for mcnpx).
--                 = 1 = fast data.
--                 = 2 = thermal data.
--                 = 3 = dosimetry data.
--                 = 4 = photo-atomic data.
--                 = 5 = photo-nuclear data.
--                 = 7 = read existing type 1 ace file to print and/or edit.
--                 = 8 = read existing type 2 ace file to print and/or edit.
--          iprint = print control.
--                   = (0/1) = minimum/maximum output to the printer.
--          ntype = ace output type.
--                   = 1/2/3 = ascii/binary/obsolete ace file format.
--          suff = zaid "id" suffix.  If reading a previously created ace file, use a negative
--                  integer to retain the existing zaid.
--                 = .00 = default value.
--           nxtra = number of (iz,aw) pairs to read (0).
-- Card 3:  hk
--          hk = character string for the ace file header (.le. 70 characters and delimited
--                with quotes).
--
-- Card 4 is only present if nxtra > 0.
-- Card 4:  (iz(i),aw(i), i=1,nxtra)
--          iz,aw = pairs of identifiers that are written to the ace file.
--
```

- Create "A Compact ENDF" file.
  - Used by MCNP(X).
- Also create an "xsdir" file record.
  - User must hand-edit the NJOY produced xsdir file entry.
  - replace "filename" with the appropriate path and name.
    - The MCNP manual, appendix K, suggests that "filename" must be ≤8 characters, but I have successfully used up to 17 characters to define and path and filename.
  - replace "route" with a zero or directory path (≤70 characters).

NJOY99 Tutorial
ACER

```
--
-- Cards 5, 6 and 7 are used when generating a fast ace file.
-- Card 5:  matd, tempd
--          matd = endf material number.
--          tempd = 300. = temperature (degrees K).
-- Card 6:  newfor, iopp
--          newfor = 0/1 = use new cumulative angle distributions (law61) and outgoing
--                         particle distributions.
--          iopp = 0/1 = (no, do not/yes, do) include detailed photon data in the ace file.
-- Card 7:  thin(1), thin(2), thin(3) … No thinning if this card is not present.
--          thin(1) =
--          thin(2) =
--          thin(3) =
--
--
-- sample input deck for a "fast" ace file:
acer
 -21 -28 0 51 52          ← (Card 1).
 1 0 1 .10 /              ← (Card 2).  Create a "fast", type 1 ace file.
 'text for ace file header' ← (Card 3).
 9228 293.6               ← (Card 5).
/                         ← (Card 6).
/                         ← (Card 7).


--
-- another sample deck, create a standard set of plots from an existing ace file
-- (only needs cards 1, 2 & 3 when card #2 iopt = 7):
acer
 0 51 61 54 55            ← (Card 1).
 7 1 1 -1/                ← (Card 2).  Create a "plot" tape from an existing ace file.
 'text' /                 ← (Card 3).
--
-- use the viewr module to create a postscript file from the acer plot file.
viewr
 61 71                    ← tape71 is a postscript plot file.
```

- Sample input decks to
  - create a "FAST", type 1 ACE library file; or
  - perform file data checks and create an output file suitable for plotting (input to VIEWR).
    - VIEWR output file (tape71) is a postscript file.

NJOY99 Tutorial
ACER

```
acer...monte carlo neutron and photon data                    1051.5s

input endf/b unit .....................        -21
input pendf unit ......................        -27
input gendf unit ......................          0
output ace format unit ................         50 <- ACE output file.
output directory unit .................         51 <- info for xsdir.

run type option .......................          1 <- "FAST" ACE file.
print option (0 min, 1 max) ...........          0 <- minimal output.
type of ace file ......................          1 <- type 1.
mat to be processed ...................       9228
temperature ...........................  2.936E+02
thermal name ..........................
new formats ...........................          1
photon option .........................          1

                                          storage  27/  180000

using endf-6 format
                                                        repacking

energy discontinuities found in gamma files
           1.09000E+06



found mt=153 with unresolved-range probability tables
  energy range:  2.2500E+03 -  2.5000E+04 ev
  tables are factors
  inelastic competition =  4
  absorption competition =  0

---message from ptleg2---negative probs found
                            1 for mt= 65 e= 1.600E+07

---message from ptleg2---negative probs found
                            1 for mt= 67 e= 1.600E+07

---message from ptleg2---negative probs found
                            1 for mt= 71 e= 1.600E+07

 adding delayed neutron data

                                                              1054.9s
 ***************************************************************
```

- ACER Output
  - identify potential issues
    - gamma discontinuity
    - angular distributions
  - note presence of URR data.
  - note presence of delayed neutron data.
- Tape51 has data needed for MCNP's xsdir file.

NJOY99 Tutorial
ACER

```
acer...monte carlo neutron and photon data                    1054.9s

input endf/b unit .....................          0
input pendf unit ......................         50 ← not pendf.
input gendf unit ......................         60 ← plot if iopt=7.
output ace format unit ................         52
output directory unit .................         53

run type option .......................          7 ← tape50 checks.
print option (0 min, 1 max) ..........          1 ← maximum output.
type of ace file ......................          1

                                                  storage  27/  180000

ace consistency checks
----------------------

check reaction thresholds against q values

check that main energy grid is monotonic

check angular distributions for correct reference frame

check angular distributions for unreasonable cosine values

check energy distributions

check delayed neutron fractions

check delayed neutron distributions

check photon production sum

check photon distributions

no problems found                                  ← Success!
```

- ACER Output, with NJOY consistency checks.
  - Much more output follows, including
    - cross sections vs mt
    - angular distributions
    - secondary energy distributions
    - photon data

NJOY99 Tutorial
RECONR / … / ACER / VIEWR

- Can run sample jobs using these modules:
  - "Job3" folder for ENDF/B-VII.0 ^{10}B (mat = 525).
    - This job runs in a few seconds.
  - "Job4" folder for ENDF/B-VII.0 ^{90}Zr (mat = 4025).
    - This job runs in approximately 1 minute.
  - "Job5" folder for ENDF/B-VII.0 ^{235}U (mat = 9228).
    - "inp1" job runs in approximately 5 minutes.
      - 1.0% reconr/broadr reconstruction; 4 bins & 2 ladders in PURR.
    - "inp2" job runs in approximately 25 minutes.
      - 0.1% reconr/broadr reconstruction; 20 bins & 64 ladders in PURR.
    - "inp3" starts with the 1.0% broadr pendf tape and runs in approximately 1 minute (4 bins & 2 ladders in PURR).

NJOY99 Tutorial

Specific Applications – Creating MCNP .t Files

- A minimum NJOY job will include:
  - reconr/broadr/thermr/acer
  - optionally, include moder to convert between ascii and binary files, or to extract data for one material from a tape with multiple materials.
- A more complete job will include:
  - reconr/broadr/leapr/thermr/acer
    - Use leapr output in lieu of an existing thermal ENDF file.
  - optionally include moder.
- May run THERMR multiple times
  - ex. H free gas, H-H_2O, H-CH_2, H-ZrH, …

NJOY99 Tutorial
LEAPR

```
--
-- See comments at the start of leapr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nout
--          nout = output tape number for the thermal file containing mf7 data.
--
-- Card 2:  title
--          title = tape id label.
--
-- Card 3:  ntempr, iprint, nphon
--          ntempr = number of temperatures.
--          iprint   = 0/1/2 = printer control (min/more/most).
--          nphon    = 100 = phonon expansion order.
--
-- Card 4:  mat, za, isabt, ilog
--          mat   = endf material number for this compound (see ENDF-102,
--                  Appendix C for guidance).
--          za    = 1000*z + a for principal scattering atom.
--          isabt       = 0/1 = S(α,β) type.
--           WARNING:  Only isabt=0 type data can be correctly processed by thermr.
--          ilog   = 0/1 = flag for S(α,β) or ln(S(α,β)) in output.
--
-- Card 5:  awr, spr, npr, iel, ncold, nsk
--          awr    = weight ratio to the neutron for the principal scattering atom.
--          spr    = free atom thermal (e=0.0253 eV) scattering cross section for the
--                   principal scattering atom.
--          npr    = number of principal scattering atoms in the compound.
--          iel    = coherent elastic scattering option.
--                 = 0 = none.
--                 = 1/2/3 = graphite/beryllium/beryllium-oxide.
--                 = 4/5/6 = aluminum/lead/iron (new to endf/b-vii).
--          ncold  = cold hydrogen option.
--                 = 0 = none.
--                 = 1/2 = ortho/para hydrogen.
--                 = 3/4 = ortho/para deuterium.
--          nsk    = deuterium scattering model option.
--                 = 0 = none.
--                 = 1 = vineyard.
--                 = 3 = skold.
--
```

- LEAPR Input
  - Only needed if User required S(α,β) ENDF/B thermal scattering law data are not available.

NJOY99 Tutorial
LEAPR

```
--
-- Card 6:  nss,b7, aws, sps, mss
--          nss    = number of secondary scattering atoms (0 or 1).
--          b7     = secondary scatter type (0/1/2 = sct only/ free/ diffusion).
--          aws    = weight ratio to the neutron for the secondary scattering atom.
--          sps    = free atom thermal (e=0.0253 eV) scattering cross section for the
--                   secondary scattering atom.
--          mss    = number of secondary scattering atoms in the compound.
--
-- Card 7:  nalpha, nbeta, lat
--          nalpha = # of alpha mesh (.le. 200).
--          nbeta  = # of beta mesh (.le. 400).
--          lat    = 0/1 = scale factor option, if .ne. 0, scale alpha and beta mesh values
--                         by 0.0253/tev (where tev = temperature in eV).
--
-- Card 8:  alpha(i), i=1,nalpha
--          alpha(i) = alpha mesh (in ascending order).
--
-- Card 9:  beta(j), j=1,nbeta
--          beta(j) = beta mesh (in ascending order).
--
-- Loop over scattering atoms.  First set of cards 10 through 19 relate to the principal
-- scattering atom.  If appropriate, a second set of cards 10 through 19 relating to the
-- secondary scattering atom will also be required (b7=0).
--
-- Card 10:  tempk
--           tempk = temperature (Kelvin).  If ntempr from card 3 is 2 or greater and this
--                   is the second or greater time this card has been read and this value
--                   of tempk is less than zero, then assume the absolute value and retain
--                   the data from the previous temperature for cards 11 through 19.
--
-- Card 11: delta, ni
--          delta  = energy interval, eV.
--          ni     = number of points in the continuous excitation function.
--
-- Card 12:  rho(k), k=1,ni
--           rho(k) = normalized frequency spectrum.
```

- LEAPR Input (con't)

NJOY99 Tutorial
LEAPR

```
--
-- Card 13:  twt, c, tbeta
--           twt     = translational weight
--           c       = diffusion constant (0.0 for free gas)
--           tbeta   = normalization factor for continuous distribution.
--
-- Card 14:  nd
--           nd = number of discrete oscillators (.le. 50).
--
--
-- Card 15:  bdel(ii), ii=1,nd
--           bdel(ii) = oscillator energies, eV.
--
-- Card 16:  adel(jj), jj=1,nd
--           adel(jj) = oscillator weights (should sum to 1.0-tbeta-twt).
--
-- Note:  Cards 17 through 19 are only required if nsk (card 5) > 0.
-- Card 17:  nka,dka
--           nka  = number of kappa values (.le. 500)
--           dka  = kappa increment (inverse angstroms).
--
-- Card 18:  ska(kk), kk=1,nka
--           ska(kk) = s(k) values (if nsk=1/2, s(k) are for the vineyard/skold method).
--
-- Note:  Card 19 is only required if nsk (card 5) = 2.
-- Card 19: cfrac
--          cfrac = coherent fraction (skold method parameter).
--
-- Repeat cards 10 through 19 as necessary for the User specified number of temperatures
-- and scattering atom options.
--
-- Card 20:  text
--           text = a User text record (.le. 66 characters) to appear in mf1, mt451 of the
--                  output tape.
--
-- Continue reading "card 20" until a blank line is read.
--
```

- LEAPR Input (con't)

NJOY99 Tutorial
LEAPR

```
leapr
 30
' H in H2O, IKE model modified at LANL'  /
9 2 200 /
1 101 /
0.99917 20.43634 2 /            latest Hale values for VII
1 1 1.585751+1 3.842443 1 / oxygen as free gas from VI.8
187 274 1 /
.001 .0015 .0025 .0035 .005 .007 .01 .015  .025 .035
 . . .
590.  597.  604.  611. 618. 625. 632.9 / 187 alpha's
0.000 0.005 0.010 0.015 0.020 0.025 0.030 0.040 0.050 0.060
 . . .
152. 154. 156. 158.1 / 274 beta's
293.6 /  temperature (K) [first of nine]
0.00215 68/  frequency distribution
0.00000E+00  1.04170E-02  4.16710E-02  9.37490E-02  1.66682E-01
. . .
1.97272E+00  9.86360E-01  0.00000E+00 / 68 frequency values
0.0192 0. 0.4904 /      weights
2 /                     discrete oscillators
0.205 0.436 /           oscillator energies (eV)
0.163467 0.326933 /  oscillator weights
350. /                  temperature (K) [second of nine]
0.00215 68/
0.00000E+00  1.01473E-02  4.05927E-02  9.13258E-02  1.62372E-01
. . .
1.80884E+00  8.99437E-01  0.00000E+00 / 68 frequency values
0.029135 0. 0.485433 / weights
2 /                       discrete oscillators
0.205 0.436 /             oscillator energies (eV)
0.161811 0.323622 /     oscillator weights

. . . (next temperature) . . .
```

- Sample input (similar to that used to create the ENDF/B-VII.0 H-H_2O thermal file).
  - See M. Mattes report, http://www-nds.iaea.org/reports/indc-nds-0470.pdf for additional details.
  - Previous, ENDF/B-VI.2, thermal kernel results are documented in “New Thermal Neutron Scattering Files for ENDF/B-VI Release 2” by Bob MacFarlane (LA-12639-MS, available from http://t2.lanl.gov/data/thermal.html).

NJOY99 Tutorial
LEAPR

- LEAPR Input (con't)

```
800./
0.00215 68/
0.00000E+00  9.20968E-03  3.68424E-02  8.29024E-02  1.47390E-01
. . .
1.11069E+00  5.27354E-01  0.00000E+00 / 68 frequency values
0.049020 0. 0.47549 / weights
2 /                      discrete oscillators
0.205 0.436 /            oscillator energies (eV)
0.158497 0.316993  /  oscillator weights
 ' H(H2O)    IKE,LANL   EVAL-mar06 MacFarlane,Keinert,Mattes      '/
 ' INDC-NDS-0470       DIST-                                      '/
 '----ENDF/B-VII       MATERIAL    1                              '/
 '-----THERMAL NEUTRON SCATTERING DATA                           '/
 '------ENDF-6 FORMAT                                           '/
 '                                                               '/
 ' Temperatures (K)                                             '/
 '       293.6  350  400  450  500  550  600  650  800           '/
 '                                                               '/
 ' This evaluation[1] was generated at IKE in January of 2004 using    '/
 ' the LEAPR module of the NJOY Nuclear Data Processing System[2]  '/
 ' and modified at LANL in March of 2006 to use a temperature grid  '/
 ' more like the other ENDF evaluations and to fit the experimental '/
 ' data slightly better.  The model is improved over the one used   '/
 ' at General Atomics in 1969 to produce the original ENDF/B-III    '/
 ' evaluation[3].  The alpha and beta grids have been extended to   '/
 ' . . .                                                         '/
 ' . . .                                                         '/
 ' . . .                                                         '/
 ' 3. J.U.Koppel and D.H.Houston, "Reference Manual for ENDF      '/
 '    Thermal Neutron Scattering Data," General Atomic report    '/
 '    GA-8774 revised and reissued as ENDF-269 by the National   '/
 '    Nuclear Data Center, July 1978.                            '/
 '                                                               '/
 ' ------------------------------------------------------------- '/
/  end leapr
stop
```

NJOY99 Tutorial
LEAPR

- Partial LEAPR Output
  - hydrogen bound in water.

Partial leapr output for hydrogen bound in water:

```
 leapr...compute thermal scattering law
3.3s

                                          storage  15/ 7500000

     h in h2o, IKE model modified at LANL

 no. of temperatures ..................          2
 print flag ...........................          2
 phonon-expansion order ...............        200
 endf mat number ......................          1
 za ...................................        101
 isabt ................................          0
 ilog .................................          0

 awr for principal scatterer ..........      0.999
 free xsec for principal scatterer ....     20.436
 number of principal atoms ............          2
 elastic option .......................          0
 cold moderator option ................          0
 s(kappa) option ......................          0

 secondary scatterer type .............      1.000
 awr for secondary scatterer ..........     15.858
 free xsec for secondary scatterer ....      3.842
 number of secondary atoms ............          1

 principal scatterer...

 doing temp =    293.60
```

NJOY99 Tutorial
THERMR

```
--
-- See comments at the start of thermr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, nin, nout
--          integers that specify endf and pendf input tapes plus an output pendf tape.
--          nendf (may be 0 when iinc=1) contains mf7 data, nin contains pointwise
--          data from reconr, broadr, … for this isotope.
--
-- Card 2:  matde, matdp, nbin, ntemp, iinc, icoh, natom, mtref, iprint
--          matde = thermal material to be processed (from nendf input file), or zero.
--          matdp = pointwise material to be processed (from nin input file).
--          nbin = number of equi-probable angles.
--          ntemp = number of temperatures (1 ≤ ntemp ≤ 10).
--          iinc = inelastic options.
--               = 0 = none.
--               = 1 = compute as free gas.
--               = 4 = read S(α,β) and compute scattering matrix.
--          icoh = elastic options (only needed for endf/b-iii thermal input tapes).
--               =  0 = none.
--               =  1 = graphite.
--               =  2 = beryllium.
--               =  3 = beryllium-oxide.
--               = 11 = polyethylene.
--               = 12 = h-zrh.
--               = 13 = zr-zrh.
--          natom = number of principal atoms in the molecule.
--          mtref = mt value used for output inelastic data (221 ≤ mtref ≤ 250).
--          iprint = 0/1/2 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
--                   2 = maximum plus intermediate results send to standard output.
--
-- Card 3:  tempk(i), i=1,ntemp
--          tempk(i) = list of temperatures in degrees Kelvin, given in ascending order.
--
-- Card 4:  tol, emax
--          tol = cross section reconstruction tolerance.
--          emax = maximum energy for thermal treatment (reduced to 10 eV if input
--                 is greater).
--
```

- Generate pointwise neutron scattering cross sections
  - THERMR results are added to an existing pendf tape.
  - THERMR accepts thermal input from endfb3, endfb6 or LEAPR.
- Inelastic scattering matrix is written in a unique file 6 format for later use by ACER.
- THERMR may be executed multiple times in a given NJOY job.

NJOY99 Tutorial
THERMR

```
--
--
-- Free gas processing for hydrogen:
thermr
 0 -26 -27 /                 ← nendf=0 when iinc=1, tape26 must exist, tape27 will be created.
 0 125 20 1 0 0 1 221 /      ← Free gas calculation, calculated σs to be saved in mt=221.
 293.6 /                     ← One temperature, since ntemp on card 2 was 1.
 0.001 10. /                 ← 0.1% σs reconstruction tolerance, calculated up to 10 eV.
--
--
-- thermr for h-h2o.
-- S(α,β) data are read from tape30.
-- temperatures must match previous broadr, leapr jobs.
thermr
 30 -27 -28                  ← tape30=thermal input, tape27=pendf input, tape28=output.
 1 125 20 2 4 0 2 222 0 /    ← process S(α,β) for h bound in h2o, σs to be saved in mt=222.
 293.6 350. /                ← Two temperatures, since ntemp on card 2 is 2.
 0.001 10. /
--
--
-- thermr for h bound in polyethylene (endf/b-vii thermal material 37).
-- S(α,β) data are read from tape31.
-- If the output tape, tape27 here, already exists it will be overwritten.
-- If these three thermr jobs are run in sequence, the final tape27 will contain scattering
-- cross sections in mf=3, mt=221, mt=222 and mt=223.
thermr
 31 -28 -27                  ← tape31=thermal input, tape28=pendf input, tape27=output.
 37 125 20 1 4 11 2 223 /    ← process S(α,β) for h bound in ch2, σs to be saved in mt=223.
 293.6 /
 0.001 10. /
```

- Sample input decks for hydrogen
  - free gas (atom, not a molecule).
  - h bound in h_2o.
  - h bound in ch_2.

NJOY99 Tutorial
THERMR

```
thermr...compute thermal scattering cross sections and matrices 93.7s

                                          storage  10/  800000

 unit for endf/b tape .................          30 ← thermal input
 unit for input pendf tape ............         -27 ← pendf input
 unit for output pendf tape ...........         -28

 material to be processed (endf) ......           1 ← thermal matn
 material to be processed (pendf) .....         125 ← neutron xs matn
 number of angle bins .................          20
 number of temperatures ...............           2
 inelastic option .....................           4 ← S(a,b) option
 elastic option .......................           0
 number of principal atoms ............           2
 reference mt .........................         222 ← thermal xs mt
 print option (0 min, 1 max) ..........           0 ← minimal output
 temperatures (kelvin) ................ 2.9360E+02
                                        3.5000E+02
 tolerance ............................ 1.0000E-03
 max energy for thermal treatment ..... 1.0000E+01

 endf uses endf-6 format

 pendf uses endf-6 format

 ***warning***max value of beta limits the allowed energy transfer
 the sct approx. will be used for transfers larger than 4.000 ev.

 wrote thermal data for temp = 2.9360E+02                     320.4s

 ***warning***max value of beta limits the allowed energy transfer
 the sct approx. will be used for transfers larger than 4.000 ev.

 wrote thermal data for temp = 3.5000E+02                     533.5s

                                        usage  123970/  800000
                                                             533.5s
*******************************************************************************
```

- THERMR Output
  - Identify i/o files.
  - Identify thermal and fast endf/b material numbers.
  - Identify temperatures.
  - Identify thermal energy range.

NJOY99 Tutorial
ACER

```
--
-- Cards 8, 8a and 9 are used when generating a thermal ace file.
-- Card 8:  matd, tempd, tname
--          matd = material id (from the endf tape, not the thermal tape).
--          tempd = 300. = temperature (degrees K).
--          tname = 'za' = thermal zaid name (must be .le. 6 characters).
-- Card 8a:  iza01, iza02, iza03
--           iza01 = za value for the first component of this moderator.
--           iza02 = 0 = za value for the second moderator component (0 = n/a).
--           iza03 = 0 = za value for the second moderator component (0 = n/a).
-- Card 9:  mti, nbint, mte, ielas, nmix, emax, iwt
--          mti = mt value for thermal incoherent data (mtref from thermr card 2).
--          nbint = number of equiprobable angular bins for incoherent scattering.
--          mte = mt value for thermal elastic data.
--          ielas = 0/1 = coherent/incoherent elastic flag.
--          nmix = (1) = number of atom types if the moderator is mixed.
--                       Note:  1 = moderator is not mixed, if 2 (e.g., endf/b-iii beo), then
--                              require that many za values on card 8a.
--          emax = (1000.) = maximum energy for thermal treatment, in eV.
--                           Note:  the default will be the maximum energy read from
--                                  the thermal input tape for mf3, mti.
--          iwt = (0/1/2) = weighting option = variable/constant/tabulated.
--
-- A sample deck for hydrogen.
acer
 -21 -28 0 51 52          ← (Card 1).
 2 0 1 0.10 /             ← (Card 2).  Create a thermal, type 1 ace file.
 'text'                   ← (Card 3).
 125 293.6 'hh2o' /       ← (Card 8).
 1001 /                   ← (Card 8a).
 222 80 0 0 1 10. 0 /     ← (Card 9).
--
-- Another sample deck (that creates a plot file).
acer
 0 51 61 53 54            ← (Card 1).  Read an existing, tape51 ace file.
 7 1 1 /
 'text' /
--
-- Use viewr to create a postscript file from the acer generated plot file.
viewr
 61 71                    ← tape71 is a postscript plot file.
```

- Thermal ACER Input
  - Cards 1, 2 & 3 described previously.
  - Cards 8, 8a & 9 are for thermal data.
- As with FAST output file, can perform data checks and create a plot file.

NJOY99 Tutorial
ACER

Minimal ACER output for h-h2o:

```
 acer...monte carlo neutron and photon data                    327.0s

 input endf/b unit .....................          20
 input pendf unit ......................          29
 input gendf unit ......................           0
 output ace format unit ................          33 ← ACE output file.
 output directory unit .................          34 ← info for xsdir.

 run type option .......................           2 ← "THERMAL" job.
 print option (0 min, 1 max) ...........           0 ← minimal output.
 type of ace file ......................           1 ← type 1.
 mat to be processed ...................         125
 temperature ...........................  2.936E+02
 thermal name ..........................        hh2o
 iza01 .................................        1001
 iza02 .................................           0
 iza03 .................................           0
 mt incoherent .........................         222
 bins for incoherent scattering ........          80
 mt elastic ............................           0
 coherent/incoherent elastic flag ......           0
 no. atoms in mixed moderator ..........           1
 max energy for thermal ................      10.000
 weight option (0 var, 1 cons, 2 tab) ..           0

                                        storage  27/  180000

 using endf-6 format

 relative weights for energy bins are  1  4  10...10  4  1

                                                               328.6s

*********************************************************************
```

- Thermal ACER Output
  - minimal output shown.
- ACE file written to tape33.
- Tape34 has data needed for MCNP's xsdir file.

NJOY99 Tutorial
ACER

```
Maximum ACER output and data checks for h-h2o:

 acer...monte carlo neutron and photon data                    328.6s

 input endf/b unit .....................          0
 input pendf unit ......................         31 ← not pendf.
 input gendf unit ......................         37 ← plot if iopt=7.
 output ace format unit ................         35
 output directory unit .................         36

 run type option .......................          7 ← tape31 checks.
 print option (0 min, 1 max) ..........          1 ← maximum output.
 type of ace file ......................          1

                                          storage  27/  180000

 ace consistency checks
 ----------------------

 check reaction thresholds against q values

 check that main energy grid is monotonic

 check angular distributions for correct reference frame

 check angular distributions for unreasonable cosine values

 check energy distributions

 check photon production sum

 check photon distributions

 checking particle production sections

   deuteron production:

   checking energy distributions

 no problems found                                  ← Success!
```

- Thermal ACER Output
  - only a small portion of the maximum output shown.
- ACE file written to tape35.
- Tape36 has data needed for MCNP's xsdir file.

NJOY99 Tutorial
(LEAPR) / THERMR / ACER / VIEWR

- Can run sample jobs using these modules:
  - "Job6" folder for ENDF/B-VII.0 H-H_2O (mats = 1 & 125).
    - This job includes LEAPR to calculate S(α,β) data used by THERMR.
      - Job "1a" uses correct input.
      - Job "1b" erroneously assigns both hydrogen and oxygen as thermal moderator components to H_2O.
        - Impact is to underestimate the hydrogen scattering cross section by a factor of 2.
  - "Job7" folder for ENDF/B-VII.0 H-H_2O (mats = 1 & 125).
    - This job uses official ENDF/B-VII.0 data tapes.
    - Process 350 °K data.

NJOY99 Tutorial

Specific Applications – ERRORJ & Covariances

- NJOY99.259 uses Go Chiba's ERRORJ-2.3 program for covariance processing.
  - ERRORJ (version 2.2 is available from RSICC as a stand-alone program) was merged into NJOY99 as update 258.
    - ERRORJ replaces NJOY's ERRORR module.
    - The ERRORR module name is retained to minimize changes to historical input decks, but …
  - ERRORJ input is different than the input used by NJOY's ERRORR module (some variables swapped between cards 2 and 3).
  - Much of the discussion for ERRORR in the original NJOY91 manual remains valid.

NJOY99 Tutorial

Specific Applications – ERRORJ & Covariances

- Typical processing sequence will include NJOY99's RECONR, BROADR, GROUPR and ERRORJ modules.
  - Restrictions in ERRORJ mean that GROUPR is only executed at one temperature, for one σ_0 value (typically 1.e+10 which is infinitely dilute) and one Legendre component.
  - Might also include COVR and VIEWR for visualization.
  - Can run ERRORR or ERRORR/COVR by themselves if the input evaluated data file is for a non-resonance nuclide.

NJOY99 Tutorial

Specific Applications – ERRORJ & Covariances

- There has been limited use of covariance data from ENDF or other internationally distributed libraries in the past.
  - Covariance data processing is an area of increasing technical interest.
  - Covariance data and its formats continue to evolve to meet the needs of the User community.
    - ERRORJ includes coding to process covariances for MF=34 & MF=35 (NJOY99's original ERRORR only handled MF=31 and MF=33).
      - There has been limited experience with these data to date.
      - JENDL-3.3 formatting for MF35 may not conform rigorously to the ENDF/B6 format.

NJOY99 Tutorial
GROUPR

```
--
-- See comments at the start of groupr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, npend, ngout1, ngout2
--          integers that specify endf and pendf input tapes plus an optional input gendf tape
--          (default=0=no gendf input) and an optional output gendf tape (default=0=no gendf
--          output).
-- Card 2:  matb, ign, igg, iwt, lord, ntemp, nsigz, iprint
--          matb = material to be processed.
--          ign = neutron group structure option.
--          igg = gamma group structure option.
--          iwt = weight function option.
--          lord = Legendre order (must be 1 when running errorj).
--          ntemp = number of temperatures to process (must be 1 when running errorj).
--          nsigz = number of sigma zeroes (must be 1 when running errorj)
--          iprint = 0/1 = printer output option.
--                   0 = minimal results send to standard output.
--                   1 = maximum results send to standard output.
--
-- Card 3:  title
--          gendf output tape id record (default is "blank", truncated at 66 characters).
--
-- Card 4:  temp(i), i=1,ntemp
--          temp(i) = temperatures, in ascending order and in Kelvin.
--
-- Card 5:  sigz(i), i=1,nsigz
--          sigz(i) = sigma-0 values, in descending order (10^10 is infinity).
--
-- Cards 6 and 6a are only required when ign (card 2) = 1.
-- Card 6:  ngn
--          ngn = number of user specified neutron energy groups.
-- Card 6a:  egn(i), i=1,ngn+1
--           egn(i) = energy group breakpoints, in ascending order and in eV.
--
-- Cards 7 and 7a are only required when ig6 (card 2) = 1.
-- Card 7:  ngn
--          ngn = number of user specified gamma energy groups.
-- Card 7a:  egn(i), i=1,ngn+1
--           egn(i) = energy group breakpoints, in ascending order and in eV.
```

- GROUPR input includes user options for group structure, weighting function, Legendre order, temperature(s) and σ_0 factors.

NJOY99 Tutorial
GROUPR

```
--
-- The presence of cards 8a, 8b, 8c and 8d depends upon User choices for iwt.
-- Card 8a is only required if iwt < 0 (card 2).
-- Card 8b is only required if iwt=+1 or iwt=-1.
-- Card 8c is only required if iwt=+4 or iwt=-4.
-- Card 8d is only required if iwt=0.
--
-- Card 8a:  not relevant for errorj processing.
-- Card 8b:  A user specified weighting function, using the ENDF TAB1 format.
-- Card 8c:  eb, tb, ec, tc
--             eb = thermal breakpoint, eV.
--             tb = thermal temperature, eV.
--             ec = fission breakpoint, eV.
--             tc = fission temperature, eV.
-- Card 8d:  not relevant for errorj processing.
--
-- Repeat card 9 until mfd=0.
-- Card 9:  mfd, mtd, mtname
--            mfd = ENDF "file" number.
--            mtd = ENDF "section" number.
--            mtname = User name for this mf/mt.
--
-- Repeat card 10 until matd=0.
-- Card 10:  matd
--             matd = next material to process (using the same input as for the previous matd).
--
-- a sample input deck:
groupr
 -21 -23 0 25 /          ← input tape21 & tape23 must exist, tape25 will be created.
 9237 1 0 2 1 1 1 0 /
 'tape id record text goes here'
 300. /                  ← One temperature.
 1.e10                   ← One sigma-0.
 1                       ← Number of energy groups.
 1.e-5 2.e7              ← Group boundaries.
 3 /                     ← Group average all file 3 mt's.
 3 251 'mubar'           ← Another file 3 derived reaction.
 3 252 'xi'              ← Another file 3 derived reaction.
 3 452 'nu-t' /          ← Another file 3 derived reaction.
 3 455 'nu-d' /          ← Another file 3 derived reaction.
 3 456 'nu-p' /          ← Another file 3 derived reaction.
 5 18  'xi' /            ← Prompt fission spectrum.
 0 /                     ← End of file 3 mt list
 0 /                     ← End of groupr input
```

- Can request automatic processing of all available file 3 mt reactions and/or user specified reactions.
- Only request one material when passing the output to ERRORJ.

NJOY99 Tutorial
GROUPR

```
groupr...compute self-shielded group-averaged cross-sections    0.4s

                                          storage  23/ 5000000

unit for endf/b tape ..................        -21
unit for pendf tape ...................        -23
unit for input gout tape ..............          0
unit for output gout tape .............         91
mat to be processed ...................       9237
neutron group structure option ........          1
gamma group option ....................          0
weight function option ................          2
legendre order ........................          1
print option (0 min, 1 max) ...........          1

run title
---------------------------------------
     test

temperatures (kelvin) .................   3.00E+02
sigma zeroes ..........................   infinity

neutron group structure......read in
    1   1.00000E-05  -  1.00000E+00
    2   1.00000E+00  -  1.00000E+02
    3   1.00000E+02  -  1.00000E+04
    4   1.00000E+04  -  1.00000E+05
    5   1.00000E+05  -  1.00000E+06
    6   1.00000E+06  -  1.00000E+07
    7   1.00000E+07  -  2.00000E+07

weight function......constant for all 1
                                          id scr    1/     356

using endf-6 format
                                          id nu     2/ 4999924
                                          xx nu             0

processing mat   9237
---------------------------------------
```

- Output summary identifies input and output tapes plus other User options.

NJOY99 Tutorial
GROUPR

```
processing mat   9237
--------------------------------------
                                                id unr    2/ 4999924
                                                xx unr           547
                                                xx unr           547
                                                id ans    3/     905
                                                id ff     4/     907
                                                id prod   5/     914
                                                id sig    6/    1270
                                                                0.7s
group constants at t=3.000E+02 deg k
for mf  3 and mt  1 (n,total) cross section.

enrgy  group constants at
group  infinite dilution

  1    1.01118+1
 flx   9.99990-1
  2    9.35920+1
 flx   9.90000+1
  3    1.92810+1
 flx   9.90000+3
  4    1.31530+1
 flx   9.00000+4
  5    8.61730+0
 flx   9.00000+5
  6    7.04422+0
 flx   9.00000+6
  7    5.96554+0
 flx   1.00000+7

                                                xx ans           -1
                                                id ans    3/     905
                                                id ff     4/     907
                                                id prod   5/     914
                                                id sig    6/    1270
group constants at t=3.000E+02 deg k                              1.6s
for mf  3 and mt  2 (n,elastic) cross section.

enrgy  group constants at
group  infinite dilution

  1    9.21567+0
  2    4.69469+1
  3    1.78799+1
  4    1.26377+1
  5    6.81428+0
  6    3.74885+0
  7    2.96897+0

                                                xx ans           -1
                                                id ans    3/     905
                                                id ff     4/     907
                                                id prod   5/     914
                                                id sig    6/    1270
```

- List multigroup cross sections for various mt's at the User requested temperature and σ_0 .

NJOY99 Tutorial
GROUPR

```
 group constants at t=3.000E+02 deg k                                  7.2s
 for mf  3 and mt455 nu-d

 enrgy  group constants at
 group  infinite dilution

   1    4.40000-2
   2    4.40000-2
   3    4.40000-2
   4    4.40000-2
   5    4.40000-2
   6    3.47276-2
   7    2.60000-2

                                                xx ans             -1
                                                id ans    3/      906
                                                id ff     4/      909
                                                id prod   5/      916
                                                id sig    6/     1272
                                                id yld    7/ 4999924
                                                xx yld               28
 group constants at t=3.000E+02 deg k                                  8.0s
 for mf  3 and mt456 nu-p

 enrgy  group constants at
 group  infinite dilution

   1    2.44809+0
   2    2.44809+0
   3    2.44827+0
   4    2.45163+0
   5    2.51020+0
   6    3.25582+0
   7    4.59408+0

                                                xx ans             -1
                                                id ans    3/      911
                                                id ff     4/      919
                                                id prod   5/      926
                                                id sed    6/      933
                                                id sc     7/ 4999924
                                                xx sc            32570
 group constants at t=3.000E+02 deg k                                  8.8s
 for mf  5 and mt 18 chi

 normalized fission spectrum

   1  9.8242-11 4.10840-7 4.13211-4 1.24751-2 3.00146-1 6.86119-1 8.47163-4

                                                xx ans             -1
                                                xx unr             -1

                                              usage   34340/ 5000000
                                                                   9.0s
 ***************************************************************************
```

- Multigroup results continue for all User requested data.
- BUT, it is a fatal error to request processing for an mt value that is not available for a given material.

NJOY99 Tutorial
ERRORJ

```
--
-- See comments at the start of errorr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nendf, npend, ngout, nout, nin, nstan
--          nendf = endf input tape.
--          npend = pendf input tape.
--          ngout = 0 = gendf input tape (not always required (see card 7), if not present group
--                      cross sections will be calculated internally).
--          nout = 0 = output covariance tape (data are appended to an existing tape).
--          nin = 0 = input covariance tape.
--          nstan = 0 = input for ratio-to-standard
--
-- Card 2:  matd, ign, iwt, iprint, irelco
--          matd = endf material number to be processed.
--          ign = 1 = neutron group option (same definition as groupr, except 19 means merge
--                    the user input grid with the existing endf covariance grid).
--          iwt = 6 = group weight function.
--          iprint = (0/1) = minimum/maximum output to the printer.
--          irelco = (0/1) = absolute/relative covariances.
--
-- Omit card 3 if ngout (card 1) is ≠ 0.
--
-- Card 3:  mprint, tempin
--          mprint = 0/1 = minimum/maximum group average print option.
--          tempin = 300.0 = cross section temperature.
--
-- Cards 4, 5 & 6 are only required when processing ENDF/B-IV tapes.
-- These cards will not be discussed here.
--
-- Card 7:  iread,mfcov,irespr,legord,ifissp
--          iread = 0/1/2 = program calculated mt list/ user input mt and energy (card 8a) list/
--                          program calculated mt list plus user mat1-mt1 pairs.
--          mfcov = 33 = endf covariance file to be processed (31, 33, 34 or 35).  Note, if 33
--                       is specified then mf=32 data will be processed also.
--          irespr = 0/1 = resonance parameter (mf=32) processing option (area/ 1% sensitivity
--                         method).
--          legord = 1 = legendre order (ignored if not processing mf=34).
--          ifissp = -1 = fission spectrum energy (ignored if not processing mf=35).  If > 0, is
--                        energy range number, if -1 is fast reactor (2 MeV).
```

- ERRORJ Input
  - "iwt" – third item on card #2 was the first item on card #3 in NJOY99's original ERRORR module.
  - The ERRORR description in the NJOY91 manual (section X) remains valid.

NJOY99 Tutorial
ERRORJ

```
--
-- The presence of absence of cards 8 through 13 depend upon user options:
--
-- Cards 8, 8a, 8b and 9 are only required when iread (card 7) is 1.
-- Cards 8b and 9 are only required when nek (card 8) ≠ 0.
-- Card 10 is only required when iread (card ) is 2.
-- Card 11 is only required when nstan (card 1) ≠ 0.
-- Cards 12a and 12b are only required when ign (card 2) is 1 or 19.
-- Card 13a is only required when iwt = 1 (same as GROUPR).
-- Card 13b is only required when iwt = 4 (same as GROUPR).
--
-- Card 8:  nmt, nek
--          nmt = # of mt's to be processed.
--          nek = # of derived cross section energy ranges (if = 0, all cross sections are
--                independent).
--
-- Card 8a, mts(i), i=1,nmt
--          mts(i) = mt value.
--
-- Card 8b, ek(j), j=1,nek+1
--          ek(j) = derived cross section energy bounds.
--
-- Card 9, akxy(j), j=1,nmt
--         akxy(j) = derived cross section coefficients (one row/line).
--
-- Card 10:  mat1, mt1
--           matl, mtl = material id and reaction mt to include in covariance reaction list.
--           Note:  repeat card 10 as necessary.  Terminate with matl = 0.
--
-- Card 11:  matb, mtb, matc, mtc
--           matb, mtb = standards reaction referenced in matd (card 2).
--           matc, mtc = standards reactioin to be used in place of matb, mtb.
--
-- Card 12a:  ngn
--            ngn = number of energy groups (if < 0, energies will be in decending order)
--
-- Card 12b:  egn(i), i=1,ngn+1
--            egn(i) = group boundaries, eV (in ascending order unless ngn < 0).
--
-- Card 13a:  user weight function, specified using the ENDF "tab1" function format.
--
-- Card 13b:  eb, tb, ec, tc
--            eb = thermal breakpoint energy, eV.
--            tb = thermal temperature, eV.
--            ec = fission breakpoint energy, eV.
--            tc = fission temperature, eV.
```

- ERRORJ Input
  - Presence, or absence, or many input cards is dependent upon specific User options.
  - In practice most User input decks will not require many of these cards.

NJOY99 Tutorial
ERRORJ

```
--
-- Meaning for ign and iwt (card 2 input variables):
--
--     *      ign          meaning                                  *
--     *      ---          -------                                  *
--     *       1        arbitrary structure (read in)              *
--     *       2        csewg 239-group structure                  *
--     *       3        lanl 30-group structure                    *
--     *       4        anl 27-group structure                     *
--     *       5        rrd 50-group structure                     *
--     *       6        gam-i 68-group structure                   *
--     *       7        gam-ii 100-group structure                 *
--     *       8        laser-thermos 35-group structure           *
--     *       9        epri-cpm 69-group structure                *
--     *      10        lanl 187-group structure                   *
--     *      11        lanl 70-group structure                    *
--     *      12        sand-ii 620-group structure                *
--     *      13        lanl 80-group structure                    *
--     *      14        eurlib 100-group structure                 *
--     *      15        sand-iia 640-group structure               *
--     *      16        vitamin-e 174-group structure              *
--     *      17        vitamin-j 175-group structure              *
--     *      18        xmas 172-group structure                   *
--     *      19        read in, supplement with endf cov. grid    *
--     *                                                           *
--     *      iwt          meaning                                  *
--     *      ---          -------                                  *
--     *       1        read in smooth weight function             *
--     *       2        constant                                   *
--     *       3        1/e                                        *
--     *       4        1/e + fission spect + thermal maxwel       *
--     *       5        epri-cell lwr                              *
--     *       6        (thermal) -- (1/e) -- (fission + fusion)   *
--     *       7        same with t-dep thermal part               *
--     *       8        thrml--1/e--fast reactor--fission+fusion   *
--     *       9        claw weight function                       *
--     *      10        claw with t-dependent thermal part         *
--     *      11        vitamin-e weight function (ornl-5505)      *
--     *      12        vit-e with t-dep thermal part              *
--     *                                                           *
--     *************************************************************
```

- ERRORJ Input
  - Many group structure and weighting function options mirror those from the GROUPR module.
- NJOY99's Standard Problem Test Suite Includes Two ERRORJ Jobs.

NJOY99 Tutorial
ERRORJ

```
--
-- NJOY test suite, problem #4.
-- (endf input tape contains endf/b-v, 235U, material #1395 data)
moder
 20 -21
reconr
 -21 -22
 'u-235 10% pendf for errorr test problem from t511'/
 1395/
 .10/
 0/
errorr
 -21 -22 0 23 0 /      ← Card #1
 1395 19 3 1 1         ← Card #2 (ign=19=endf input + user grid).
 0 0                   ← Card #3
 0 33 /                ← Card #7
 1                     ← Card #12a (required since card #2's ign=19).
 1.e0 1.e3             ← Card #12b (required since card #2's ign=19).
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/       ← Card #1
 1395 1 2 1 1          ← Card #2 (ign=1=user energy grid)
 0 31/                 ← Card #7 (no card #3 since card #1's ngout≠0).
 7                     ← Card #12 (required since card #2's ign=1).
 1.e0 1.e1 1.e2 1.e3 1.e4 1.e5 1.e6 1.e7    ← Card 12b
stop
```

- Input deck for NJOY99 Test Problem #4.
  - Process fission nu covariance data.

NJOY99 Tutorial
COVR

```
--
-- See comments at the start of covr.f for the latest input instructions.
-- Bold, italicized variables have internal default values.
--
-- Card 1:  nin, nout, nplot
--          integers that specify the input covariance file (output from errorj) and optional
--          (default=0=none) output and plot tapes.  The plot tape will serve as input to the
--          VIEWR module, which will produce a postscript formatted output tape.
--
-- Cards 2, 2a and 3a only appear when nplot ≠ 0.
-- Card 2:  icolor
--          icolor = 0/1 = produce monochrome (cross-hatch) / color plots.
--
-- Card 2a:  epmin
--           epmin = minimum plot energy (default = 0.0 eV).
--
-- Card 3a:  irelco, ncase, noleg, nstart, ndiv
--          irelco = 0/1 = absolute/relative covariances are on nin.
--          ncase = 1 = number of plots to produce.
--          noleg = -1/0/1 = legend label option (first plot only/all plots/no legend label).
--          nstart = 1/n = first figure to realize.
--          ndiv = 1 = # of gray shades.
--
-- Cards 2b, 3b and 3c only appear when nout > 0.
--These cards are not needed to produce an output plot file.
-- Card 2b:  matype, ncase
--           matype = 3/4 = output library matrix (covariances/correlations) option.
--           ncase = 1 = number of cases to process.
--
-- Card 3b:  hlibid
--           hlibid = 6-character id.
--
-- Card 3c:  hdescr
--           hdescr = 21-character descriptive message.
--
-- Card 4 contains a quartet of data, specifying materials and mt numbers for covariance
-- matricies.  This card is repeated "ncase" (card 3a) times.  If this card appears once with
-- mat ≠ 0 and mt=mat1=mt1=0, then all possible covariance plots (up to 60) are generated.
-- Card 4:  mat, mt, mat1, mt1
--          mat = material number.
--          mt = reaction number from mat.
--          mat1 = material1 number.
--          mt1 = reaction number from mat1.
--
```

- Use COVR to produce a plot file.
- Follow with VIEWR to produce postscript plots.

NJOY99 Tutorial
COVR

```
--
-- a sample errorj/covr input series (fission nu covariances from file 31).
-- moder/reconr/broadr/groupr not shown here.
--
errorr
 -21 0 91 25 0 0 /
 9237 3 6 1 1 /
 0 31 1 1 -1 /
--
-- covariance plotting (mf31 data) with covr.
covr
 25 0 35/
 1/
 /
 /
 9237/
--
-- make postscript plot file.
viewr
 35 45/
```

- Another input deck – processing JENDL-3.3 ^{238}U nu (file 31) with ERRORJ/COVR/VIEWR.
  - tape21 is original JENDL-3.3 data (binary).
  - tape91 is GROUPR output.
  - tape25 is ERRORJ output.
  - tape35 is COVR plot output.
  - tape45 is VIEWR postscript formatted plot file.

NJOY99 Tutorial
COVR

- Another input deck – processing JEFF-3.1 ^{56}Fe pointwise cross sections (file 33).

```
--
-- a sample errorj/covr input series (cross section covariances from file 33).
-- moder/reconr/broadr/groupr not shown here.
--
errorj
 20 0 91 26 0 0 /
 2631 19 2 1 1 /
 0 33 /
 7 /
 1.e-5 1.e0 1.e3 1.e4 1.e5 1.e6 1.e7 2.e7 /
--
--
covr
 26 0 36 /                  ← input tape26 must exist, plot tape36 will be produced.
 1 /                        ← Card 2.  icolor=1=color plots
 1.e3 /                     ← Card 2a.  E(min) on plot axis is 1 keV.
 1 5 /                      ← Card 3a. Relative covariances, card 4 will appear 5 times.
 2631    1 2631    1       ← Card 4 (repeated "ncase"=5 times).
 2631    2 2631    2
 2631    3 2631    3
 2631   16 2631   16
 2631  102 2631  102
```

NJOY99 Tutorial
RECONR / … / ERRORR / COVR / VIEWR

- Can run sample jobs using these modules:
  - "Job8" folder for ENDF/B-V Carbon.
    - Carbon is a non-resonance nuclide; therefore run MODER/ERRORR/COVR (NJOY99 test suite, problem #5).
  - "Job9" folder for JENDL-3.3 ^{238}U.
    - ERRORJ processes file 31 (total, prompt and delayed υ).
  - "Job10" folder for JEFF-3.1 ^{56}Fe
    - ERRORJ processes file 33; COVR plots user specified reaction list.

NJOY99 Tutorial

References

- Web Sites:
  - http://t2.lanl.gov/codes/njoy99/index.html
  - http://www.nea.fr/lists/njoy.html
- Reports:
  - R.E.MacFarlane & D.W.Muir, "The NJOY Nuclear Data Processing System, Version 91" (distributed with the NJOY99 code package).
  - H.R.Trellue *et al*, ENDF70: A Continuous-Energy Neutron Data Library Based on ENDF/B-VII.0 (ICRS-11 conference).
  - J.M.Campbell *et al*, "ENDF66: A Continuous-Energy Neutron Data Library Based on ENDF/B-VI Release 6" (RPSD-2002 conference).
  - Oscar Cabellos, "Processing of the JEFF-3.1 Cross Section Library into a Continuous energy Monte Carlo Radiation Transport and Criticality Data Library", NEA/NSC/DOC(2006)18 (http://www.nea.fr/html/dbprog/Njoy/Cabellos-report_mcjeff31-v36.pdf).

NJOY99 Tutorial
Conclusions

- During This Tutorial User's have Learned:
  - How to Maintain the NJOY99 Code System.
    - Where to Find and How to Apply Update Files to Create a New NJOY99 Executable.
  - Where to Find Information on Historical NJOY99 Test i/o Files.
  - How to Setup NJOY99 Input Decks to Produce:
    - Continuous Energy Neutron Cross Section (MCNP .c cross section) Files.
    - Thermal Kernel (MCNP .t cross section) Files.
    - Use ERRORJ to Process Covariance Data.
- Further Questions, Comments, Feedback?
  - send email to akahler@lanl.gov and/or ryxm@lanl.gov.

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