The NJOY Nuclear Data Processing System - Current Status and Future Plans

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The base version of NJOY99 is distributed by ORNL’s RSICC and the NEA Data Bank.

Updates are maintained at Los Alamos and distributed freely at http://t2.lanl.gov/codes/njoy99.

- Machine dependent updates and sample makefiles for a variety of compilers and hardware/OS configurations are included here.

- The current version of the code is 99.259.

- In-house updates through 99.279 will be posted at the end of November.

A new base version, NJOY2008, is nearing completion with distribution to ORNL’s RSICC anticipated by the end of 2008.
NJOY - Introduction

NJOY is a collection of discrete programs that are run in sequence to accomplish a specific goal.

- Most common usage includes
  - Creation of continuous energy cross section files in “ace” fast format for use with the LANL MCNP(X) continuous energy Monte Carlo programs.
  - Creation of scattering kernel (“ace” thermal) files.
  - Processing covariance data.
    - Version 2.3 of ERRORJ was merged into NJOY99.259; several of the new updates described below expand this processing capability.
  - Data visualization.
    - NJOY’s PLOTR/VIEWR modules can be used to create postscript formatted plots.
      - Can display continuous energy cross sections, multigroup cross sections, angular distributions, secondary energy spectra, correlation matrices and uncertainties.
NJOY - Introduction

Code Management

RSICC or NEA Data Bank distribution includes the basic, uncompiled f77 NJOY99 source code, “src”; the source code for an updating utility program, “upd.f”; various test problem i/o files and various sample makefiles.

To create an executable

- Create an executable version of upd.
- Download the latest available update and appropriate machine dependent patches from [http://t2.lanl.gov/codes/njoy99](http://t2.lanl.gov/codes/njoy99).
- Merge the update file and machine dependent patch files, creating “upn”.
- With “scr” and “upn” in the same directory, execute upd.
  - Output will be a series of *.f files for the latest version of NJOY99
  - Compile and link these files to create the NJOY executable.
NJOY - Introduction

Code Management (con’t)

- Changes to NJOY99 embodied in these patches mean that the sample test problem files accompanying the original distribution are no longer valid.
- Obtain the latest test files from the “t2” web site.
- Small differences are acceptable
  - Test10 which uses random numbers will likely produce different answers (a deficiency that will be rectified in NJOY2008) as a function of User platform.
NJOY - Introduction

NJOY interprets a combination of User input instructions plus an ENDF-formatted evaluated data file.

- NJOY output files conform closely to basic ENDF-formatting rules.
  - A pointwise cross section file output from a given NJOY module is termed a “pendf” file, and is suitable for input to the next NJOY module in the User processing sequence.
  - A groupwise cross section file output by NJOY’s GROUPR module is termed a “gendf” file. While not a formal endf-formatted file, subsequent NJOY modules that further process groupwise data can read this file.
  - ERRORJ’s output file contains a combination of groupwise and covariance matrices that can be read by NJOY’s COVR module which generates correlation matrix, cross section and cross section uncertainty plots.
NJOY – Create Fast ACE Files

Creation of fast ACE files:

- **reconr**: expand file2/file3 data to create linearly interpolable continuous energy cross sections.
- **broadr**: doppler broaden reconr (or previous broadr) output to the desired temperature.
- **unresr** (optional): calculate unresolved resonance cross sections.
- **heatr** (optional): calculate energy deposition and damage “cross sections”.
- **purr**: calculate unresolved resonance probability tables.
- **gaspr** (optional): calculate gas ($^1\text{h}$, $^2\text{h}$, $^3\text{h}$, $^3\text{he}$ and $^4\text{he}$) production cross section.
- **acer**: recast output from previous NJOY modules into MCNP fast “ace” format.
NJOY – Fast ACE Plots

Doppler broadened continuous energy, linearly interpolable cross sections.
NJOY – Fast ACE Plots

Example of inelastic cross section plotting.
NJOY – Fast ACE Plots

- MF4, MT2 (elastic scattering) angular distributions.
NJOY – Fast ACE Plots

First inelastic level angular distributions – clearly not isotropic which may be an approximation in older codes.
NJOY – Fast ACE Plots

Secondary neutron emission spectra.
NJOY – Create Thermal ACE Files

Creation of thermal ACE files

- leapr (optional): use this module to create mf7 thermal scattering kernel data, if not available from a previously generated endf-formatted source.
- thermr: use this module to process leapr output or an endf-formatted thermal kernel input tape.
- acer: convert thermr output to MCNP thermal ace format.
NJOY – Thermal ACE Plots

- Hydrogen bound in water, inelastic scattering.
NJOY – Fast ACE Plots

- Free-gas hydrogen
- Note difference in elastic scattering at low energy.
NJOY – Covariance Processing

- **reconr**: expand file2/file3 data to create linearly interpolable continuous energy cross sections.
- **broadr**: doppler broaden reconr (or previous broadr) output to the desired temperature.
- **unresr**: calculate unresolved resonance cross sections.
- **groupr**: calculate group averaged cross sections, angular distributions and emission spectra.
- **errorj**: process mf31, mf32, mf33, mf34 and mf35 covariance data.
- **covr**: create plot file for mf31 (nu), mf33 (cross sections), mf34 (mu-bar) or mf35 (spectra), their uncertainties and correlation matrices;
- **viewr**: convert covr plot file to postscript format.
Covariance Plots – MF31

- New plotting features
  - Uncertainty in data on one frame.
  - Data on the second frame.
  - Use log-log scale for the ordinate when min-to-max ratio is large (currently 10x).
  - Additional color scale so virtually all correlation matrix elements are displayed.

- These data are from JENDL-3.3 $^{238}\text{U}$.
Covariance Plots – MF33

- **New plot feature**
  - Warn user when uncertainty data are truncated to fit within the fixed ordinate axis limits.

- Unexpected discontinuities, especially in a derived cross section uncertainty, may indicate a deficiency in the underlying covariance data.
Covariance Plots – MF33

- Axis limits are adjusted to minimize plotting of “zero” data.
Covariance Plots – MF33

Again, some features seem unphysical.
Covariance Plots – MF34

- Plotting of mu-bar uncertainty (mt251) is new in NJOY99.279.

- This plot is a 618-group calculation for JENDL-3.3 $^{238}$U.
Covariance Plots – MF35

Plotting of fission spectrum uncertainty (mf5, mt18) is new in NJOY99.279.

This plot is a 618-group calculation for JENDL-3.3 $^{238}$U.
NJOY – Visualization

Visualization

- NJOY produces a predefined suite of plots, on user option, from the groupr, acer and covr modules.

- User’s can also create plots using the plotr and viewr modules.
  - Example follows.
NJOY – PLOTR/VIEWR

- User input to PLOTR to set axis limits, specific MT’s, plot title, curve legend, individual curve colors and individual curve line texture.
- This plot generated from GROUPR output.
NJOY2008

All NJOY99 coding now converted to Fortran 90/95.
   No more machine-dependent updates!
      Can use Fortran 90/95 intrinsic functions to define these variables.
      No more “set sw” to get real*8 precision – now use “kind” definition.

Historical test problems reproduce NJOY99 results.
   New coding includes a “physics” module with various constants collected in one location for easy upgrade.

A new User manual will accompany the new code.
   No more references to NJOY91!
NJOY – Future Developments

Future Developments (think about this for Friday’s NJOY User Group Meeting)

- Continuing evolution of Covariance formats
  - Scattering radius uncertainty (Rochman/Chiba & revised ERRORJ).
- An NJOY/CINDER module?
  - A new version of CINDER90 is near release and will contain a room temperature, 63-group, ENDF/B-VII.0 based cross section library.
    - May also contain JEFF-3.1 and JENDL-3.3 based libraries.
  - Is there User demand to make their own CINDER90 library?
- Calculate elastic scattering angular distributions from resolved resonance parameters.
  - This capability exists but is not yet tested nor formally implemented in NJOY2008 for LRF=7 (Limited Reich-Moore) evaluations.
    - Recent data testing of selected ICSBEP benchmarks indicates a large sensitivity in calculated eigenvalue for systems with large axial reflectors as a function of elastic scattering angular distributions.
NJOY – Future Developments

Future Developments (con’t)

- Additional training & web page upgrades.
  - Half-day tutorials at recent technical society meetings have been well attended; *may* next occur during the ANS general meeting in Atlanta.
  - On-line training was partially implemented for NJOY97 and remains relevant, but is incomplete.

- When should NJOY recognize a deficiency in the basic input file and automatically make corrections?
  - int=2 → int=22 for interpolation of emission spectra.
  - ???

- ???

Funding for future developments?