The NJOY Processing Code

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OF NUCLEAR DATA FOR APPLICATIONS

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Outline

- Where did the ENDF system come from?
- Where did NJOY come from?
- A review of the ENDF format
  - You can't speak NJOY if you don't speak ENDF.
- A brief summary of NJOY i/o for creating ACE files
  - .c (continuous energy)
  - .t (thermal scattering law) – **second lecture starts here…**
  - .y (dosimetry)
- A brief summary of NJOY's plotting capability
  - Cross Sections; Angular distributions; Secondary emission spectra
- Criticality Validation
- Some NJOY references

ENDF Introduction - I

- The Evaluated Nuclear Data File (ENDF) is the United States' 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

- The Evaluated Nuclear Data Format was initially developed during the mid-1960s.
- Was an effort to develop an agreed upon common set of cross section data among US practitioners (an effort that remains a work in progress among the broader, international community!)
  - ENDF/B-I was released in ~1968.
  - Quickly followed by ENDF/B-II (~1970) … and ENDF/B-III (~1972).
  - ENDF/B-IV was released in 1975.
  - -V, -VI, -VII followed in the 80s, 90s and 2000s.
- Some cross sections are known as “Standards”; when they change the next ENDF release is a new generation.

ENDF Introduction - III

- 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.
  - … more
- 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 - IV

- 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 NEA (http://www.oecd-nea.org/dbdata/) and the IAEA.

NJOY History - I

- Before NJOY
  - ENDF/B allowed users to say they were using the same basic data, but processing techniques varied …
  - LANL had MINX = Multigroup Interpretation of Nuclear X-Sections …
    - http://www.nndc.bnl.gov/endfdocs/ENDF-237.pdf
  - … and other stand-alone processing codes ...
    - Some pre-NJOY codes include LAPHAN0, GAMLEG, ETOPL, …
      - 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, 2016) .
      - NJOY has evolved as ENDF has evolved.
    - NJOY has benefitted from constructive feedback and collaboration with national and international peers.
  - The latest release is NJOY2016 … open source … see http://njoy.lanl.gov
    - NJOY2016 … works with legacy (cardimage) ENDF formatted files.
    - NJOY21 … a future release under active development for use with GND formatted files.

The ENDF Format - 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)

The ENDF Format - 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.

The ENDF Format - 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.

The ENDF Format - 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 with associated interpolation code(s).
    - "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 information.
  - Review the "Procedures …" section of each chapter for additional guidance and restrictions on data structure usage.

The ENDF Format – 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).

The ENDF Format – 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.

The ENDF Format – 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.

The ENDF Format – 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.

The ENDF Format - 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.

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.
  - The basic energy unit in ENDF is eV.

ACE .c:

- xs's are linear-linear interpolable on a common energy mesh at a user defined temperature; need probability tables for the URR region.
- The basic energy unit in ACE is MeV.

MCNP ACE .c - II

Differences between ENDF and ACE (A Compact ENDF) …

- 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 (A Compact ENDF) …

- 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, or NJOY module, requires …
    - User input unique to that module;
    - Input file(s) named “tape##”, where ## is part of the user input.
  - Each module 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 their 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; extract a single evaluation (matn) from a multi-matn tape; add an evaluation to an existing tape (*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 Input Summary …

- The following slides describe these NJOY modules in more detail, and summarize their input.
  - These slides serve as reference material to assist users in creating NJOY input decks.
  - It is not practical to discuss this material in a lecture setting.
    - We skim through the highlights here and reserve detailed discussions for the computer exercises.

NJOY's "MODER" Module - I

- What does MODER 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.***
    - ***use of binary mode allows intermediate results to be saved with greater precision than ENDF's 11-column fixed-format.***

NJOY's "MODER" Module - II

- **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 matn from nin to nout.**
  - **Can continue with more materials from additional input tapes; set nin = 0/ to terminate MODER.**
  - **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 or pendf input
    = abs(nin) = 2 = gendf input
    = abs(nin) = 3 = errorr input
  - *nout = output tape number*

- *card 2: tapeid*
  - *tape id record for nout*

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

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

NJOY's "RECONR" Module - I

- What does RECONR 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; CIELO ^{56}Fe, maybe ^{16}O).

NJOY's "RECONR" Module - II

- What does RECONR 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 original interpolation to within a User specified tolerance (typically 0.1%).

NJOY's "RECONR" Module - III

- What does RECONR do?
  - Unionization
    - The energy mesh of a derived cross section must be the union of the energy mesh from all constituent cross sections.
    - Note: All NJOY versions 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 and later does re-calculate these derived cross sections.

NJOY's "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.**
  - **matn = 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: matn,ncards,ngrid*
  - *matn = endf material 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's "BROADR" Module - I

- What does BROADR do?
  - Doppler broadening
    - User specifies the initial temperature and final temperature.
    - Can specify multiple final temperatures (NJOY99 is ≤ 10, NJOY2012 and later is ≥ 1).
    - Note: NJOY99 does not re-calculate derived cross sections such as, for example, mt107 if mt800 – mt849 are present but NJOY2012 and later do re-calculate derived cross sections.
    - Tallies standard thermal data when requested T = ~293.6 °K.
    - Energy mesh reconstruction tolerances can differ from those used by RECONR.
    - Some characteristics of Doppler broadened cross sections …
      - 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's "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.

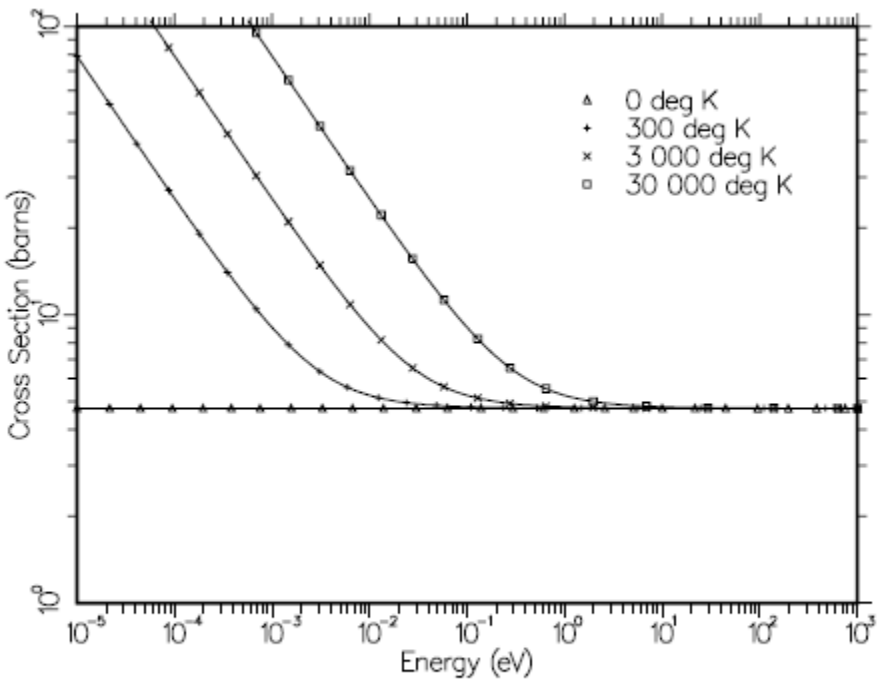


Figure 5: The elastic cross section for carbon from ENDF/B-V showing that Doppler-broadening a constant cross section adds a $1/v$ tail.

NJOY's "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.

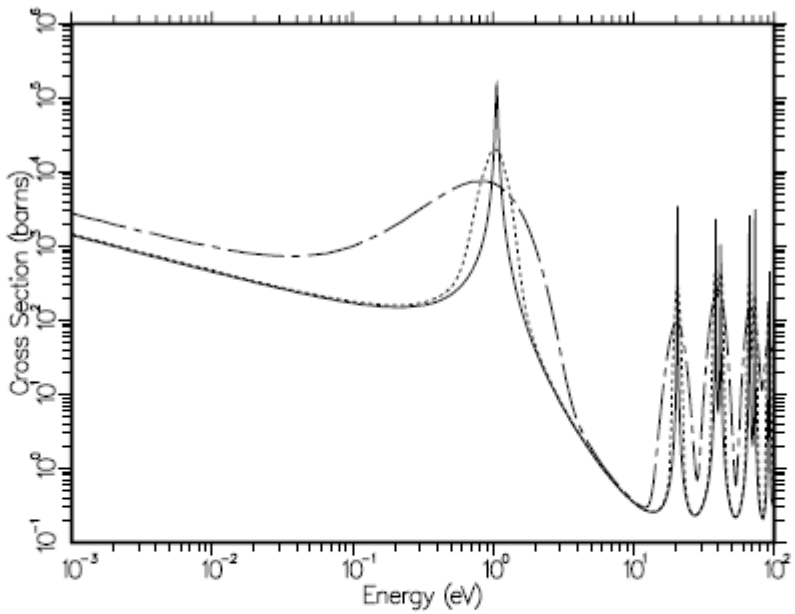


Figure 6: The (n,γ) cross section for ^{240}Pu for several temperatures showing the effects of Doppler broadening on resonances. The temperatures are 0K (solid), 30 000K (dotted), and 300 000K (dash-dot). The higher resonances behave in the classical manner even at 30 000K; note that the line shape returns 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's "BROADR" Module - IV

- **nendf, nin, nout must be the same mode.**
- **Temperatures are given in °K.**
- **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 depends upon NJOY version.**
- **Card 5 specifies additional materials (matl) to broaden**
  - **Set matl = 0/ to terminate BROADR.**

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 nin temperature (**0.**)*
- *card 3: errthn,thnmax,errmax,errint*
  - *errthn = fractional thinning tolerance*
  - *thnmax = possible maximum energy*
  - *errmax = integral thinning **(10*errthn)***
  - *errint = integral thinning (**errthn/2.e4**)*
- *card 4: temp2*
  - *temp2 = ntemp2 output temperatures*
- *card 5: matl*
  - *next material, terminate with matl=0/.*

NJOY's "UNRESR" Module - I

- What does UNRESR 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 and later is ≥ 1).
    - Can specify multiple self-shielding factors (NJOY99 is ≤ 10, NJOY2012 and later is ≥ 1).
    - Data are saved in a local "pendf" output file as mf2/mt152.
      - This is not a sanctioned ENDF definition; it is only used internally by NJOY.
  - NJOY simply copies the input tape to the output tape if no urr data are present.
    - Therefore there is no harm if UNRESR is invoked when processing an evaluation that does not include urr data.

NJOY's "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 and later.**

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's "HEATR" Module - I

- What does HEATR 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's "HEATR" Module - II

- What does HEATR 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 HEATR chapter in the NJOY manual for more details.

NJOY's "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 HEATR multiple times if more partial kerma calculations are needed.**
- **Reaction Q-value input, by MT and can be energy-dependent, is an old feature to overcome limited data found in elemental evaluations.**
  - **See the NJOY manual for a description of cards 4, 5 and 5a .**

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 (**0**/1/2 = min/max/check)*
  - *ed = displacement energy (**internal table; see the NJOY manual**)*

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

- *cards 4, 5 & 5a: allow user input of Q-values. Not described here; see the NJOY manual.*

NJOY's "PURR" Module - I

- What does PURR 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 in order to develop these tables.

NJOY's "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 (≥ 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*

- *repeat card 2 to process additional materials; set matd=0/ to terminate purr.*

NJOY's "GASPR" Module - I

- What does GASPR 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.
    - These input tapes should only contain the material to be processed, but multiple temperature pendfs are allowed.

NJOY's "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's "ACER" Module - I

- What does ACER 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's "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 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 is 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's "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)*
  - *nace = output (ace) file*
  - *ndir = output for ace 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) = ascii/binary ace format*
  - *suff = mcnp zaid suffix (default = **.00**)*
  - *nxtra = number of (iz,aw) pairs to read (**0**)*

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

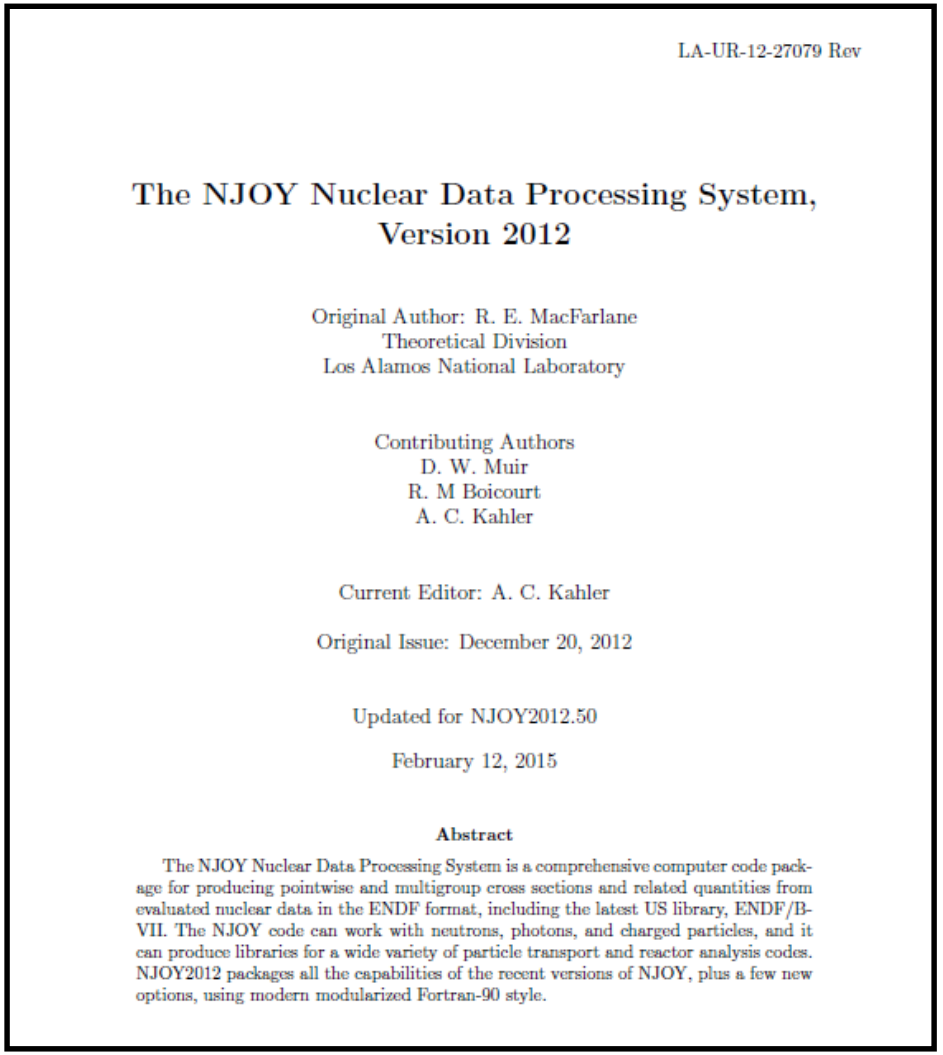
NJOY's "ACER" Module - IV

- **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 ace and
xsdir output files.
```

NJOY Documentation - I

- hyperlinked NJOY2012 and NJOY2016 manuals are available …
- http://t2.lanl.gov/nis/codes/NJOY12/NJOY2012.82.pdf
- https://github.com/njoy/NJOY2016-manual/blob/master/njoy16.pdf



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
Nuclear Data Sheets 111 (2010) 2739–2890
Nuclear Data Sheets
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”.

- Additional reports on “NJOY Data Processing” can be found under the “Nuclear Data and Physics” category in the MCNP Reference Collection.

NJOY Documentation - IV

- … 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).
  - "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 (https://www.oecd-nea.org/dbprog/Njoy/Cabellos-report_mcjeff31-v36.pdf).
- … and other JEF documents issued through the OECD Nuclear Energy Agency.