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Title: Using NJOY to Create MCNP ACE Files and Visualize Nuclear Data

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Using NJOY to Create MCNP ACE Files and Visualize Nuclear Data

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UNCLASSIFIED

Abstract

- We provide lecture materials that describe the input requirements to create various MCNP ACE files (Fast, Thermal, Dosimetry, Photo-nuclear and Photo-atomic) with the NJOY Nuclear Data Processing code system. Input instructions to visualize nuclear data with NJOY are also provided.

Course Outline

- History of NJOY (lecture).
- How to obtain the NJOY2012 code package and update the code (lecture).
- Introduction to the Evaluated Nuclear Data File (ENDF) system (lecture).
  - ENDF data structures (lecture).
- Creating MCNP ACE .c and .t files (interactive).
  - Also provide notes for dosimetry, photo-nuclear and photo-atomic files.
- Visualizing nuclear data with NJOY (interactive).

NJOY History

NJOY History - I

- LANL has a long history in nuclear data processing to support its in-house transport codes
  - Pre-NJOY = MINX, LAPHAN0, GAMLEG, ETOPL, …
    - MINX = Multi-group Interpretation of Nuclear X-sections.
    - LAPHAN0 = photon production.
    - GAMLEG = photon interaction.
    - ETOPL = MCN (pre-MCNP) Monte Carlo library generator.
  - MINX-II = early-1970s development effort to bring the various processing codes into a single code.
    - NJOY is what you get when your 1970s impact printer slips a cog and each letter is off by one!

NJOY History - II

- The NJOY Nuclear Data Processing System
  - Original developer … Bob MacFarlane
    - LANL retiree, in 2005, but remains active in NJOY development.
      - "… a strange retirement hobby …" according to his wife.
  - NJOY is used world-wide
    - NJOY has been in continuous development for nearly 40 years
      - First public release was in 1977 (additional major updates in 1978, 1981, 1983, 1989, 1991, 1994, 1997, 1999, 2012).
      - Many new "upn" updates between major releases.
      - NJOY has evolved as ENDF has evolved.
    - NJOY has benefitted from constructive feedback and collaboration with national and international peers.
    - See Section 1.4 in the NJOY2012 manual.

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How do I get NJOY2012?

Obtaining NJOY2012 - I

- NJOY2012 is distributed by LANL's Feynman Center for Innovation.
  - Sadly, for most users, it costs money.
  - Working to make the next release, NJOY2016 (and NJOY21), open source.
- Current contact information is available at http://t2.lanl.gov/nis/codes
- LANL point-of-contact for license information:
  - Christine Ramos
  - Email: ctramos@lanl.gov
  - Phone: 505-665-6846

Obtaining NJOY2012 - II

- The next generation NJOY code … NJOY21 …
  - "NJOY for the 21st Century".
  - Approved for Open Source release.
  - Will work with the new Generalized Nuclear Data (GND) format currently under development.

NJOY Installation and Updating

NJOY Installation & Updating - I

- I have downloaded the distribution zip file, or have an NJOY2012 CD … now what?
  - The NJOY2012 distribution contents include …
    - A source file, src.
    - A code maintenance control program, upd.f90.
    - Miscellaneous input files to run test jobs, output files from LANL, sample make files, figure files for the manual …
    - A “readme0” file.
  - The distribution does NOT include an executable version of NJOY2012.
    - NJOYx has always been distributed as source code only.
  - We do not tell you how to layout the various code components on your system’s HDD.

NJOY Installation & Updating - II

- The directory layout expected if using Windows *.bat files …
  - njoy (contains src)
    - njoy/manual (contains *.tex)
      - njoy/manual/figs (contains *.ps)
    - njoy/test (contains endf tapes used by various test jobs)
      - njoy/test/test## (contains input and output files)
    - njoy/up# (contains update instructions)
  - upd (contains upd.f90, to be compiled by the user)

NJOY Installation & Updating - III

- Steps to create an NJOY2012 executable
  - Compile upd.f90 …
  - Execute upd (specifically upd x)…
    - The folder where upd is executed must also contain the distribution media supplied “src” file and an update file, “upn”.
      - Update, up0, is included in the distribution media;
      - The latest up# file, currently up50, can be downloaded from http://t2.lanl.gov/nis/codes/NJOY12/index.html;
      - Simply rename your “up#” file to “upn”.
  - Will now have a suite of NJOY2012 .f90 source code files and *.tex LaTeX files.
  - Sample makefiles are included on the distribution media.

NJOY Installation & Updating - IV

- Steps to create an NJOY2012 executable (con't)
  - I work in the PC/Windows world.
    - Batch files/scripts to create an NJOY executable, and the latest version of the NJOY2012 manual, are included in the distribution.
    - Users may need to customize the sample makefiles to use the fortran compiler and LaTex distribution available to them.
      - Intel, g95, gfortran examples are provided.
    - If using the "makeNJOY.win#.bat" files you must have the Microsoft "nmake" program and MiKTeX's "texify" program installed in your path.
    - Sample files used by Bob MacFarlane on a Mac laptop are also included on the distribution media.

NJOY Installation & Updating - V

- Updating NJOY2012
  - upd is a simplified version of the CDC “update” program.
    - upd is a line editor … each line in the “src” input file contains a unique identifier.
    - The “upn” file contains comments, commands and source code that is inserted, deleted and/or inserted & deleted in “src”.
    - The “src” file is broken into “decks” and after applying the required commands each “deck” becomes either a .f90 fortran source file or a .tex LaTeX file.
    - A new “list” file, where each line contains the latest identifiers, may also be created for each .f90 and .tex file to support future revisions.
      - Execute “upd l”.

NJOY Installation & Updating - VI

```
*deck njoy.f90
program njoy
!-----------------------------------------------------------------------
!
!    NJOY Nuclear Data Processing System
!    Version 2012
!
!-----------------------------------------------------------------------
!
! NJOY is a system of processing modules intended to convert evaluated
! nuclear data in the ENDF format into forms useful for practical
…
```

- A portion of NJOY2012's "src" file …
  - "*deck NAME" is an identifier used by upd to assign line numbers needed to execute subsequent upd commands.
  - "program njoy" is the opening Fortran statement.
  - ! lines are Fortran comment statements.

NJOY Installation & Updating - VII

```
njoy.2    : program njoy                                                    njoy
njoy.3    : !-------------------------------------------------------------  njoy
njoy.4    : !                                                               njoy
njoy.5    : !    NJOY Nuclear Data Processing System                        njoy
njoy.6    : !    Version 2012                                               njoy
njoy.7    : !                                                               njoy
njoy.8    : !-------------------------------------------------------------  njoy
njoy.9    : !                                                               njoy
njoy.10   : ! NJOY is a system of processing modules intended to convert evaluated   njoy
njoy.11   : ! nuclear data in the ENDF format into forms useful for practical       njoy
…
```

- The “njoy.lst” file produced by upd I …
  - Line identifier is “NAME” from *deck NAME plus a sequentially increasing integer.
    - Line 1 is the *deck NAME record, but does not appear in the *.lst or *.f90 files.

NJOY Installation & Updating - VIII

```
*ident ver
*/ 21dec12
*/ This is the initial release of the NJOY2012 package,
*/ the new version written using modern Fortran-90 style.
*/ set the locale variables for lab and mx
*/ set the version and date
*d njoy.6
!    Version 2012.0
*d vers.7,vers.8
   character(8),public::vers='2012.0'
   character(8),public::vday='21Dec12'
*d locale.15,locale.16
   character(8),public::lab='lanl t2'
   character(8),public::mx='pc-ifort'
```

- Part of the “up0” file …
  - “ver” in *ident ver is the name that upd will apply to any inserted code.
  - Lines beginning with “*/” are upd comments.
  - *d njoy.6 plus next line says to delete line 6 and replace with that line.
  - “vers” and “locale” are other njoy2012 decks with code version, lab and machine specific info that can be customized.

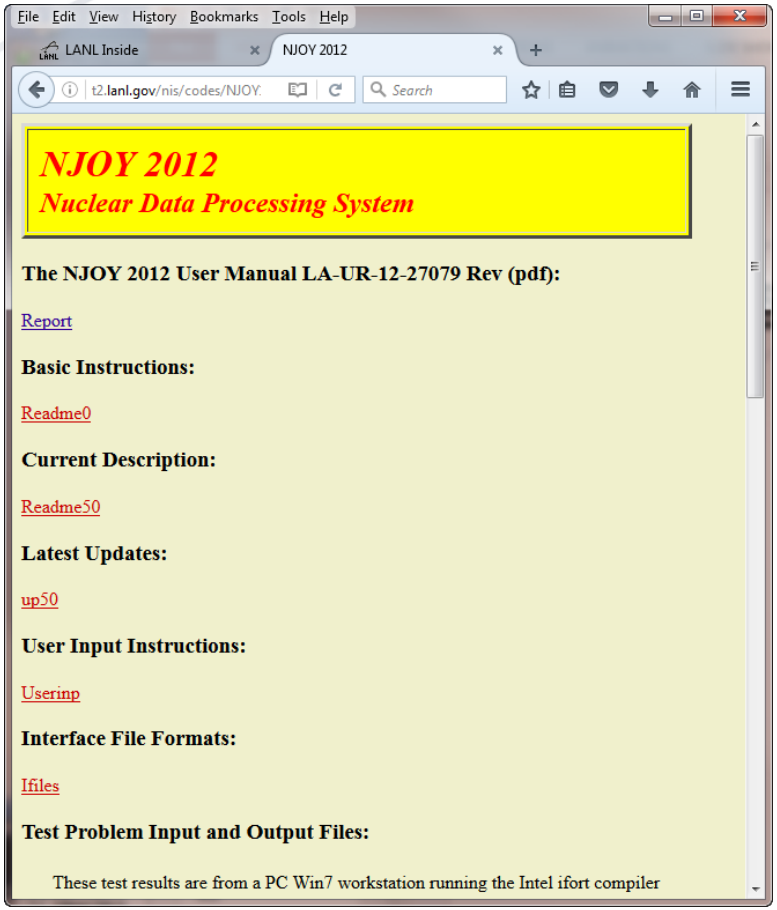
NJOY Installation & Updating - IX

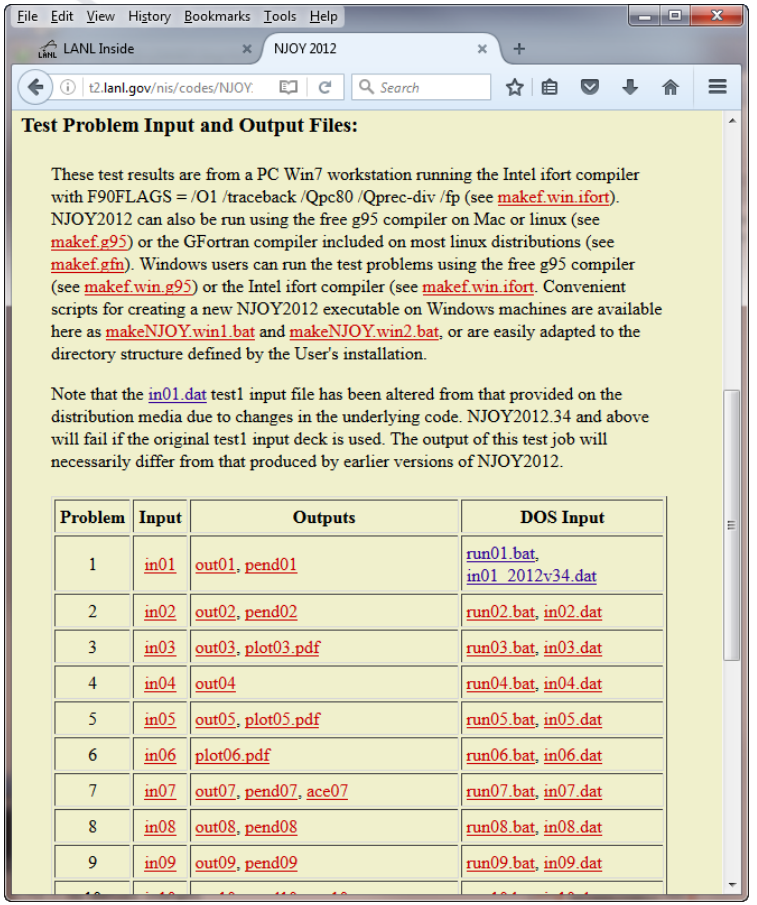
```
njoy.2    : program njoy                                                        njoy
njoy.3    : !-------------------------------------------------------------------njoy
njoy.4    : !                                                                   njoy
njoy.5    : !    NJOY Nuclear Data Processing System                            njoy
 ver.8    : !    Version 2012.0                                                 njoy
njoy.7    : !                                                                   njoy
njoy.8    : !-------------------------------------------------------------------njoy
njoy.9    : !                                                                   njoy
njoy.10   : ! NJOY is a system of processing modules intended to convert evaluated njoy
njoy.11   : ! nuclear data in the ENDF format into forms useful for practical  njoy
…
```

- The “lst” after executing upd with the up0 update file …
  - The original njoy.6 line has now been replaced.

NJOY Installation & Updating - X

Where can I get the latest updates and manual?





- http://t2.lanl.gov/nis/codes/NJOY12/index.html

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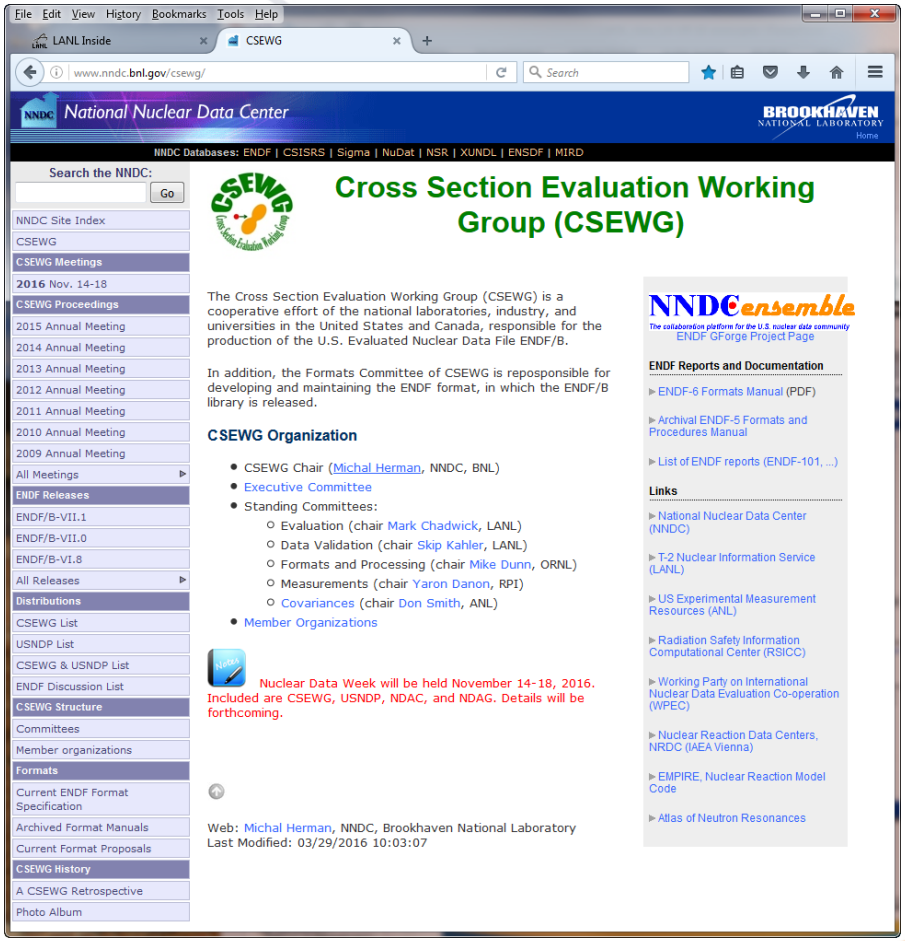
Introduction to ENDF

ENDF Introduction - I

- The Evaluated Nuclear Data File (ENDF) is the nation's nuclear reaction cross section database.
  - The file is maintained and is publicly available from the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL, http://www.nndc.bnl.gov/).
  - ENDF content is determined by the Cross Section Evaluation Working Group (CSEWG, http://www.nndc.bnl.gov/csewg/).
    - CSEWG members come from national labs, academia, (industry).
    - CSEWG members collaborate with international colleagues.
      - CSEWG members are not all-knowing … if the data you care about isn't available perhaps your organization needs to be involved in our community.

ENDF Introduction - II



NNDC web pages … http://www.nndc.bnl.gov/ & http://www.nndc.bnl.gov/csewg/

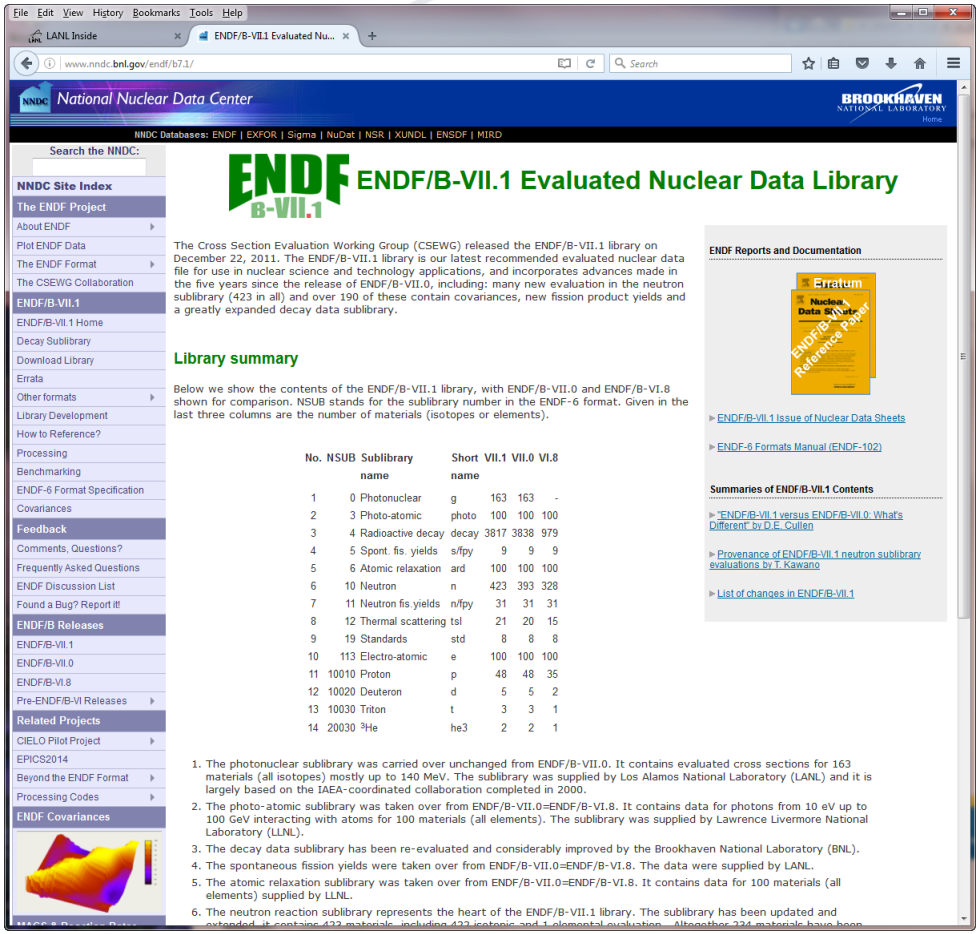
ENDF Introduction - III

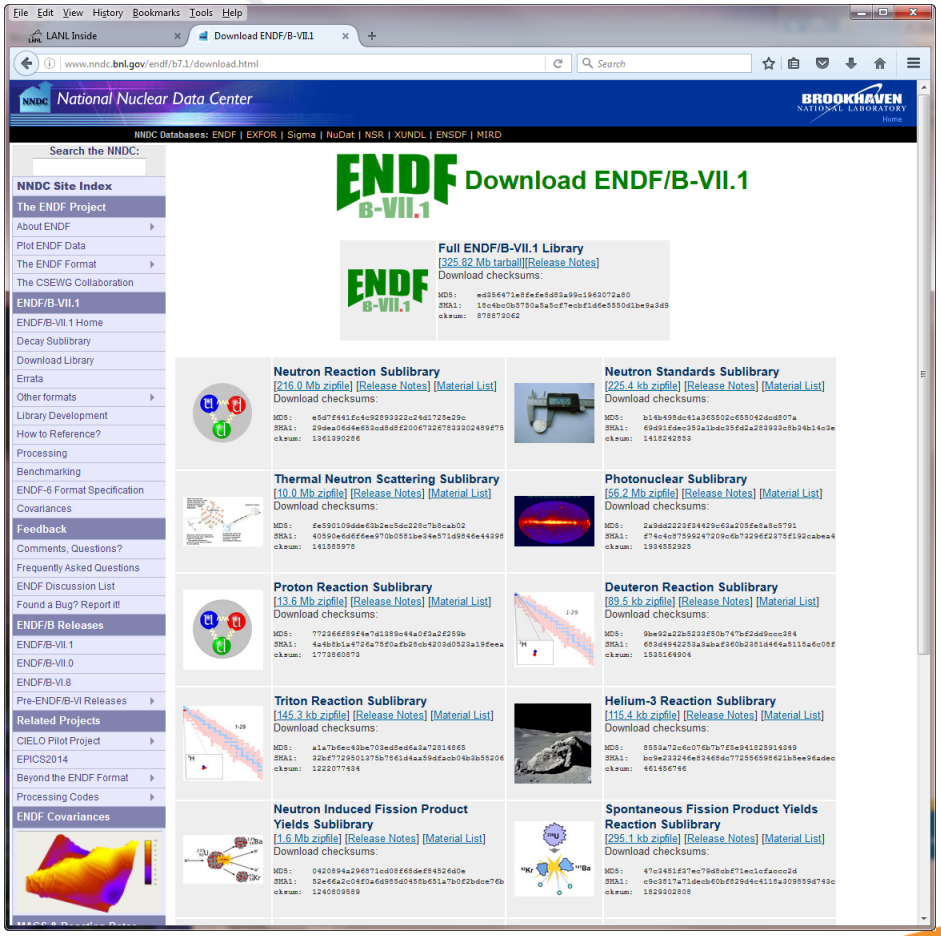
- ENDF evaluations are designated “A” or “B” files.
  - “A” = a preliminary, perhaps partial file.
  - “B” = a complete file in the sense that it can be used for a neutron transport simulation.
    - Complete means that cross sections, angular distributions and secondary emission spectra are defined from 1.0e-5 eV to at least 20 MeV for major cross sections.
- The concept of a national cross section database dates from the mid-1960s.
  - ENDF/B-I was released in 1966.
    - ENDF/B-roman numeral = data version.
    - ENDF/B-arabic number = format version.

ENDF Introduction - IV

- Latest version is ENDF/B-VII.1
  - Released in 2011; next release planned for the 2017 – 2018 timeframe (ENDF/B-VIII.0).
- Neutron cross section data are given for 424 materials (423 isotopes, 1 (carbon) element).
- Thermal scattering law (tsl) files are given for 21 materials (H-H_2O, H-CH_2, Be, Be-BeO, O-BeO, graphite, …).
- Many other specialty files … decay, photo-atomic, photo-nuclear, incident CP - see http://www.nndc.bnl.gov/endf/b7.1/).

ENDF Introduction - V





http://www.nndc.bnl.gov/endf/b7.1/ & http://www.nndc.bnl.gov/endf/b7.1/download.html

ENDF Introduction - VI

- Evaluated data files are available from a variety of world-wide sources …
  - JEFF = Joint European Fission/Fusion File.
  - JENDL = Japanese Evaluated Nuclear Data Library.
  - CENDL = Chinese Evaluated Nuclear Data Library.
  - TENDL = TALYS Evaluated Nuclear Data Library.
    - Mainly a model evaluated library … TALYS being a nuclear reaction code developed largely by Arjan Koning (current Head of the IAEA Nuclear Data Section).
  - All recent evaluated data files use the ENDF-6 format and so what you can do with NJOY/ENDF can also be done with these other libraries.

ENDF Introduction - VII

- Some Internet resources …
  - ENDF: http://www.nndc.bnl.gov/endf/b7.1/
  - JEFF: https://www.oecd-nea.org/dbdata/jeff/
  - JENDL: http://wwwndc.jaea.go.jp/jendl/j40/j40.html
  - TENDL: https://tendl.web.psi.ch/tendl_2015/tendl2015.html
  - IAEA: http://www-nds.iaea.org

  - Other special-purpose libraries also available from the OECD/Nuclear Energy Agency (NEA) and the IAEA.

ENDF Data Structures - I

```
 9.223500+4 2.330248+2          1          1          0          79228 1451    1
 0.000000+0 1.000000+0          0          0          0          69228 1451    2
 1.000000+0 2.000000+7          1          0         10          79228 1451    3
 0.000000+0 0.000000+0          0          0        798        1329228 1451    4
 92-U -235 ORNL,LANL,+EVAL-SEP06 Young,Chadwick,Talou,Madland,Leal9228 1451    5
                     DIST-DEC06 REV-                 20111222   9228 1451    6
----ENDF/B-VII.1     MATERIAL 9228         REVISION -           9228 1451    7
-----INCIDENT NEUTRON DATA                                      9228 1451    8
------ENDF-6 FORMAT                                            9228 1451    9
```

- ENDF information is given as card-image data records.
  - 80 characters per card … 66 characters are “data”; 14 characters are control parameters.
  - The control parameters are 4 integers …
    - matn (i4) = material id
    - mf (i2) = “file” id (see ENDF Manual, Table 4)
      - each “file” contains a unique type of data.
    - mt (i3) = “section” id (see ENDF Manual, Appendix B)
      - each “section” contains data for a unique reaction.
    - ns (i5) = sequence id (now obsolete, NJOY doesn’t care if its not present)

ENDF Data Structures - II

- Each evaluation contains a number of “files”, and each “file” contains a specific type of information
  - MF = 1: comments, dictionary, fission data;
  - MF = 2: resonance parameters;
  - MF = 3: cross sections;
  - MF = 4: emitted neutron angular distributions;
  - MF = 5: emitted neutron energy distributions;
  - MF = 6: coupled energy-angle distributions for all emitted particles;
  - MF = 7: thermal scattering law data;
  - MF = 12 – 15: photon data;
  - MF = 30+: covariance data.

ENDF Data Structures - III

- Each “file” contains one or more “sections”
  - Within a given “file”, or MF, section numbers appear in ascending order and are not contiguous
    - MF = 1
      - MT = 451: evaluator comments and “dictionary”
      - MT = 452: total $\overline{\nu(E)}$; mt=455,456,458,460 = other fission data
    - MF = 2
      - MT=151: resolved and unresolved resonance parameters
    - MF = 3
      - MT = 1,2, …: mt=1=total xs; mt=2=elastic scattering; mt=16=(n,2n); mt=18=(n,f), mt=51-90 = inelastic scattering, mt=102=(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 what mt sections are present in an earlier file.

ENDF Data Structures - IV

- "Data" can be various combinations of text, integers and real numbers.
  - Integers and real numbers are constrained to fit in 11 column fields. Data structures include …
    - "CONT" record - a single card (a66 or 2e11.0,4i11).
    - "LIST" record – one or more cards to define a simple list (6e11.0).
    - "TAB1" record – multiple cards to define (x_i,y_i) data such as cross sections or secondary emission spectra with associated interpolation codes (6e11.0).
    - "TAB2" record – a wrapper to combine multiple LIST or TAB1 records.
- See http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf for the latest ENDF format info.

ENDF Data Structures– V (CONT)

```
 9.223500+4 2.330248+2          1          1          0          79228 1451    1
 0.000000+0 1.000000+0          0          0          0          69228 1451    2
 1.000000+0 2.000000+7          1          0         10          79228 1451    3
 0.000000+0 0.000000+0          0          0        798        1329228 1451    4
 92-U -235 ORNL,LANL,+EVAL-SEP06 Young,Chadwick,Talou,Madland,Leal9228 1451    5
                      DIST-DEC06 REV-                 20111222   9228 1451    6
----ENDF/B-VII.1      MATERIAL 9228         REVISION -           9228 1451    7
-----INCIDENT NEUTRON DATA                                      9228 1451    8
------ENDF-6 FORMAT                                            9228 1451    9
…
```

- Part of ENDF/B-VII.1 ^{235}U (matn=9228) …
  - In MF=1, MT=451 …
    - Lines 1 through 4 are **CONT(data)** records.
      - Fortran read statement is 2e11.0,4i11
    - Lines 5 through 9 are **CONT (text)** records.
      - Fortran read statement is a66
  - Other CONT records specify the end of a section (mt=0); end of a file (mf=0), end of an evaluation (matn=0) and end of a tape (matn=-1).

ENDF Data Structures– VI (LIST)

```
…
 2.330200+2 9.602000-1          0          0      19158       31939228 2151    5
-2.038300+3 3.000000+0 1.970300-2 3.379200-2-4.665200-2-1.008800-19228 2151    6
-1.812100+3 3.000000+0 8.574000-4 3.744500-2 7.361700-1-7.418700-19228 2151    7
-1.586200+3 3.000000+0 8.284500-3 3.443900-2 1.536500-1-9.918600-29228 2151    8
-1.357500+3 3.000000+0 5.078700-2 3.850600-2-1.691400-1-3.862200-19228 2151    9
…
```

- Part of ENDF/B-VII.1 ^{235}U (matn=9228) …
  - In MF=2, MT=151 (resolved resonance data)…
    - Line 5 marks the beginning of a **LIST** record.
      - The list contains 19,158 entries, and these entries may be broken up into 3,193 items.
      - Fortran read statement is 6e11.0
        - Fortran does not require the “e” exponent, and embedded blanks are acceptable since this is a fixed format.

ENDF Data Structures– VII (TAB1)

```
…
 5.010000+3 9.926921+0          0          0          0          0 525 3107     1
 2.789520+6 2.789520+6          0          0          2        191 525 3107     2
         32          5        191          2                      525 3107     3
 1.000000-5 1.932772+5 2.530000-2 3.842558+3 9.400000+0 1.990185+2 525 3107     4
 1.500000+2 4.956277+1 2.500000+2 3.831832+1 3.500000+2 3.233614+1 525 3107     5
…
 1.650000+7 4.015499-2 1.700000+7 3.870001-2 1.750000+7 3.722898-2 525 3107    65
 1.800000+7 3.576560-2 1.850000+7 3.430929-2 1.900000+7 3.285713-2 525 3107    66
 1.950000+7 3.141235-2 2.000000+7 2.998125-2                       525 3107    67
 0.000000+0 0.000000+0          0          0          0          0 525 3  099999
…
```

- Part of ENDF/B-VII.1 ^{10}B (matn=525) …
  - In MF=3, MT=107 (n,α cross section)…
    - Line 2 marks the beginning of a **TAB1** record.
      - There are two interpolation intervals and 191 (E_i,σ_i) data pairs.
      - The first interpolation interval is log-log (code 5) for the first 32 data pairs followed by linear-linear (code 2) for the remaining data pairs.

ENDF Data Structures– VIII (TAB2)

```
…
 0.000000+0 0.000000+0          0          0          1         209228 5 18     5
         20          2                                               9228 5 18     6
 0.000000+0 1.000000-5          0          0          1        6439228 5 18     7
        643          2                                               9228 5 18     8
 0.000000+0 0.000000+0 1.000000+1 1.850569-9 1.100000+1 1.940894-99228 5 18     9
 1.200000+1 2.027196-9 1.300000+1 2.109973-9 1.400000+1 2.189621-99228 5 18    10
 1.500000+1 2.266473-9 1.600000+1 2.340803-9 1.700000+1 2.412844-99228 5 18    11
…
 2.960000+7 1.49306-16 2.980000+7 1.26309-16 3.000000+7 1.06854-169228 5 18   222
 3.100000+7 0.000000+0                                           9228 5 18   223
 0.000000+0 5.000000+5          0          0          1        6439228 5 18   224
        643          2                                               9228 5 18   225
 0.000000+0 0.000000+0 1.000000+1 1.837674-9 1.100000+1 1.927368-99228 5 18   226
 1.200000+1 2.013070-9 1.300000+1 2.095269-9 1.400000+1 2.174363-99228 5 18   227
…
```

- Part of ENDF/B-VII.1 ^{235}U (matn=9228) …
  - In MF=5, MT=18 (prompt fission neutron spectrum, PFNS)…
    - Line 5 marks the beginning of a **TAB2** record.
      - There is one interpolation range among the 20 TAB1 records to follow.
      - PFNS for E_{inc} = 1.e-5 eV contains 643 data points, lines 9 to 223.
      - Next spectrum is for E_{inc} = 500 keV.

ENDF Data Structures– IX

- Some Cross Section Data are “derived” …
  - “derived” = can be obtained from other data in the file.
    - e.g. MT=1=“Total” cross section = sum of all other cross sections.
      - ENDF interpolation rules mean that a derived cross section that is a sum can only be defined at the union energy points.
      - Common MTs derived as a sum of other MTs are listed in Table 14 of the ENDF Format Manual.
  - “derived” = a data type of interest, such as “gas production”, “heating” or “radiation damage”.
    - Created by a processing code and generally not part of the original ENDF evaluation.

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Creating an MCNP ACE .c File

MCNP ACE .c - I

Differences between ENDF and ACE (A Compact ENDF) …

- ENDF:
  - xs's may contain RR/URR parameters plus multiple interpolation intervals; each reaction has its own energy mesh; zero °K.
- ACE .c:
  - xs's are lin-lin on a common energy mesh at a user defined temperature; need probability tables for the URR region.

MCNP ACE .c - II

Differences between ENDF and ACE …

- ENDF:
  - Scattering angular distributions are given via Legendre polynomial coefficients, or tabulated probability distributions in cosine, or a combination of both (Legendre coefficients from 1.0e-5 eV to E'; tables from E' to E_{max}).
- ACE .c:
  - Angular distributions are defined using probability and cumulative density functions on a cosine grid.

MCNP ACE .c - III

Differences between ENDF and ACE …

- ENDF:
  - A variety of “laws” are allowed to define the secondary emission spectrum (tabulated, evaporation, Maxwellian, Watt, Madland-Nix)
- ACE .c:
  - Tabulated secondary distributions are converted into probability and cumulative density functions; other ENDF law parameters are copied for internal sampling in MCNP.

MCNP ACE .c - IV

- Converting a general purpose ENDF evaluation into an ACE file requires several NJOY processing steps.
  - Each step requires
    - User input unique to that step;
    - Input files named “tape##”, where ## is part of the user input.
  - Each step produces an output pointwise-ENDF, or pendf, tape named “tape##’”, where ##’ is part of the user input.
    - Often output tape##’ from one NJOY module serves as part of the input to another NJOY module;
    - User values for ## and ##’ must range from 20 to 99.
      - Values from 10 to 19 are reserved for NJOY scratch file use.

MCNP ACE .c - V

- A generic input deck steps through a sequence of NJOY modules …
  - moder, reconr, broadr, unresr, heatr, purr, gaspr, acer, viewr.

```
--
-- "--" signifies an optional
--  njoy comment card;
--  moder, reconr, broadr, etc are njoy
--  modules, each requiring its own input.
--
moder
 "user input cards go here"
--
-- (optional), more user comment(s)
reconr
 "user input cards go here"
--
-- (optional), more user comment(s)
broadr
 "user input cards go here"
…
-- all done
stop
```

MCNP ACE .c - VI

- MODER – ascii to binary conversion; also extract a single evaluation (matn) from a multi-matn file (*optional, but highly recommended*).
- RECONR – resonance reconstruction, linearization and mesh unionization.
- BROADR – doppler broadening to user specified temperature (can be more than one), mesh thinning.
- UNRESR – urr processing (recommended if including HEATR in the job stream).

MCNP ACE .c - VII

- HEATR (*optional*) – heating and radiation damage.
  - Derived data types, can specify total heating and/or heating by reaction.
- PURR – unresolved resonance probability tables.
  - User controls amount of random sampling to develop these tables.
- GASPR (*optional*) – gas production.
  - Another derived data type … all reaction mt's are combined to yield total p,d,t,^{3}He and α production.
- ACER – create an MCNP .c "ACE" file.

NJOY's "MODER" module - I

- What does MODER really do?
  - Copy a tape from ascii/binary format to binary/ascii.
  - Extract an individual material from a multi-material tape and copy (including ascii/binary or binary/ascii conversion) to a new tape.
  - Create a custom multi-material tape (including ascii/binary or binary/ascii conversion).
  - ***We strongly recommend that MODER be the first module executed by the User, to create a binary tape.***
    - ***use binary tapes for i/o between the various NJOY modules and only convert the final binary pendf tape to ascii.***

NJOY's "MODER" module

- **A positive tape number denotes an ascii tape; a negative tape number denotes a binary tape.**
  - ***This ASCII/binary definition is true for all NJOY modules.***
- **Tape numbers from 10 to 19 are reserved for NJOY scratch usage.**
- **When abs(nin) ≥ 20, simply copy nin to nout, with or without mode conversion (depending upon the signs of nin and nout).**
- **When abs(nin) = 1, 2 or 3, write a new tapeid (from card 2) to nout, then copy matd from nin to nout.**
  - **Can continue with more materials from additional input tapes.**
  - **When copying multiple materials, they should appear on nout in increasing matn order (ENDF format rule).**

```
Input …
 - card 1:  nin,nout
   - nin = input tape number (if abs(nin) ≥ 20)
   - nout = output tape number

or

 - card 1:  nin,nout
   - nin = input option
         = abs(nin) = 1 = endf i/o
         = abs(nin) = 2 = gendf i/o
         = abs(nin) = 3 = errorr i/o
   - nout = output tape number

 - card 2:  tapeid
   - tape id record for nout

 - card 3:  nin,matn
   - nin = input tape
   - matd = endf material (matn) number

 - repeat card 3, nin=0 denotes end of MODER
   input
```

NJOY's "RECONR" module - I

- What does RECONR really do?
  - Resonance reconstruction, linearization, grid unionization, derived cross sections …
  - Resonance reconstruction …
    - ENDF formats allow the evaluator to define a variety of resolved resonance formats (LRF #).
      - SLBW (1), MLBW (2), Reich-Moore (3), Adler-Adler(4), General R-Matrix (5), Hybrid R-Function (6), Limited Reich-Moore (7).
      - SLBW only appears in old evaluations, MLBW used for many non-actinides, R-M in modern actinide evaluations, LRF=7 is relatively new (ENDF/B-VII.1 ^{35}Cl; JEFF-3.2 ^{63,65}Cu; maybe future ^{16}O, ^{56}Fe).
        - Users need a special patch to calculate angular distributions from LRF=7 resonance parameters.

NJOY "RECONR" module - II

- What does RECONR really do?
  - Resonance reconstruction (con't) …
    - Within the resolved resonance region, define an initial energy grid.
      - RRR limits, RR energies, RR widths, extra User specified energies.
      - Given energy grid points E_1 and E_2 …
        - Calculated the cross sections at end points and at the mid-point.
        - Compare the mid-point calculation to linear interpolation from the end points.
        - Continue to insert new grid points until linear interpolation is accurate over the entire energy interval to within a User specified tolerance (typically 0.1%).
  - Linearization
    - Add energy points so that linear-linear interpolation reproduces the specified interpolation to within a User specified tolerance.

NJOY "RECONR" module - III

- What does RECONR really do?
  - Unionization
    - The energy mesh of a derived cross section must be the union of the energy mesh from all constituent cross sections.
    - Note: NJOYxx will re-calculate the total (mt1) cross section.
    - Note: NJOY99 does not re-calculate derived cross sections such as, for example, mt107 if mt800 – mt849 are present but NJOY2012 does re-calculate the derived cross section.

NJOY "RECONR" module - IV

- **nendf and npend must both be the same mode (+ = ascii; - = binary).**
- **Cards 1 through 4 are required.**
  - **Default inputs noted by *X*.**
- **Can use psi-chi broadening (non-zero tempr) with SLBW, MLBW.**
- **Card 5 is omitted if ncards=0, or must appear ncards times.**
- **Card 6 is omitted if ngrid=0, or ngrid entries are required.**
  - **These energies are forced onto the reconstructed energy grid.**
  - **… but no linkage to BROADR so they may not last, ☹.**
- **Can process multiple materials in a single RECONR execution.**
  - **Return to card 3 for input to process the next material.**
  - **mat = 0 denotes end of RECONR input.**

```
Input …
 - card 1:  nendf,npend
   - nendf = input (endf) tape number
   - npend = output tape number

 - card 2:  tlabel
   - tlabel = tape id label for npend

 - card 3:  mat,ncards,ngrid
   - mat    = endf material (matn) number
   - ncards = number of text records (0)
   - ngrid  = number of User grid points (0)

 - card 4:  err,tempr,errmax,errint
   - err    = reconstruction tolerance
   - tempr  = output temperature (SLBW, MLBW)
   - errmax = integral thinning (10*err)
   - errint = integral thinning (err/2.e4)

 - card 5 (repeat ncards times): text
   - text records for npend mf1/mt451

 - card 6:  enode
   - ngrid energy points
```

NJOY "BROADR" module - I

- What does BROADR really do?
  - Doppler broadening
    - User specifies the initial temperature and final temperature.
    - Can specify multiple final temperatures (NJOY99 is ≤ 10, NJOY2012 is ≥ 1).
    - Note: NJOY99 does not re-calculate derived cross sections such as, for example, mt107 if mt800 – mt849 are present but NJOY2012 does re-calculate the derived cross section.
    - Tallies standard thermal data when requested T = ~293.6 °K.
    - Energy mesh reconstruction tolerances can differ from those used by RECONR.
      - 1/v cross sections are invariant; constant cross sections develop a 1/v tail; resonance peaks decrease and broaden.
      - Usually have fewer energy mesh points after Doppler broadening.

NJOY "BROADR" module - II

Doppler broadening of a constant cross section (such as is commonly seen for low energy elastic scattering) adds a 1/v tail to that cross section.

Figure 5 is from the NJOY2012 manual.

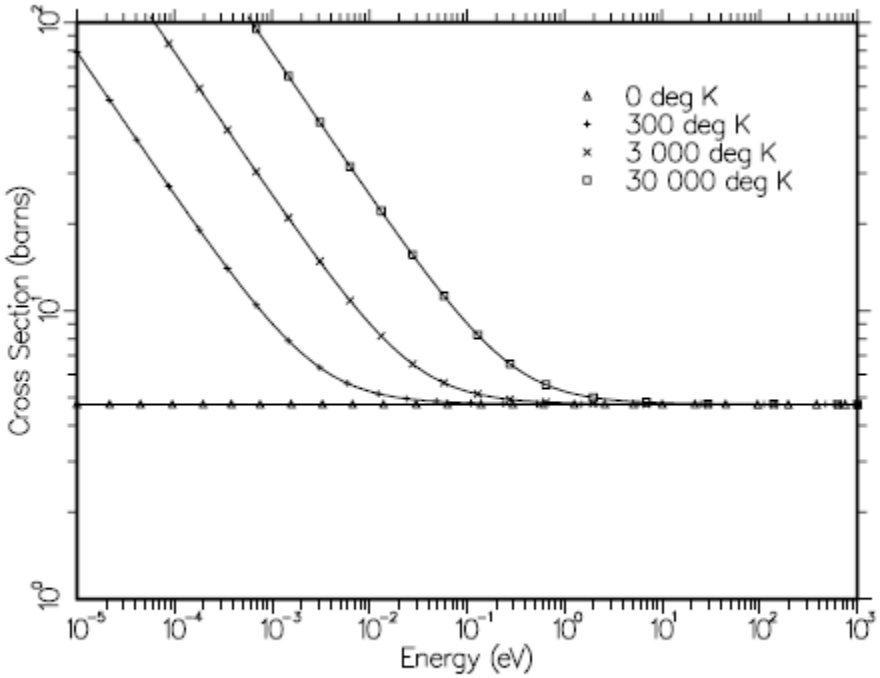


Figure 5: The elastic cross section for carbon from ENDF/B-V showing that Doppler-broadening a constant cross section adds a $1/v$ tail.

NJOY "BROADR" module - III

Doppler broadening of resonances will decrease the peak cross section value, and increase the resonance width.

Figure 6 is from the NJOY2012 manual.

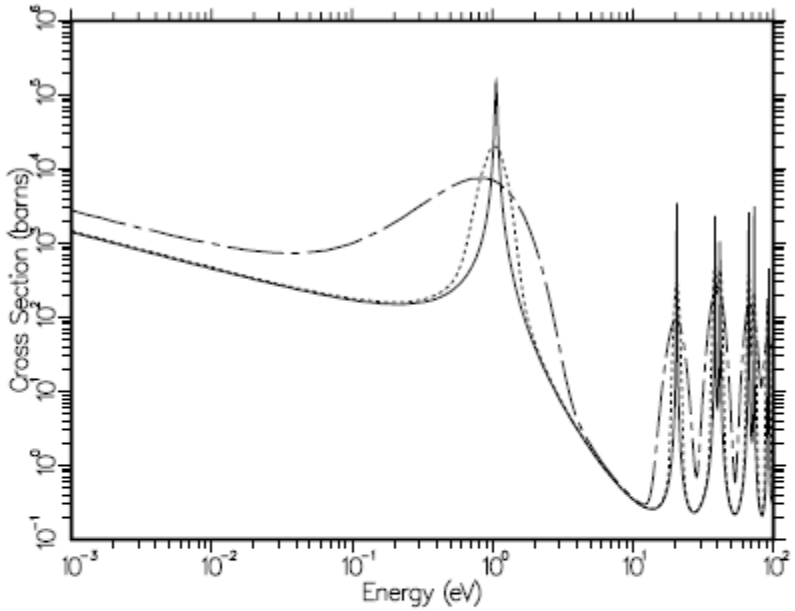


Figure 6: The (n,γ) cross section for ^{240}Pu for several temperatures showing the effects of Doppler broadening on resonances. The temperatures are 0K (solid), 30 000K (dotted), and 300 000K (dash-dot). The higher resonances behave in the classical manner even at 30 000K; note that the line shape returns to the asymptotic value in the wings of the resonance. All resonances at 300 000K (and to a lesser extent the first resonance for 30 000K) show the additional $1/v$ component that appears when kT/A is large with respect to the resonance energy.

NJOY "BROADR" module - IV

- **nendf, nin, nout must be the same mode.**
- **Temperatures are given in °K.**
- **Repeat cards 2, 3 & 4.**
  - **mat1 = 0 denotes end of BROADR input.**
- **istart = restart option**
  - **no = nout is a new output tape.**
  - **yes = copy nin to nout through temp1, then append temp2(i).**
- **istrap = bootstrap option**
  - **no = broaden each final temperature, temp2(i), from temp1.**
  - **yes = broaden each final temperature, temp2(i), from the previous temp2(i-1).**
- **errthn, etc … see RECONR discussion.**
- **thnmax**
  - **If < 0, defines maximum broadening energy; if > 0 the smaller of thnmax, top of RRR or non-threshold xs.**

```
Input …
 - card 1:  nendf,nin,nout
   - nendf = input, endf, tape number
   - nin   = input pendf tape number
   - nout  = output tape number

 - card 2:  mat1,ntemp2,istart,istrap,temp1
   - mat1   = material number from nin
   - ntemp2 = number of final temperatures (1)
   - istart = restart (no/yes = 0/1)
   - istrap = bootstrap (no/yes = 0/1)
   - temp1  = starting temperature from nin (0.)

 - card 3:  errthn,thnmax,errmax,errint
   - errthn = fractional thinning tolerance
   - thnmax = possible maximum energy (1.e6)
   - errmax = integral thinning (10*errthn)
   - errint = integral thinning (errthn/2.e4)

 - card 4:  temp2
   - temp2  = ntemp2 output temperatures
```

NJOY "UNRESR" module - I

- What does UNRESR really do?
  - Unresolved resonance (urr) processing …
    - Calculate "flux weighted" cross sections on the evaluated file energy grid using the Bondarenko method.
      - Total, Elastic Scattering, Capture, (Fission).
    - Can specify multiple final temperatures (NJOY99 is ≤ 10, NJOY2012 is ≥ 1).
    - Can specify multiple self-shielding factors (NJOY99 is ≤ 10, NJOY2012 is ≥ 1).
    - Data are saved in a local "pendf" output file as mf2/mt152.
      - This is not a sanctioned ENDF mt definition; it is only used internally by NJOY.
  - NJOY simply copies the input tape to the output tape if no urr data are present.

NJOY "UNRESR" module - II

- **nendf, nin, nout must be the same mode.**
- **Temperatures are given in °K.**
- **Repeat cards 2, 3 & 4.**
  - **matd = 0 denotes end of UNRESR input.**
- **NJOY will simply copy nin to nout if there are no URR data for this material.**
- **ntemp, nsigz was ≤ 10 in njoy99; no limit in njoy2012.**

```
Input …
 - card 1:  nendf,nin,nout
   - nendf = input, endf, tape number
   - nin   = input pendf tape number
   - nout  = output tape number

 - card 2:  matd,ntemp,nsigz,iprint
   - matd   = material number from nin
   - ntemp  = number of final temperatures (1)
   - nsigz  = number of sigma zeroes (1)
   - iprint = print option (min/max = 0/1)

 - card 3:  temp
   - temp = ntemp output temperatures

 - card 4:  sigz
   - sigz = nsigz sigma-0 values
```

NJOY "HEATR" module - I

- What does HEATR really do?
  - Total Heating, Heating by Reaction, Radiation Damage
    - Heating is described using "KERMA" (Kinetic Energy Release in Materials), $k_{ij}(E)$ such that $H(E) = \sum_i \sum_j \rho_i k_{ij}(E)\varphi(E)$, where ρ_i is number density, $k_{ij}(E)$ is KERMA for material *i* and reaction *j* at incident energy *E*, and $\varphi(E)$ is the neutron or photon scalar flux.
      - With many modern files, can use a "direct method" … $k_{ij}(E) = \sum_l \overline{E_{ijl}}\,(E)\sigma_{ij}(E)$, where the sum is carried over all charged products, including the recoil nucleus. $\overline{E_{ijl}}$ is the kinetic energy carried away by the l^{th} secondary particle.
      - If such data are not available, use "energy balance" … the energy allocated to neutrons and photons is subtracted from the available energy … $k_{ij}(E) = (E + Q_{ij} - \overline{E_{ijn}} - \overline{E_{ij\gamma}})$.

NJOY "HEATR" module - II

- What does HEATR really do?
  - Total Heating, Heating by Reaction, Radiation Damage
    - Radiation Damage has many sources … direct heating, gas production, lattice defect production. Atomic displacement depends upon total available energy and the energy required to displace an atom … $DPA = \frac{E_a}{2E_d}$.
      - NJOY calculates E_a, which depends upon the recoil spectrum and the division of recoil energy between atomic motion and electronic excitation.
      - NJOY output is a "damage energy production cross section" (eV-barns) which when multiplied by material density and flux yields eV/sec; and dividing by $2E_d$ yields displacements/sec.
        - In practice a 0.8 "efficiency" factor is applied.
    - See the NJOY manual, chapter 6, section 5 for more details.

NJOY "HEATR" module - III

- **nendf, nin, nout must be the same mode; nplot is ascii.**
- **Temperatures are given in °K.**
- **Heating "mt" numbers are normal reaction mt + 300.**
- **Total heating is calculated by default.**
- **A maximum of 7 (npk) partial kerma mtk values are allowed; execute the HEATR module multiple times if more partial kerma calculations are desired.**
- **Reaction Q-value input, by MT and can be energy-dependent, is an old feature to overcome limited data found in elemental evaluations.**

```
Input …
 - card 1:  nendf,nin,nout,nplot
   - nendf = input, endf, tape number
   - nin   = input pendf tape number
   - nout  = output tape number
   - nplot = output tape for check plots

 - card 2:  matd,npk,nqa,ntemp,local,iprint,ed
   - matd   = material number from nin
   - npk    = number of partial kermas (0)
   - nqa    = number of user Q-values (0)
   - ntemp  = number of temperatures (0 = all)
   - local  = (0/1) = transport/deposit local
              photon energy (0)
   - iprint = print option (min/max = 0/1/2)
   - ed     = displacement energy (internal
              table, NJOY manual Ch. 6, Table 2.)

 - card 3:  (only if npk > 0)
   - mtk = list of partial kermas

 - cards 4, 5 & 5a:  allow user input of Q-values
```

NJOY "PURR" module - I

- What does PURR really do?
  - Calculate unresolved resonance probability tables from urr parameters.
    - Generate tables that yield the probability that the total cross section is less than some value, σ_t, for a range of incident energies.
      - Also have conditional probability tables for elastic scattering, capture and fission.
    - Use average resonance parameters and known distribution functions to calculate multiple sample cross sections.
      - NJOY calls this a "ladder". Calculate, and average, the results from multiple ladders.

NJOY "PURR" module - II

- **nendf, nin, nout must be the same mode.**
- **Temperatures are given in °K.**
- **Use 1.e+10 for infinite σ_0.**
- **Bonderenko-style self-shielded cross sections are calculated from the probability tables and written as mf2/mt152 on nout.**
  - ***Existing mt=152 data will be overwritten.***
- **Probability table data are written to mf2/mt153 on nout.**
- **Repeat card 2 with matd = 0 to signify the end of PURR input.**

```
Input …
 - card 1:  nendf,nin,nout
   - nendf = input, endf, tape number
   - nin   = input pendf tape number
   - nout  = output tape number

 - card 2:  matd,ntemp,nsigz,nbin,nladr,iprint,
            nunx
   - matd   = material number from nin
   - ntemp  = number of final temperatures (1)
   - nsigz  = number of sigma zeroes (1)
   - nbin   = number of probability bins (must be
              ≥ 15)
   - nladr  = number of resonance ladders
   - iprint = bootstrap (min/max = (0/1)
   - nunx   = number of energy points (0=all)

 - card 3:  (ntemp values)
   - temp = list of temperatures

 - cards 4:  (nsigz values)
   - sigz = list of sigma zero values
```

NJOY "GASPR" module - I

- What does GASPR really do?
  - Uses built-in MT tables, including "LR" flags, to accumulate the total cross section for producing protons (mt=203), deuterons (mt=204), tritons (mt=205), ^{3}He (mt=206) and alphas (mt=207).
    - "LR" flags denote a multi-step break-up reaction … for example inelastic scattering where the residual nuclide is in a particle unbound level.
  - Will overwrite existing mt=203 to mt=207 sections.
  - User input only specifies input and output tapes.
    - The input tape should only contain the material to be processed, but multiple temperature pendfs are allowed.

NJOY "GASPR" module - II

- **nendf, nin, nout must be the same mode.**
- **GASPR will insert (or overwrite) mt=203 to mt=207 on nout.**
- **nendf and nin should only contain the material of interest (but multiple temperatures are permitted).**
- **Need nendf to determine file version number and to check for mf6/mt5 data.**

```
Input …
 - card 1:  nendf,nin,nout
   - nendf = input, endf, tape number
   - nin   = input pendf tape number
   - nout  = output tape number
```

NJOY "ACER" module - I

- What does ACER really do?
  - Creates an ACE (A Compact ENDF) format file for MCNP.
    - "fast" (continuous energy); thermal; dosimetry; photo-atomic; photo-nuclear;
    - Can write files in ascii (type 1) or binary (type 2) format;
      - We recommend that users create ascii formatted files for ease of portability.
    - Creates an "xsdir" record;
    - Performs rudimentary data checks.

NJOY "ACER" module - II

- What does ACER really do … in NJOY's own words:

```
!    --- continuous (fast) data ---
!
! Reaction cross sections are reconstructed on the grid of the total cross section from the input
! pendf tape (assumed to be linearized and unionized).  Redundant reactions (except for MT1,
! MT452, and reactions needed for photon yields) are removed.  MT18 is considered redundant if
! MT19 is present.  Angular distributions are converted into either 32 equally probable bins, or into
! cumulative probability distributions.  Tabulated energy distributions are converted into "law 4"
! probability distributions.  Analytic secondary-energy distributions are converted into their ACE
! formats.  Coupled energy-angle distributions (File 6) are converted into ACE laws.  The old format
! supports law44 for tabulated data with Kalbach systematics, law67 for angle-energy data, and
! law66 for phase space.  The newer format adds law61 with cumulative angle distributions for
! Legendre or tabulated distributions (see newfor).  All photon production cross sections are combined
! on the cross section energy grid.  If provided, multigroup photon production data are summed and
! converted into a set of equally probable emission energies for each input group.  Detailed photon
! production data can be generated directly from Files 12, 13, 14, 15, and 16 from the input ENDF
! tapes and written out using the "law 4" cumulative energy distribution format.
```

NJOY "ACER" module - III

- **We recommend accepting all default options.**
- **Card 2 iopt = 1 to create a ".c" ACE file.**
- **Card 2 itype = 1 for an ascii file.**
- **Card 2 suff is easily changed at any time via text editor.**
- **Card 2 nxtra is obsolete. Set to zero and there is no card 4.**

```
Input …
 - card 1:  nendf,npend,ngend,nace,ndir
   - nendf = input endf tape
   - npend = input pendf tape
   - ngend = unit for multigroup photon data
             (obsolete), or plots if iopt=7
   - nace  = output (ace) file
   - ndir  = xsdir information

 - card 2:  iopt,iprint,itype,suff,nxtra
   - iopt = ace file type (1/2/3/4/5/7/8 = fast/
            thermal/dosimetry/photo-atomic/photo-
            nuclear/read type 1/read type 2
            (iopt<0 for mcnpx format)
   - iprint = (0/1) = min/max print
   - itype  = (1/2) = ace output type
   - suff   = mcnp zaid suffix (default = .00)
   - nxtra  = number of (iz,aw) pairs to read (0)

 - card 3:  hk
   - hk = descriptive character string
          (≤ 70 characters)
```

NJOY "ACER" module - IV

- **Card 4 is obsolete.**
- **We recommend no thinning (card 7); this is a somewhat obsolete option that was sometimes used in the past due to computer memory limitations.**
- **The input card is simply a slash "/" when accepting default values for all input parameters on that card.**

```
Input …
 - card 4:  (only if nxtra > 0)
   - iz,aw = nxtra pairs of iz,aw for the ace
             file

 *** Cards 5,6,7 for fast (iopt=1) output ***
 - card 5:  matd,tempd
   - matd  = material id
   - tempd = temperature (°K, 300)

 - card 6:
   - newfor = (0/1) = no/yes use law61 for out-
              going particle distributions
   - iopp   = (0/1) = no/yes, use detailed photon
              distributions

 - card 7: thinning options.  Three entries,
           default=0 = no thinning

 *** If iopt=7, card 3 (or 4) was the last input
card.  Card 1 will have nendf=0, npend=ace file
to check, if ngend .ne. 0 it will receive plot
commands.  nace,ndir are newly generated output.
```

Creating an MCNP ACE .t File

MCNP ACE .t - I

Differences between ENDF and ACE (A Compact ENDF) …

- ENDF:
  - A thermal kernel evaluation may include data to represent “coherent” elastic or “incoherent” elastic, and always contains “incoherent” inelastic scattering (S(α,β)).
- ACE .t:
  - Coherent elastic is a linearly interpolable (E_i,σ_i) array.
  - Incoherent elastic is the same, or may contain σ_i/E.
  - Incoherent inelastic energy-angle probability distributions.

NJOY Sequence for ACE .t

- MODER/RECONR/BROADR – as before, if want "free gas" scattering for that isotope.
- (LEAPR, optional) – create a tsl tape from user defined α and β mesh, temperature(s), and the molecular phonon spectrum (*not covered in this class*).
- THERMR – create coherent and incoherent cross sections and scattering matrices, from one of (i) LEAPR output, or (ii) an evaluated thermal scattering library (tsl) file.
- ACER – create mcnp thermal (.t) file.

NJOY "THERMR" module - I

- What does THERMR really do?
  - Produces pointwise neutron scattering cross sections in the thermal range.
    - Works with legacy, ENDF/B-III, or ENDF/B-VI and later thermal data.
    - Inelastic scattering and energy-transfer matrices for free and bound scatterers are determined from ENDF $S(\alpha,\beta)$ scattering functions.
    - Incoherent elastic scattering cross sections from non-crystalline materials (e.g., polyethylene, ZrH) are generated from ENDF/B-VI data or internal data.
    - Coherent elastic scattering cross sections from crystalline materials (e.g., graphite) are also generated from ENDF/B-VI data or internal data.

NJOY "THERMR" module - II

- **nendf, nin, nout must be the same mode.**
- **THERMR card 2 input has changed from NJOY99 to NJOY2012.**
  - **iin S(α,β) option is 2 (is 4 in NJOY99).**
  - **iform is new (iform=0 is typical).**
- **Use matde=0 when computing free gas scattering for matdp.**
- **nbin = 20 is typical, but a new continuous representation option in acer makes this obsolete.**

```
Input …
 - card 1:  nendf,nin,nout
   - nendf = input, endf, tape with mf7 data
   - nin   = input pendf tape number
   - nout  = output tape number

 - card 2:  matde,matdp,nbin,ntemp,iin,icoh,
            iform,natom,mtref,iprint
   - matde = material from nendf tape
   - matdp = material from nin (pendf) tape
   - nbin  = number of equiprobable angles
   - ntemp = number of temperatures (1)
   - iin   = inelastic options
             [0/1/2 = none/free_gas/S(α,β)]
   - icoh  = elastic options
             [0/1 = none/use ENDF6], or if
             processing earlier formats, see the
             NJOY2012 manual, section 7.6
   - iform = inelastic output format
             [0/1 = E-E'-μ (MF6 special), or
                    E-μ-E' (MF6/Law7).
```

NJOY "THERMR" module - III

- **mtref+1 is automatically assigned for elastic scattering.**
- **See NJOY2012 manual, Table 4 for a list of ENDF/B moderator materials and recommended "mtref" values.**
- **tempr must match that on nendf.**
- **tol = 0.1% is typical**
- **emax = 10 eV is typical; there is no harm in specifying a value that exceeds the maximum tsl input tape energy.**
- **THERMR may be executed multiple times in the same NJOY job.**
- **For example, a job might process "free gas" ^{1}h, h-h_2o, and h-ch_2.**

```
Input (con't) …
 - card 2:  matde,matdp,nbin,ntemp,iin,icoh,
            iform,natom,mtref,iprint
   - natom  = number of principal atoms
   - mtref  = inelastic reaction mt (must be
              between 221 and 250)
   - iprint = print option (0/1/2 = minimum/
              maximum/maximum + intermediate
              results) (0)
 - card 3:  temperatures (°K)
   - tempr = list of temperatures

 - card 4:  tol,emax
   - tol    = reconstruction tolerance
   - emax   = maximum energy for thermal treatment
              (for free gas and T > 3000, emax and
              the energy grid are scaled)
```

NJOY "ACER" module - I

- What does ACER really do?
  - Creates an ACE (A Compact ENDF) format file for MCNP.
    - "fast" (continuous energy); thermal; dosimetry; photo-atomic; photo-nuclear;
    - Can write files in ascii (type 1) or binary (type 2) format;
      - We recommend that users create ascii formatted files for ease of portability.
    - Creates an "xsdir" record;
    - Performs rudimentary data checks.

NJOY "ACER" module - II

- What does ACER really do … in NJOY's own words:

```
!    --- thermal data ---
!
! The data from the pendf tape as prepared by the thermr module is read in.  Inelastic and
! incoherent elastic cross sections are stored directly.  Coherent elastic cross sections are
! converted to a cumulative "stair step" form and stored.  The angular representation for incoherent
! elastic is stored directly.  None is needed for coherent elastic.  The incoherent inelastic energy
! distributions are converted into probability bins with the equally probable angles left unchanged.
! The bins can have equal probabilities or variable probabilities.  In the latter case, outlying bins with
! smaller probabilities are provided to extend the sampling to rare events.  A new tabulated option
! uses a continuous tabulated probability distribution (pdf/cdf) (requires a MCNP5.1.50 or later) and
! provides extended plotting.
!
! WARNING … the continuous tabulated probability distribution format is identical to earlier
! thermal kernel ACE formats … meaning that older versions of MCNP will read this file but
! not interpret the data properly and yield incorrect answers.
```

NJOY "ACER" module - III

- **We recommend accepting all default options.**
- **Card 2 iopt = 2 to create a ".t" ACE file.**
- **Card 2 itype = 1 for an ascii file.**
- **Card 2 suff is easily changed at any time via text editor.**
- **Card 2 nxtra is obsolete. Set to zero and there is no card 4.**

```
Input …
 - card 1:  nendf,npend,ngend,nace,ndir
   - nendf = input endf tape
   - npend = input pendf tape (from previous job)
   - ngend = unit for multigroup photon data
             (obsolete)
   - nace  = output (ace) file
   - ndir  = xsdir information

 - card 2:  iopt,iprint,itype,suff,nxtra
   - iopt = ace file type (1/2/3/4/5/7/8 = fast/
            thermal/dosimetry/photo-atomic/photo-
            nuclear/read type 1/read type 2
            (iopt<0 for mcnpx format)
   - iprint = (0/1) = min/max print
   - itype  = (1/2) = ace output type
   - suff   = mcnp zaid suffix (default = .00)
   - nxtra  = number of (iz,aw) pairs to read (0)

 - card 3:  hk
   - hk = descriptive character string
          (≤ 70 characters)
```

NJOY "ACER" module - IV

- **Thermal values such as mti, nbint and mte must be consistent with those used in the previous THERMR job.**

```
Input …
 *** Cards 8,8a,9 for thermal (iopt=2) output ***
 - card 8:  matd,tempd,tname
   - matd  = material id
   - tempd = temperature (°K, 300)
   - tname = thermal zaid (≤ 6 characters,
             default is za

 - card 8a:
   - iza01 = moderator component za value
   - iza02 = moderator component za value (0)
   - iza03 = moderator component za value (0)

 - card 9:  mti,nbint,mte,ielas,nmix,emax,iwt
   - mti   = mt value for thermal inelastic data
   - nbint = number of bins for incoherent sct
   - mte   = mt value for thermal elastic data
   - ielas = 0/1=coherent/incoherent elastic
   - nmix  = number of atom types in mixed
             moderator (1/2 = not mixed/mixed)
   - emax  = max energy for thermal
   - iwt   = (0/1/2 = variable/const/tabulated)
             weighting option
```

Creating an MCNP ACE .y File

- .y is a dosimetry ACE file …

NJOY Processing of IRDFF Data Sets

```
--
-- NJOY processing of the IRDFF dosimetry file into ACE format
-- - IRDFF is one large file with many materials
--    - use moder to extract the material of interest
--      - make two copies for ACER
--
moder
 1 -21
 'IRDFF v1.02 for mat xxx'
 20 xxx
 0/ end of moder
--
-- make a second copy of this material
moder
 -21 -22
--
-- acer/dosimetry processing
acer
 -21 -22 0 31 32/                          card 1
 3 1 1 .10/                                card 2
 'IRDFF v1.05 data for material xxx'/ card 3
 xxx 300./                                 card 10
--
-- end of job
stop
```

NJOY input script to create an MCNP dosimetry file … replace "xxx" with the appropriate material number.

Nonlinear interpolation is allowed in MCNP Dosimetry files (NJOY99, p. XVII-29); NJOY2012, p. 513,514).

Creating an MCNP ACE .u File

- .u is a photo-nuclear ACE file

NJOY Processing of Photo-Nuclear Data Files

```
--
-- extract 235u file and convert to binary
moder
 1 -21/
 'e71 235u photonuclear'/
 20 9228/
 0/
--
-- standard reconr processing
reconr
 -21 -22/
 'e71 235u photonuclear pendf'/
 9228 1 0/
 .001 0./
 'e71 photonuclear pendf for 235u at 0.1% reconstruction'/
 0/
acer
 -21 -22 0 31 32/                card1
 5 0 1 .10/                      card2
 'e71 235u photonuclear data'/   card3
 9228/                           card12
--
-- finished
stop
```

NJOY input script to create an MCNP photo-nuclear file.

See Chapter 17, Section 15 in the NJOY manual for details.

Creating an MCNP ACE .p File

- .p is a photo-atomic ACE file

NJOY Processing of Photo-Atomic Data Files

```
--
-- Photo-atomic processing to ACE ...
-- - no pre-processing required;
-- - only input an endf formatted
--   photo-atomic input tape;
-- - "ZA" is simply 100*Z.
--
acer
 20 0 0 31 32/                  card1
 4 1 1 .00/                     card2
 'e71 92u photoatomic data'/    card3
 9200/                          card11
--
-- finished
stop
```

NJOY input script to create an MCNP photo-atomic file.

See Chapter 17, Section 14 in the NJOY manual for details.

Course Outline

- History of NJOY (lecture).
- How to obtain the NJOY2012 code package and update the code (lecture).
- Introduction to the Evaluated Nuclear Data File (ENDF) system (lecture).
  - ENDF data structures (lecture).
- Creating MCNP ACE .c and .t files (interactive).
  - Also provide notes for dosimetry, photo-nuclear and photo-atomic files.
- Visualizing nuclear data with NJOY (interactive).

Visualizing Nuclear Data

Visualizing Nuclear Data - I

- NJOY produces postscript formatted plots.
  - Use the “PLOTR” module to create a plot command file.
  - Use the “VIEWR” module to create a .ps file.
- The minimum input to PLOTR is (i) an output tape number (ascii) and an input card specifying the pendf tape (ascii or binary), matn, mf, mt and temperature.
- The only input to VIEWR is the PLOTR output tape number and VIEWR’s output tape number (ascii).

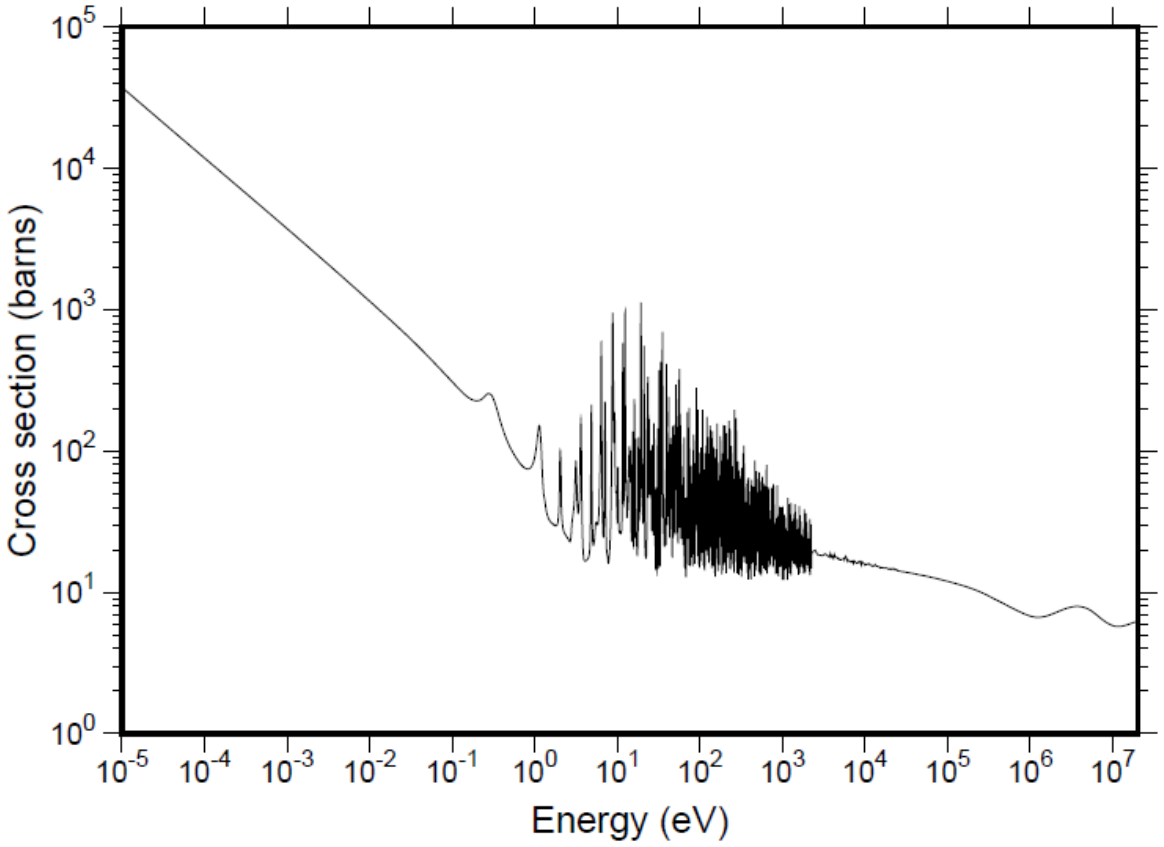
Visualizing Nuclear Data - II

- What does PLOTR really do … in NJOY's own words:

! plot cross sections
!
! Handles ENDF data, PENDF or GENDF data at specified temperatures, or experimental input
! data. Several plots can be given on each set of axes, with both left and right scales. Also,
! several graphs can be given on each page or display. Error bars may be included for input
! data. Flexible titles and legend blocks are allowed. All standard combinations of log and
! linear axes are supported, either grids or tick marks can be requested, and scales can be
! chosen automatically or set by the user. In some cases, the x axis is thinned. In other cases,
! extra points are added so that, for example, linear-linear data plots correctly on a log-log
! graph. A limited capability for 3-d plots of angle and energy is included, and the ENDF-6
! File 6 format is supported. Percent difference and ratio plots can be requested.
!
! Plotr writes plot commands on an output file for later use by the viewr module or an external
! graphics program.

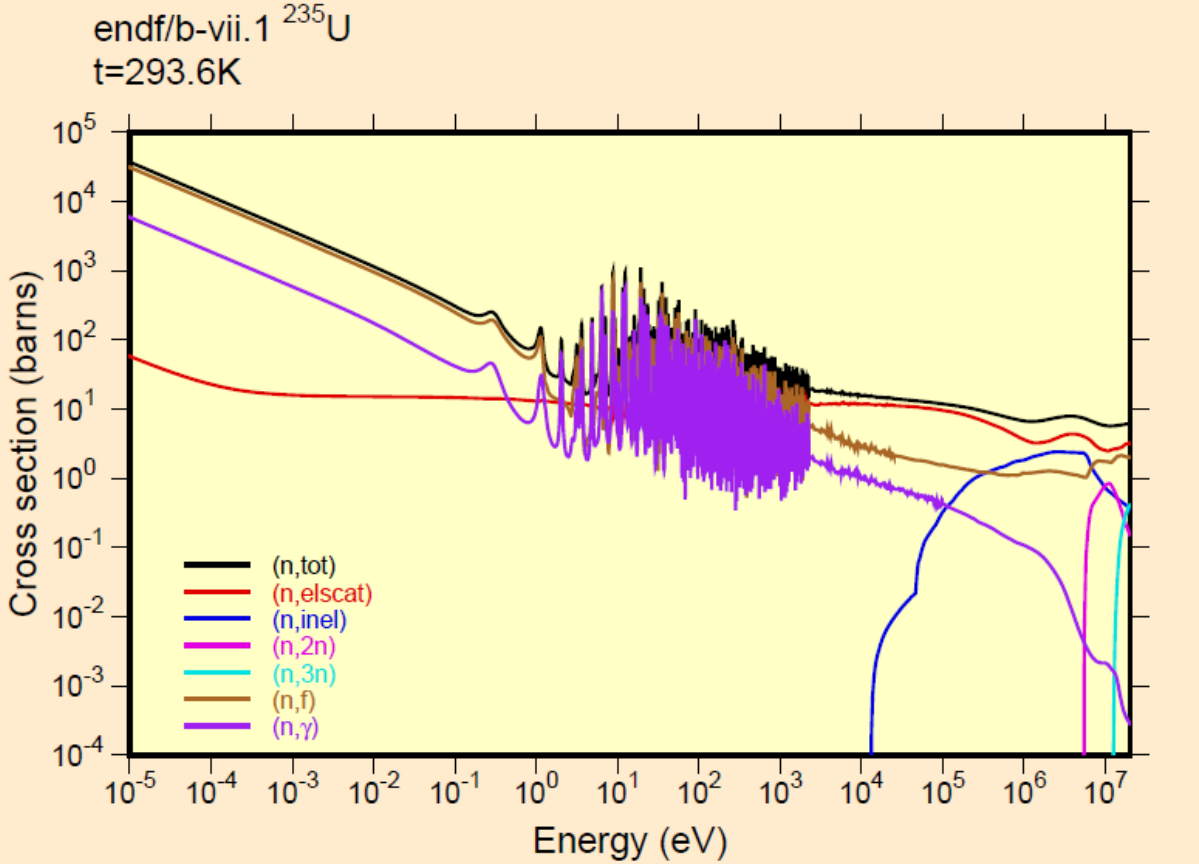
Visualizing Nuclear Data - III

- A plot with minimal user input …
- matn = 9228
- mf = 3
- mt = 1
- temper = 293.6 °K



Visualizing Nuclear Data - IV

- Something a little more informative



NJOY "PLOTR" module - I

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
 - card 0:  nplt,nplt0
   - nplt  = output file
   - nplt0 = input file (0)

 - card 1:  lori,istyle,size,ipcol
   - lori   = page orientation
              (0=portrait/1=landscape).
   - istyle = character font (1=roman/2=roman).
   - size   = character size (+=page unit;
              -=fraction of subplot (+0.3).
   - ipcol  = page color (0 = white).

 *** Repeat cards 2 thru 13 for each curve ***
 - card 2:  iplot,iwcol,factx,facty,xll,yll,
            ww,wh,wr
   - iplot = plot index (1 = new axes, new page).
   - iwcol = window color (default to ipcol).
   - factx = x-axis scaling (1.0)
   - facty = y-axis scaling (1.0)
   - xll,yll = lower left corner of plot area
               (0.0,0.0).
   - ww,wh,wr = window width, height & rotation
                angle (default is one plot/page).
```

NJOY "PLOTR" module - II

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
 * cards 3 through 7 for iplot = +1 or -1 only *

 - card 3:  t1
   - t1 = up to 60 character title (line 1)
          (default is blank).

 - card 3a:  t2
   - t2 = up to 60 character title (line 2)
          (default is blank).

 - card 4:  itype,jtype,igrid,ileg,xtag,ytag
   - itype = 1/2/3/4 = linx-liny/linx-logy/
             logx-liny/logx-logy axes.
   - jtype = 0/1/2 = none/linear/log
             alternate y or z axis.
   - igrid = 0/1/2/3 = grid & tic mark control;
             none/grid/tic outside/tic inside.
             -=fraction of subplot (+0.3).
   - ileg  = 0/1/2 = legend options;
             none/yes/yes with pointer.
   - xtag  = legend upper left x value
   - ytag  = legend upper left y value
             (default is upper left corner).
```

NJOY "PLOTR" module - III

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
 * cards 3 through 7 for iplot = +1 or -1 only *

 - card 5:  el,eh,xstep
   - el    = plot E_min.
   - eh    = plot E_max.
   - xstep = x-axis step for tic marks.
   - default is automatic scales; if el & eh are
     given with linear scaling xstep is required.

 - card 5a:  xlabl
   - xlabl = x-axis label (up to 60 characters,
             default = energy (ev)).

 - card 6:  yl,yh,ystep
   - yl    = lowest value of y-axis.
   - yh    = highest value of y-axis
   - ystep = y-axis step for tic marks.
   - default is automatic scales; if yl & yh are
     given with linear scaling ystep is required.

 - card 6a:  ylabl
   - ylabl = y-axis label (up to 60 characters,
             default = cross section (barns)).
```

NJOY "PLOTR" module - IV

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
 * cards 3 through 7 for iplot = +1 or -1 only *
 * cards 7 and 7a for jtype > 0 only *

 - card 7:  el,eh,xstep
   - el    = plot E_min.
   - eh    = plot E_max.
   - xstep = x-axis step for tic marks.
   - default is automatic scales; if el & eh are
     given with linear scaling xstep is required.

 - card 7a:  rl
   - rl = alternate y-axis or z-axis label (up to
          60 characters, default = blank).
```

NJOY "PLOTR" module - V

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
 *** card 8 is always present ***

 - card 8:  iverf,nin,matd,mfd,mtd,temper,
            nth,ntp,nkh
   - iverf = endf version (0=user input on cards
             12 & 13 plus ignore the remaining
             parameters on this card; 1=gendf).
   - nin   = input endf/pendf/… tape.
   - matd  = material id.
   - mfd   = material file.
   - mtd   = material section.
   - temper = temperature (degK, default = 0.).
   - nth,ntp,nkh = control parameters for special
                   plots (default = 1,1,1).  See
                   the NJOY manual.

 *** cards 9 & 10 are used for 2D plots ***

 - card 7a:  rl
   - rl = alternate y-axis or z-axis label (up to
          60 characters, default = blank).
```

NJOY "PLOTR" module - VI

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
  *** cards 9 & 10 are used for 2D plots ***

 - card 9:  icon,isym,idash,iccol,ithick,ishade
   - icon = 0/-i/i = plot symbol and connection
            (default = points connected, no
             symbols).
   - isym = plot symbol code (see manual 0=none).
   - idash = line type (see manual, 0=solid).
   - iccol = curve color (see manual, 0=black).
   - ithick = curve thickness (1).
   - ishade = shade pattern (0=none).  A somewhat
              obsolete option from days when b&w
              printers ruled the day.

*** card 10 is required when ileg ≠ 0 ***
- card 10:  aleg
   - aleg = legend or curve title (up to
            60 characters, default = blank).

*** card 10a is required when ileg = 2 ***
- card 10a:  xtag,ytag,xpoint
   - xtag,ytag = x,y position of title
   - xpoint    = x position of pointer (≤ 0 to
                 omit the pointer).
```

UNCLASSIFIED

NJOY "PLOTR" module - VII

- **PLOTR reads plot commands from nplt0 or card input and creates a plot command file on nplt to be interpreted by VIEWR.**
- **Refer to the NJOY2012 manual, Chapter 20, Section 8 for a summary of PLOTR input commands.**
  - **Numerous PLOTR examples are provided throughout this chapter.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**
- **Other NJOY modules creating a plot command file include HEATR, ACER, GROUPR, and COVR.**

```
Input …
  *** card 11 is used for 3D plots ***

 - card 11:  xv,yv,zv,x3,y3,z3
   - xv,yv,zv = coordinates of view point
                (default = 15.,-15.,15).
   - x3,y3,z3 = side of "work box"
                (default = 2.5,6.5,2.5).

 *** cards 12 & 13 are required when iverf=0 ***
 - card 12:  nform
   - nform = input data format code.

 - card 13:  xdata,ydata,yerr1,yerr2,xerr1,xerr2
   - xdata = x-axis data
   - ydata = y-axis data
   - yerr1,yerr2 = lower & upper y value limit
   - xerr1,xerr2 = lower & upper x value limit
   - repeat card 13 until an empty (/) record is
     read.
   - yerr1,yerr2,xerr1,xerr2 default is zero.
```

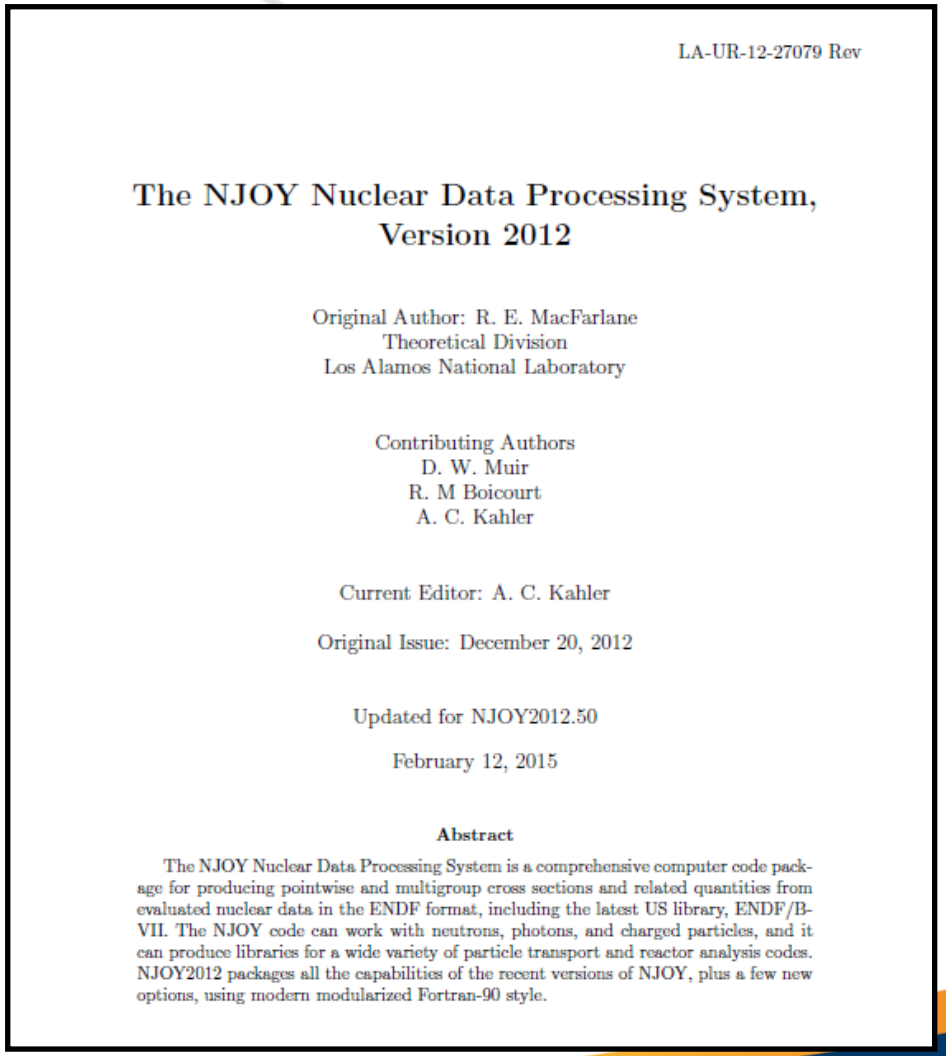
NJOY "VIEWR" module - I

- **VIEWR reads plot commands from infile and creates a postscript formatted output tape.**
- **infile can be generated by one of HEATR, ACER, GROUPR, COVR or PLOTR.**
- **Refer to the NJOY2012 manual, Chapter 21 (VIEWR) for special command sequences to generate greek letters and to create subscript and/or superscript characters in text strings.**

```
Input …
 - card 1:  infile,nps
   - infile = input tape with plot commands
   - nps    = output file containing postscript
              (.ps) formatted plots.
```

NJOY Documentation - I

- A .pdf hyperlinked NJOY2012 manual is included in the NJOY Distribution (and in the “docs” folder of this class).



LA-UR-12-27079 Rev

The NJOY Nuclear Data Processing System, Version 2012

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Abstract

The NJOY Nuclear Data Processing System is a comprehensive computer code package for producing pointwise and multigroup cross sections and related quantities from evaluated nuclear data in the ENDF format, including the latest US library, ENDF/B-VII. The NJOY code can work with neutrons, photons, and charged particles, and it can produce libraries for a wide variety of particle transport and reactor analysis codes. NJOY2012 packages all the capabilities of the recent versions of NJOY, plus a few new options, using modern modularized Fortran-90 style.

NJOY Documentation - II

Title page from a recent NJOY paper …

Available online at www.sciencedirect.com
ScienceDirect
ELSEVIER
Nuclear Data Sheets
Nuclear Data Sheets 111 (2010) 2739–2890
www.elsevier.com/locate/nds

Methods for Processing ENDF/B-VII with NJOY

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The NJOY Nuclear Data Processing System is widely used to convert evaluations in the Evaluated Nuclear Data Files (ENDF) format into forms useful for practical applications such as fission and fusion reactor analysis, stockpile stewardship calculations, criticality safety, radiation shielding, nuclear waste management, nuclear medicine procedures, and more. This paper provides a descrip-

NJOY Documentation - III

- Data Processing references included in the MCNP Documentation …
  - LA-UR-13-20137, “Continuous Energy Neutron Cross Section Data Tables Based Upon ENDF/B-VII.1”
  - LA-UR-12-00800, “Release of Continuous Representation for S(α,β) ACE Data”.
- Also see “NJOY Data Processing” under the “Nuclear Data and Physics” category in the MCNP Reference Collection.
- … and from Europe: “A Validated MCNP(X) Cross Section Library based upon JEFF 3.1” (http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/42/097/42097803.pdf) and other JEF documents issued through the OECD Nuclear Energy Agency.