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Workshop on Neutron Cross Sections for Nuclear Engineers

NJOY Processing for MCNP

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Workshop on Neutron Cross Sections for Nuclear Engineers

NJOY Processing for MCNP

Abstract

We discuss the characteristics of the general purpose ENDF nuclear data file and the application specific ACE file. Use of the NJOY Nuclear Data Processing System to go from ENDF to ACE is reviewed. Other NJOY capabilities are also noted.

The NJOY Nuclear Data Processing System

- NJOY is a general purpose processing tool for ENDF formatted files.
  - NJOY usage in this presentation will focus on creating continuous energy (.c formatted) ACE files for MCNP.
  - Will briefly discuss thermal kernel files (ACE .t files).
  - Other NJOY uses include covariance file processing and general plotting … examples will be shown.
  - Will not discuss multigroup processing, photoatomic processing, photonuclear processing.

NJOY Processing for MCNP

- ENDF/B is a “general purpose” file.
- ACE is an application specific file.
- Use NJOY to go from an ENDF-formatted nuclear data file to an ACE file.
  - ENDF – United States
  - JEFF – Europe
  - JENDL – Japan
  - CENDL – China
  - BROND – Russia
  - Specialized (e.g. Dosimetry, Activation, …) – IAEA
- Will focus on an ACE “FAST” file, briefly discuss “THERMAL” files and other uses of NJOY.

NJOY Processing for MCNP

- ENDF file characteristics:
  - Arbitrary energy mesh for each cross section.
  - Arbitrary (and possibly multiple) interpolation schemes for intermediate energies – histogram, lin-lin, lin-log, log-lin, log-log.
  - Mix of resonance parameters and (E,xs(E)) list.
    - Cross sections are for zero degrees.
  - Scattering angular distributions can be a mix of energy-dependent Legendre polynomials (up to N=64; N can change with energy) or energy-dependent probability distributions.
  - Outgoing particle distributions given as a simple incident energy-dependent table of outgoing energy and probability, or through various analytic functions (e.g., Maxwellian, Evaporation, Watt, …) or other parameterization (e.g. Kalbach-Mann).

NJOY Processing for MCNP

- ACE file characteristics:
  - A single energy grid for all cross sections.
    - Linearly interpolable (E,xs(E)) list, Doppler broadened to the User temperature of interest.
      - Use probability tables for unresolved resonance representation.
  - Scattering distributions are given as probability distributions.
  - If tabulated, energy distributions are also converted to probability functions; analytic functions are sampled directly.
  - May contain “extra” cross sections for User defined tallies.
    - “Heating”.
    - Gas (p, d, t, ^{3}He or α) production.

NJOY Processing for MCNP

- NJOY is a modular program.
- User input, an ENDF "tape" and the output "tape" from a previous module serve as input to NJOY.
  - MODER: Used to convert files from ascii text to binary.
  - RECONR: Used to convert resonance parameters to a simple (E,xs(E)) list, also create a unionize energy grid based upon all energies from the ENDF input tape plus additional energy points to allow linear interpolation to within a User specified accuracy.
    - NJOY99 handles SLBW, MLBW, Reich-Moore, Adler-Adler and hybrid R-function resolved resonance formats.
    - NJOY2010 handles the above plus the Limited Reich-Moore format (will be used by ^{19}F and ^{35}Cl in ENDF/B-VII.1).
    - The output file is commonly referred to as a "Pointwise-ENDF", or PENDF tape.

NJOY Processing for MCNP

- NJOY is a modular program (con't)
  - BROADR: Doppler broaden RECONR's pointwise output file to a User specified temperature.
    - Also thin or expand the energy mesh to maintain linear interpolation accuracy to User specified limits.
    - Output includes a tabulation of representative data such as thermal cross sections and resonance integrals.

```
broadened mat9228 from  0.0000E+00 to  2.9360E+02 k
        points in= 242593  points out=  76519
        mt   2  18 102

   thermal quantities at 293.6 K = 0.0253 eV
   -----------------------------------------
          thermal fission xsec:  5.8490E+02
         thermal fission nubar:  2.4367E+00
          thermal capture xsec:  9.8665E+01
      thermal capture integral:  8.6639E+01
    capture resonance integral:  1.4043E+02
      thermal fission g-factor:  9.7628E-01
        thermal alpha integral:  1.6828E-01
          thermal eta integral:  2.0859E+00
           thermal k1 integral:  6.4040E+02
                 equivalent k1:  7.2262E+02
    fission resonance integral:  2.7596E+02
```

NJOY Processing for MCNP

- NJOY is a modular program (con't)
  - HEATR: Created specialized "cross sections" to allow heating and energy deposition calculations.
  - PURR: Create probability tables for cross section calculation in the unresolved resonance region. User specifies the number of random "resonance ladders" and probability bins over which average cross sections are determined.
    - … (my) typical values are 20 bins and 64 ladders.

NJOY Processing for MCNP

- NJOY is a modular program (con't)
  - GASPR: Gas ($^{1\text{-}3}$H, $^{3\text{-}4}$He) production can result from a variety of discrete reactions ("mt" numbers in ENDF-speak).
    - Use this module to combine them into a single cross section for tally use in MCNP.
      - For example, the following reactions produce alpha (among other) particles: mt22 (n,n'α), mt23 (n,n'3α), mt24 (n,n'2nα), mt25 (n,n'3nα), mt29 (n,n'2α), mt30 (n,2n'2α), mt35 (n,n'd2α), mt36 (n,n't2α), mt45 (n,n'pα), mt107(n,α), mt108(n,2α), mt109 (n,3α) mt112(n,pα), mt113(n,t2α), mt114 (n,d2α) and mt117(n,dα).
      - Sometimes the ENDF file will contain an "LR" flag in the inelastic scattering to discrete level (mt's 51 to 90) cross section to indicate particle emission from the compound nucleus.
      - New mt numbers can be added to the ENDF system (mt152 through mt199 were added in 2010 and are used in the latest activation files).
      - Mt103 to mt107 are for (n,p), (n,d), (n,t), (n,^{3}He) and (n,α); use mt203 to mt207 for the corresponding summation cross sections.

NJOY Processing for MCNP

- NJOY is a modular program (con't)
  - ACER: create an ACE formatted file for use with MCNP.
    - MCNP ACE formats written by NJOY include:
      - "FAST" – previous module sequence yields this library.
      - "THERMAL"
      - "DOSIMETRY"
      - "PHOTONUCLEAR"
      - "PHOTOATOMIC"
    - For "FAST" files, can also run in check/plot mode (sample output follows).

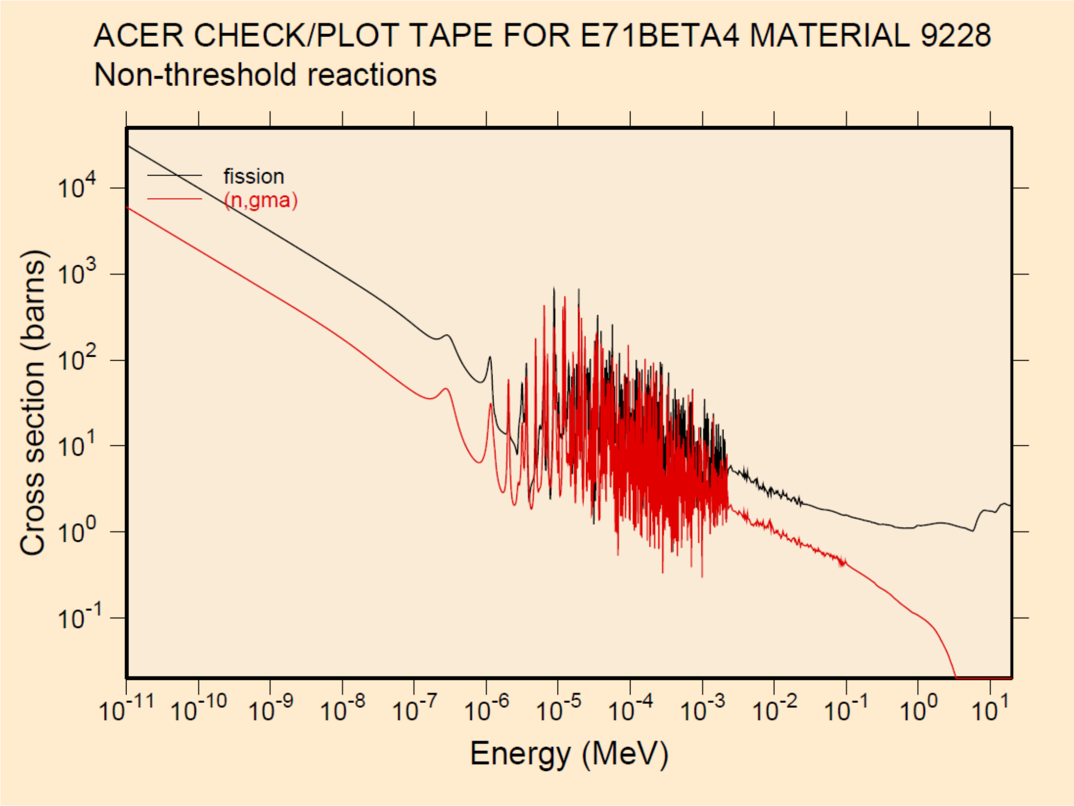
NJOY Processing for MCNP

- ACER "check/plot" output (not noted, but is ^{235}U):

```
acer...monte carlo neutron and photon data                              1450.3s

input endf unit ......................         0
input pendf unit .....................        31
input gendf unit .....................        33
output ace format unit ...............        34
output directory unit ................        35

run type option ......................         7
print option (0 min, 1 max) ..........         1
type of ace file .....................         1

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

check reaction thresholds against q values

check that main energy grid is monotonic

check angular distributions for correct reference frame

check angular distributions for unreasonable cosine values

check energy distributions

check delayed neutron fractions

check delayed neutron distributions

check photon production sum

check photon distributions

no problems found
```

NJOY Processing for MCNP

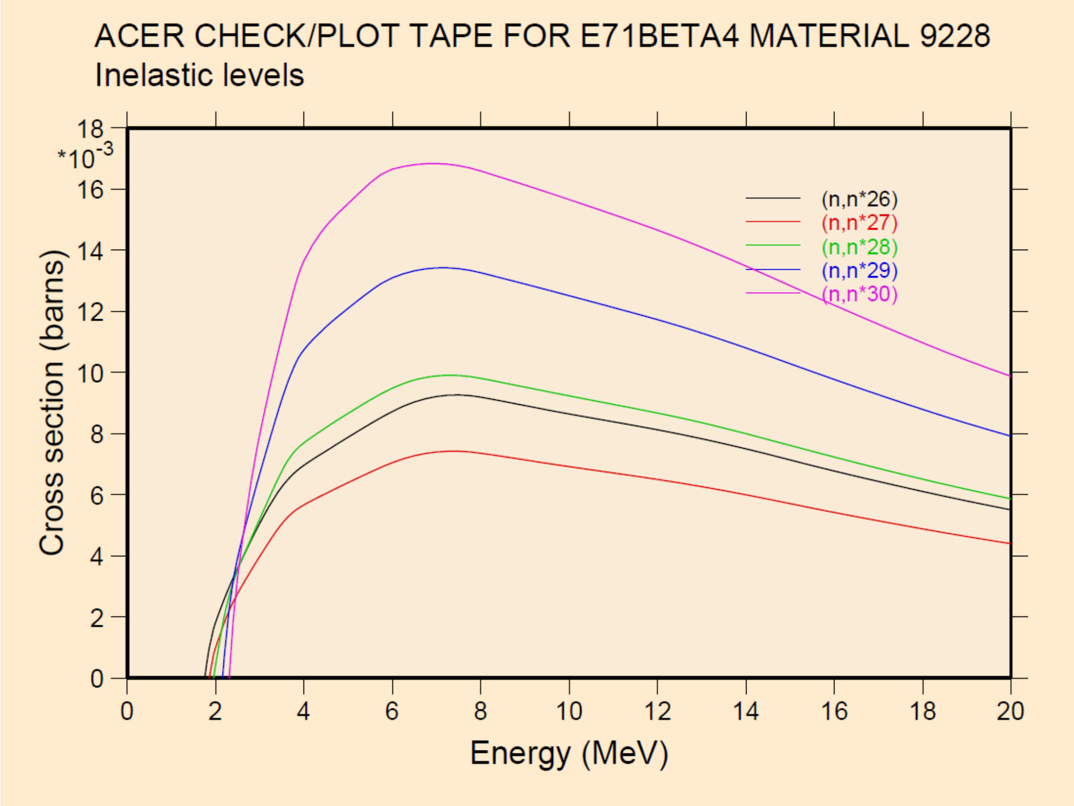
Sample plot from NJOY/ACER showing selected cross sections.



NJOY Processing for MCNP

Sample plot from NJOY/ACER showing selected cross sections.

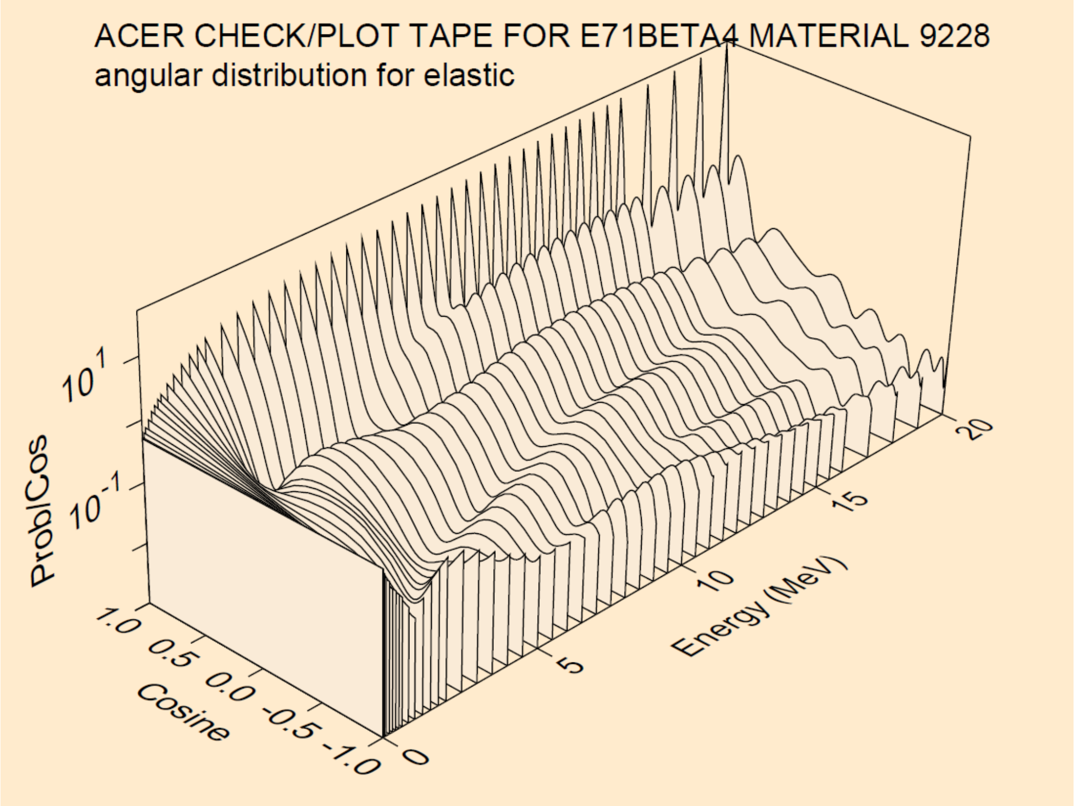
Step through all inelastic levels, with up to five discrete level cross sections shown per page.



NJOY Processing for MCNP

Sample plot from NJOY/ACER showing energy dependent elastic scattering angular distributions.

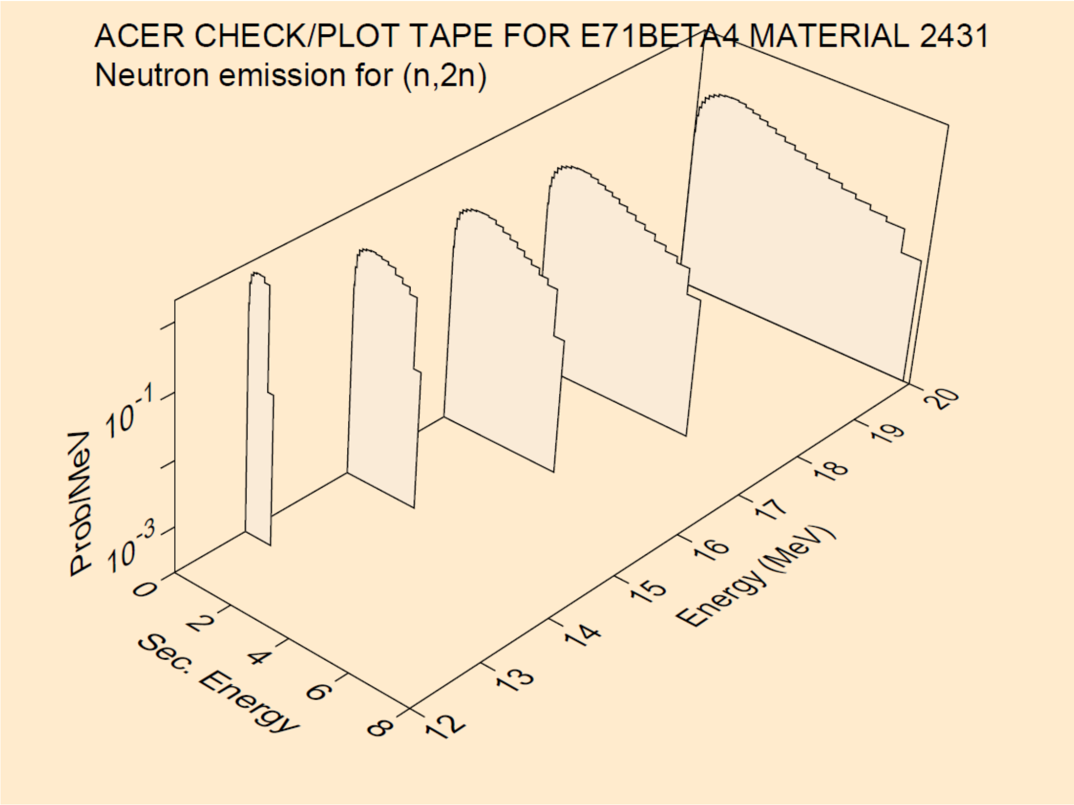
Shown as a probability distribution, where a flat curve such as observed at low energy represents an isotropic scattering distribution (i.e., equal probability as all angles).



NJOY Processing for MCNP

Sample plot from NJOY/ACER showing energy dependent neutron emission spectra.

Shown as a probability distribution, where the emission spectra approaches a delta function for decreasing incident neutron energy toward threshold.



NJOY Processing for MCNP

- ACE files are defined for a variety of nuclear data.
  - ACER: NJOY's module to create an ACE formatted file for use with MCNP.
    - MCNP ACE formats written by NJOY include
      - "FAST" – previous discussion focused on this option.
      - "THERMAL" – a few words about thermal scattering.
      - "DOSIMETRY"
      - "PHOTONUCLEAR"
      - "PHOTOATOMIC"

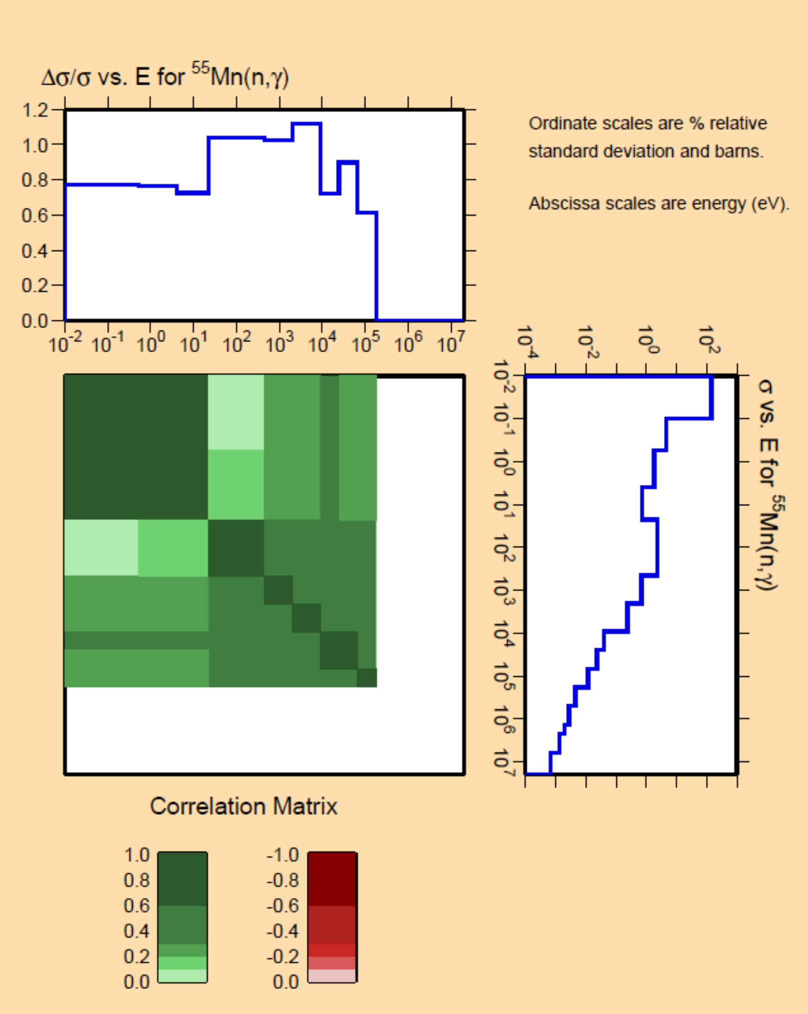
NJOY Processing for MCNP

- Thermal kernels
  - Below a few eV in energy, the impact of atoms bound in molecules may be important.
    - In practice, is only a concern for the principal scattering atom, most commonly hydrogen in typical reactor applications.
      - Scattering kernels are only defined for a few molecules (20 thermal kernel scattering files in ENDF/B-VII.0 versus 393 incident neutron files).
      - As discussed earlier in this Workshop, scattering can be “coherent elastic”, “incoherent elastic”, or “incoherent inelastic”.
    - Use NJOY’s “THERMR” module to process these data.
      - THERMR output goes to ACER.
    - Can use NJOY’s “LEAPR” module to create an ENDF-formatted file for input to THERMR.

Other NJOY Processing - Covariances

Combine the ERRORR, COVR, PLOTR and VIEWR modules to create plots of cross section uncertainty and correlation matrices.

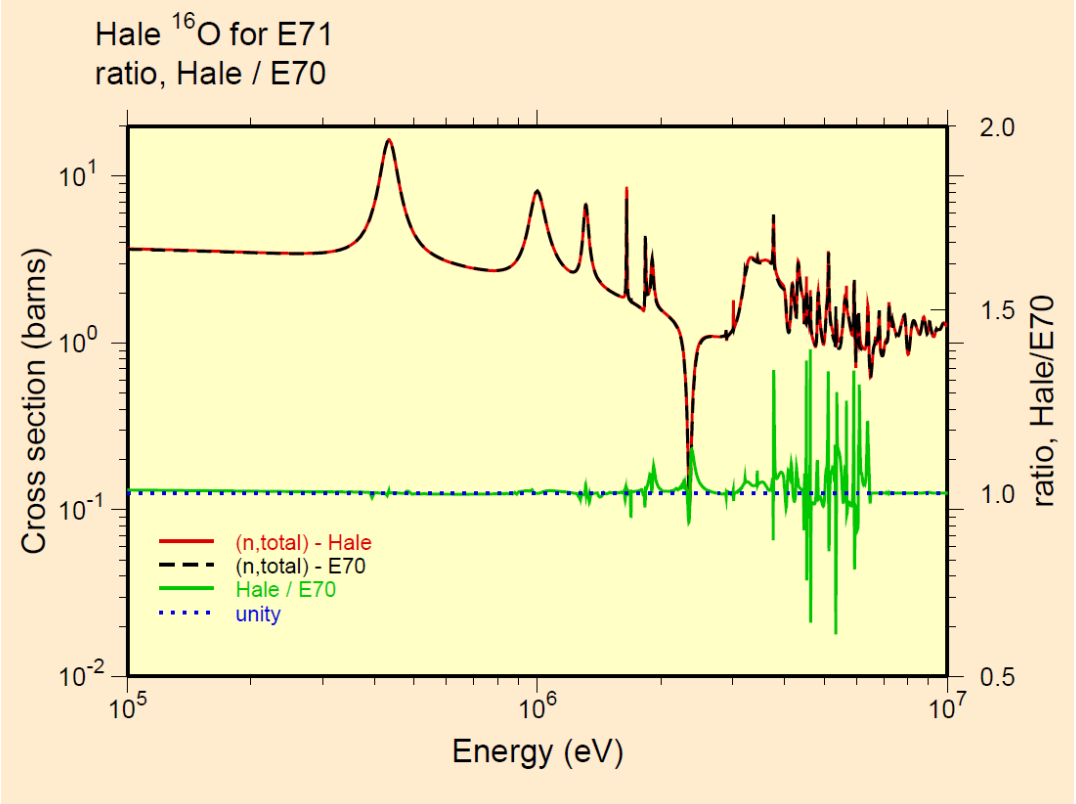
Also process nu-bar uncertainties (MF31), elastic scattering P_1 moment uncertainty (MF34), prompt fission emission spectrum uncertainty (MF35) and radioactive isotope production (MF40) uncertainty.



Other NJOY Processing - Plots

Use PLOTR and VIEWR to create plots of cross sections (including summation and ratio), angular distributions, emission spectra.

Plots can be for continuous energy data or multigroup data produced by the GROUPR module.

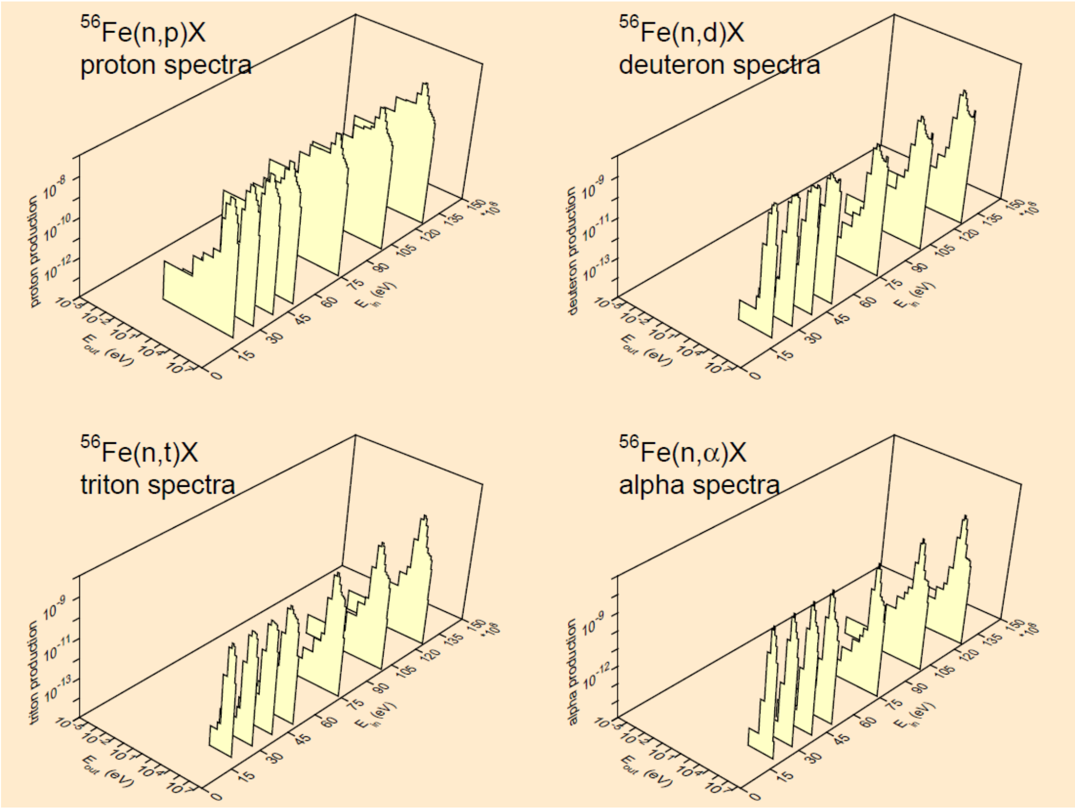


Other NJOY Processing - Plots

Use PLOTR and VIEWR to create plots of cross sections (including summation and ratio), angular distributions, emission spectra.

Plots can be for continuous energy data or multigroup data produced by the GROUPR module.

Can scale plots to yield multiple curves in a given frame.



NJOY Resources

- **Web Sites:**
  - http://t2.lanl.gov/codes/ and http://www.nea.fr/lists/njoy.html
- **Reports:**
  - R. E. MacFarlane & A. C. Kahler, "Methods for Processing ENDF/B-VII with NJOY," Nuclear Data Sheets **111**, 2739-2890 (2010).
  - R. E. MacFarlane & D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91" (distributed with the NJOY99 code package).
  - H. R. Trellue *et al*, ENDF70: A Continuous-Energy Neutron Data Library Based on ENDF/B-VII.0 (ICRS-11 conference).
  - J. M. Campbell *et al*, "ENDF66: A Continuous-Energy Neutron Data Library Based on ENDF/B-VI Release 6" (RPSD-2002 conference).
  - Oscar Cabellos, "Processing of the JEFF-3.1 Cross Section Library into a Continuous energy Monte Carlo Radiation Transport and Criticality Data Library", NEA/NSC/DOC(2006)18 (http://www.nea.fr/html/dbprog/Njoy/Cabellos-report_mcjeff31-v36.pdf).

ANS Summer Meeting Sessions

- **The United States' cross section community is finalizing the next release of the ENDF neutron library – ENDF/B-VII.1**
  - Scheduled for release at the end of 2011.
- **The Summer ANS meeting will feature two special sessions on ENDF/B-VII.1:**
  - "Initial Experience with ENDF/B-VII.1"
  - "ENDF/B-VII.1: Data Measurements, Evaluation and Processing"
  - Prove to your boss that the money to attend this workshop was well spent by submitting paper(s) to one or both of these sessions by January 13th, 2012, ☺!