The NJOY Nuclear Data Processing System

A. C. (Skip) Kahler & R. E. MacFarlane akahler@lanl.gov

T-2, Nuclear & Particle Physics, Astrophysics & Cosmology Group Theoretical Division Los Alamos National Laboratory

Presented at the OECD/NEA NJOY User's Group Meeting



November 2008

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396



NJOY - Introduction

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 <u>http://t2.lanl.gov/codes/njoy99</u>.
 - Machine dependent updates and sample makefiles for a variety of compilers and hardware/OS configurations are included here.
- \blacktriangleright 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.





- up260: includes several patches to the newly installed ERRORJ module to correct omissions from the original merge (J-Ch Sublet and C. Broeders assisted).
- up261: replace a data statement with an assignment statement in GROUPR (Lahey compiler issue identified by C. Broeders).
- up262-up264: revise RECONR, UNRESR and PURR, respectively, to recognize an energy-dependent scattering radius when calculating unresolved resonance region cross sections. Also recognize NAPS and NRO flags when
 processing URR region data (CEA/Trkov request).





- up265: replace GROUPR's abort condition introduced in up167 with a warning (not a good idea in my opinion, but I'm responding to strong user demand).
- up266: revise the minimum legal mtref value from 201 to 221 in THERMR. In practice the 221 lower limit has existed for many years but program comments and "if" test embedded in the code were never revised (Peters, UMC).
- up267: eliminate "thermal" (iopt=2) related text from ACER's standard "fast" (iopt=1) output; also revise a check for ordinate axis limits in ACER's standard plotting to assure ymin < ymax.





- up268: revise THERMR to include NS (up to 3) nonprincipal scattering atoms. Current coding only supports NS=1 (which is sufficient for today's kernels).
- up269: revise average energy calculation for thermal scattering in ACER to avoid numerical issues; also make sure the pointer for printing Bragg edge data is properly incremented when have more than 200 edges (Mattes).
- up270: make sure the q-value is defined in ACER when processing photonuclear files; revise color code definition logic when have more than 16 plots on a frame (a common occurrence with photo-nuclear plots).





- up271: revise the light particle production calculation in ACER when processing file 6 photon data. ENDF/B-VII ¹H switched from MF12/MF14 to MF6 for photon data and deuteron production was being double counted. This patch was developed to support the official MCNP5 ENDFB7 library (Trellue, LANL).
- up272: a number of additional patches in ERRORJ, mostly related to memory management - expanding array limits to handle larger numbers of multigroups; also minor bug patches per Go Chiba emails (Arcilla, Trkov, Chiba, Rochman).





• up273: COVR patches to handle larger numbers of multigroups (to maintain consistency with ERRORJ's capability); also revise plotting routines to handle MF=34 and MF=35 data; change between linear and log scales; expand color intervals for the correlation matrix; add user warning when uncertainty data exceed the ordinate scale limits and replace the redundant uncertainty plot with a plot of the underlying multigroup data; expand 60 character plot title limit to 80 characters (Trkov).

 up274: VIEWR patches to remain consistent with previous module changes that allow up to 80 characters for various titles.



- up275: implement 3D plotting of few-group emission spectra in PLOTR. A long-standing omission in this module.
- up276: revise the definition of enext in GROUPR when iwt=2 to be consistent with the coding used for other iwt values; make sure EHIGH is always defined.
- up277 & up278: revise MODER and NJOY to handle all possible integer modes for the compact covariance format (Trkov).



Operated by Los Alamos National Security, LLC for NNSA

Slide 7

- up279: revise ERRORJ coding to properly read LCOMP=2, MF32 formatted files (Trkov).
- Additional updates, just recommended by Andre last week and posted to the NJOY listserver, are under review and are expected to be included in the new release.





NJOY2008 – Ongoing Efforts

• 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!



NJOY2008 – Ongoing Efforts

Ongoing Efforts

- NJOY2008 will be consistent with NJOY99.279, but not all NJOY2008 features will be replicated in NJOY99.x
 - LRF=7 Limited Reich-Moore resolved resonance processing will only reside in NJOY2008.
 - Evaluated files using this format can be found in ENDF/A (¹⁹F & ³⁵CI).
 - The capability to calculated elastic scattering angular distributions from LRF=3 or 7 (Reich-Moore or Limited Reich-Moore) will become available in a future NJOY2008 version only.
 - Covariance processing of LRF=7 evaluations will only be possible with NJOY2008.
- We expect to maintain NJOY99 for approximately 1 year after formal release of NJOY2008 by RSICC.

UNCLASSIFIED

Significant errors will always be patched.







- Eliminate redundant uncertainty plots; replace with multigroup data.
- Use log scale on the ordinate when min-to-max data range gets large.
- Add warning when underlying data are truncated to fit within fixed axis limits.
- Extend color scale so virtually all correlation matrix elements are displayed.









Operated by Los Alamos National Security, LLC for NNSA





Slide 12



• Los Alamos



MT251 from GROUPR.







- MF35 (MT18) fission spectrum
 - MF5 MT18 'chi' out of GROUPR.





- NJOY produces a predefined suite of plots, on user option, from the groupr, acer and covr modules.
- However, based upon tutorial feedback, many User's are unaware of NJOY's other user selectable plotting options (PLOTR/VIEWR to produce postscipt formatted plot files).

Examples follow.







 Example for ENDF/B-VII.0 ¹⁰B.

> User specified axis limits, log/linear scales, titles, legends, curve colors and patterns, specific xs data to plot, background color and frame color.







- More ¹⁰B
 - Labels can include subscripts or superscipts and greek letters.
 - Curve legend can include pointer.







- More ¹⁰B
 - Can plot ratio of selected cross sections
- Nothing new in these last three pages – just a reminder to User's of NJOY's plotting capability.







 This plot generated from GROUPR output.





NJOY – Future Developments

• Future Developments

- 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 inplemented 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; <u>may</u> 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 \rightarrow int=22 for interpolation of emission spectra.
 - ♦ ???
- ♦ ???

• Funding for future developments?



