

NJOY User Group Meeting

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NJOY User Group Meeting

- Introduction
 - Skip Kahler – who is he and where is Bob?
- Recent program updates
- Focus on ERRORJ
- Open Discussion



NJOY – Introduction

- Skip Kahler –
 - Joined LANL in September 2005.
 - Previously at Bettis Atomic Power Laboratory (from 1981 to 2005).
 - Bettis is one of two Reactor Design laboratories for the US DOE Naval Reactors Program (but its really the US nuclear navy).
 - Involved in Cross Section Data Testing & served as Bettis' representative to CSEWG for 18 years.
 - A “casual” NJOY user since ~1989, but it is not the primary xs processing code for Bettis' design codes.



NJOY – Introduction

- Bob officially retired from LANL in June 2005.
 - Remains active in NJOY development and Cross Section Data Testing.
 - “Working” ~ 1/2 time.
 - Current contract extends to April 2008.
 - Hopes to continue longer, but LANL budget uncertainties make this difficult to predict – a voluntary reduction in staff is currently underway and may be followed by an involuntary reduction early in 2008.
 - Email continues to be the best way to communicate.
 - His voicemail is full (and he’s happy with it that way!)



NJOY – Current Status

- Recent Program Information

- NJOY99.259 was Uploaded on October 16, 2007.

- A generic moder/reconr/broadr/unresr/heatr/thermr/purr/gaspr/acer/groupr job can process all ENDF/B-VII.0, JEFF-3.1 and JENDL-3.3 neutron files*.

- Important new feature was inclusion of ERRORJ.

- Separate topic of discussion, later today.

- Many other updates over the last couple of years.

- NJOY99.112 -161 were used for ENDF/B-VII beta processing.
 - NJOY99.90 was posted for over two years (summer 2003).



NJOY – Current Status

- Most recent updates:
 - 259: GROUPR (Sinistra/Kahler)
 - Use prompt nu-bar for neutron multiplicity with file6 fission spectra.
 - 258: ERRORJ (Go Chiba/Kahler).
 - Replace ERRORR.
 - 257: GROUPR (MacFarlane/Kahler)
 - Photon yields; force int=22 in mf6, law1; option to modify secondary energy spectra.
 - 256: THERMR (Altiparmokov/Kahler)
 - Better checking of input file for LEAPR options.
 - 255: LEAPR (Altiparmokov/Kahler)
 - Add ilog and isabt flags to the output file.



NJOY – Current Status

- Most recent updates (con't):
 - 254: GROUPR (MacFarlane)
 - Delete obsolete coding affecting analytic fission spectra.
 - 253: HEATR (Kahler)
 - Don't extrapolate beyond EMAX.
 - 252: HEATR (Kahler)
 - Shade degenerate energy mesh points to avoid TERP floating point overflow runtime error (JEFF ^{152}Eu issue).
 - 251: RECONR (Kahler)
 - Improve dimension allocation calculation for the dictionary.
 - 250: VIEWR (Kahler)
 - Predefine more colors (for plotting 8 delayed neutron group data).



NJOY – Current Status

- Most recent updates (con't):
 - 249: ACER (Kahler)
 - Expand format field.
 - 248: RECONR (Kahler)
 - Expand format field.
 - 247: GASPR (Trellue/Kahler)
 - Continuation of up244, to handle multi-temperature tapes.
 - 246: BROADR (Daily)
 - Correct typo in up240.
 - 245: PURR (Trellue/MacFarlane)
 - Revise sampling algorithm to eliminate zero width bins.



NJOY – Current Status

- Most recent updates (con't):
 - 240, 242-244: BROADR, RECONR, ACER, GASPR (Kahler)
 - Process partial cross sections (MT>600) when MT=103 to 107 are not present (format violation?).
 - 241: THERMR (Mattes)
 - Correct liquid H & D processing for LASYM=1 and LAT=1.
 - 239: ACER (Kahler)
 - Add *set sw construct for implicit real*8 (a-h,o-z) declarations.
 - 238: GROUPR (Kahler)
 - Move Character definition out of *set sw; add *set sw to new subroutine introduced in up212 coding.



NJOY – Current Status

- Most recent updates (con't):
 - 237: HEATR (Kahler)
 - Add *set sw to new subroutine introduced in up208.
 - 236: CCCCR (Broeders/Kahler)
 - Process the number of delayed neutron groups based upon information from the input file (typically 8 for JEFF; 6 otherwise).
 - 235: NJOY (Trkov/Kahler)
 - Improve up180 coding to prohibit printing 10.00000+n when the correct value is 1.000000+n.
 - 234: ACER (Kahler)
 - Explicit variable initialization (not an issue if the compiler presets undefined variables to zero).



NJOY – Current Status

- Most recent updates (con't):
 - 233: ERRORR (Kahler)
 - Restructure multiple condition “if” test (may be needed to avoid run-time errors with un-optimized code).
 - 232: PLOTR (Kahler)
 - Explicit variable initialization (not an issue if the compiler presets undefined variables to zero).
 - 231: GAMINR (Kahler)
 - Add missing SAVE (not an issue when compiled with static allocation).
 - 230: GROUPR (Kahler)
 - Variable initialization; missing SAVE.



NJOY – Current Status

- Most recent updates (con't):
 - 229: THERMR (Broeders/Kahler)
 - Expand format field.
 - 228: VIEWR (Kahler)
 - Variable initialization.
 - 225-227: HEATR, ACER, GROUPR (Kahler/MacFarlane)
 - Get maximum energy from input file, if possible.
 - 224: PLOTR (Kahler)
 - Variable initialization.
 - 223: RECONR (Trkov/Kahler)
 - Revise up215 (mt definition for photonuclear file processing).



NJOY – Current Status

- Most recent updates (con't):
 - 222: VIEWR (Kahler)
 - Format revision.
 - 221: ACER (Kahler/MacFarlane)
 - Correction to up219.
 - 220: ACER (Kahler)
 - Extend up70 to handle $\ln u=1$ for nu-bar plot.
 - 219: ACER (MacFarlane)
 - New smoothing options for secondary energy distributions (overriding the evaluated file interpolation specification).
 - 218: ACER (Kahler)
 - Format revision.



NJOY – Current Status

- Most recent updates (con't):
 - 217: HEATR (Kahler)
 - Increase dimension limits
 - 216: ACER (MacFarlane)
 - Revise acephn for more efficient processing of all endf/b-vii.0 photonuclear files.
 - 215: RECONR (Kahler)
 - More photonuclear file processing revisions.
 - 214: POWR (Kahler)
 - Format revision.
 - 213: ACER (MacFarlane)
 - Revisions to standard plots.



NJOY – Current Status

- Most recent updates (con't):
 - 212: GROUPR (MacFarlane)
 - New routine to process file 6 discrete photons.
 - 211: HEATR (MacFarlane)
 - Variable initialization for phase space law (^2H) processing.
 - 210: GROUPR (Broeders/Kahler)
 - Avoid infinite loop if group structure energies contain 7 or more significant digits.
 - 209: ACER (Trellue/Little/MacFarlane)
 - Correct recoil heating error for file 6 law 4 ($^6\text{Li}(n,t)\alpha$, for example).
 - 208: HEATR (MacFarlane)
 - New routine to process file 6 discrete photons.



NJOY – Current Status

- Most recent updates (con't):
 - 207: GROUPR (Altiparmakov/Kahler)
 - Avoid bounds overflow in flux calculator.
 - 206: ACER (Kahler)
 - Variable initialization.
 - 205: GROUPR (Kahler)
 - Make single and double precision data statements consistent.
 - 204: HEATR (Altiparmakov/Kahler)
 - Revise logic for energy balance test based upon User input.
 - 203: NJOY (Kahler)
 - Single/double precision consistency.



NJOY – Current Status

- Most recent updates (con't):
 - 202: ERRORR (Kahler)
 - Error in group structure (ANL-27) initialization.
 - 201: ACER (Little/Trellue/MacFarlane)
 - Revise charged particle heating from isotropic file 4 distributions.
 - 197-200: BROADR, GAMINR, ERRORR, THERMR (Kahler)
 - Single/double precision consistency.
 - 196: ACER (Kahler)
 - Set sw corrections; single/double precision consistency.
 - 195: GROUPR (Kahler)
 - Include up107 group data in single precision; set sw corrections.



NJOY – Current Status

- Most recent updates (con't):
 - 191-194: LEAPR, COVR, HEATR, NJOY(Kahler)
 - Single/double precision consistency.
 - 189-190: HEATR, GROUPR (upnea)
 - Increase array space for discrete photons.
 - 188: HEATR (Kahler)
 - Insert missing SAVE.
 - 187: HEATR (MacFarlane/Kahler)
 - Revise energy limits for discrete photon production.
 - 186: ACER (MacFarlane)
 - Revise lower energy limit for discrete photon production.




NJOY – Current Status

- Most recent updates (con't):
 - 185: HEATR (MacFarlane)
 - Correct recoil heating error from up115.
 - 184: HEATR (MacFarlane)
 - Increased array size for JEFF ^{239}Pu prompt nu(E).
 - 183: ACER (MacFarlane)
 - Extend up177 to handle multiple subsections.
 - 182: BROADR (Kahler)
 - Omit small cross sections when creating energy mesh; also similar coding as up180, up182.
 - 180,181: NJOY, RECONR (Lubitz/Kahler)
 - Use “F” format for extra digit, if necessary between 0.1 & 1.0 eV.



NJOY – Current Status

- Most recent updates (con't):
 - 179: VIEWR (Kahler)
 - Include additional %% commands to plot file.
 - 178: ACER (Kahler)
 - Variable initialization for plotting.
 - 177: THERMR (MacFarlane)
 - Revise free gas energy mesh for temperature dependence.
 - 176: BROADR (Kahler/MacFarlane)
 - Increase scratch space for larger ΔT ; allow doppler broadening of partial cross sections.
 - 175: BROADR (MacFarlane)
 - Increase number of reactions that may be simultaneously broadened.
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NJOY – Current Status

- Most recent updates (con't):
 - 174: ACER (MacFarlane)
 - Use EMAX when available for discrete photon production processing.
 - 173: ACER (Sutton/Kahler)
 - Revise TAB1 processing (eliminate multiple $f(e)=0.0$ data).
 - 172: PURR (Trellue/MacFarlane)
 - Fix up62 for unresolved resonance region heating when $lssf=1$.
 - 170,171: CCCCR, MATXSR (Broeders/Kahler)
 - Increase various array limits.
 - 169: MATXSR (Sinistra/Kahler)
 - Correct coding type (array “a” should be “b”).



NJOY – Current Status

- Most recent updates (con't):
 - 168: THERMR (Kahler)
 - Variable initialization.
 - 167: GROUPR (various users/Kahler/MacFarlane)
 - Various fixes (variable initialization, missing SAVE, missing EXTERNAL, abort on unresr $\sigma < 0$, up161 correction, ...)
 - 163-166: ACER,VIEWR,MODER (various users/Kahler)
 - Variable initialization & external declaration.
 - 162: PURR (Kahler)
 - Revise logic for mt loop (can now process ^{253}Es).



NJOY – Current Status

- Summary of Recent Updates
 - New or revised capability.
 - New, but optional, capability.
 - Format revisions.
 - Revisions to Eliminate Compiler Issues.
 - Eliminate Single / Double Precision Inconsistencies.
 - Corrections, or ☹, corrections on corrections.



NJOY – Current Status

- Future Plans

- Return to development of NJOY 200x.

- Fortran 90/95 based version.

- Work started in the early 2000s but was suspended when the RSICC/NEA code sharing agreement expired.

- ERRORJ is still f77 based; other modules were converted previously but debugging is ongoing.

- Intel compiled executable runs; G95 compiled executable aborts.

- We Plan to Release this Version, and a New Manual, in 2008.

- Ongoing NJOY99 development during ENDF/B-VII “beta” testing and an internal decision to use NJOY99 to process ENDF/B-VII for the next LANL sanctioned MCNP cross section library meant continued delay for the new version.



NJOY – Current Status

- Future Plans

- Expect to freeze NJOY99 very soon.

- Some ERRORJ related updates are pending.
 - Possible new COVR plotting options (BNL request).
 - Energy dependent scattering radii for URR region.
 - Need to Verify Single Precision Mode on 64-bit Platforms.
 - ...

- Will continue to fix serious NJOY99 technical errors for the foreseeable future.



NJOY – ERRORJ

- ERRORJ

- Started from ERRORR from NJOY94.105.
- Preliminary Merge Performed by Go Chiba into NJOY99.125 (Fall 2006 visit to LANL).
- Preliminary Merge Performed by Ramon Arcilla (BNL) into NJOY99.161 (also by J-Ch Sublet, others?).
- “Official” Merge Performed by LANL into NJOY99.259.
 - Includes bug-fixes identified in “Bug-Fix for ERRORJ-2.3”, dated October 3, 2007.
 - Added Three New Test Problems.
 - Largely reproduced the standard output provided by Go Chiba for these test jobs.



NJOY – ERRORJ

- Some details of the NJOY/ERRORJ Merge:
 - Use existing NJOY common blocks for consistent definition of physical and numerical constants.
 - Consistent use of “implicit real*8” declarations in lieu of “double precision”.
 - Consistent use of “d” exponents in data declarations.
 - Miscellaneous text changes to the source code to resolve various compiler issues:
 - Split multiple condition “if” tests into multiple “if” tests (to resolve potential run-time issues when compiled without optimization).
 - Move variable initialization statements out of “if” constructs.
 - Use x(*) in lieu of x(1) in dimension declarations.
 - Eliminate use of obsolete “H” edit descriptor in format statements.

NJOY – ERRORJ

- ERRORJ Issues in NJOY99.259

- Thanks to J-Ch Sublet, C. Broeders & Go Chiba:

- Need “external error” declaration for Lahey compiler .
- Coding errors – character declarations, dimension declarations, variable initialization:
 - “hmt” and “uline” are undeclared character variables.
 - “small” in ggrmat is undefined.
 - dimension flux(10,10) not uniformly declared.
 - undefined “temp(jtemp)” in subroutine egtwtf.
 - erroneously carried over from subroutine getwtf in groupr.
- Delete unused subroutine (ggrmatorg).
- Remove restriction for MT < 870 (needed for ^9Be).
- Maximum number of reaction types = 60. Enough? (^{28}Si)
- More Checking When Processing MF35?
- ???

NJOY – ERRORJ

- My experience with ERRORR/ERRORJ is very limited.
- Feedback is needed so that I can make sure what the code does is really what the User needs.



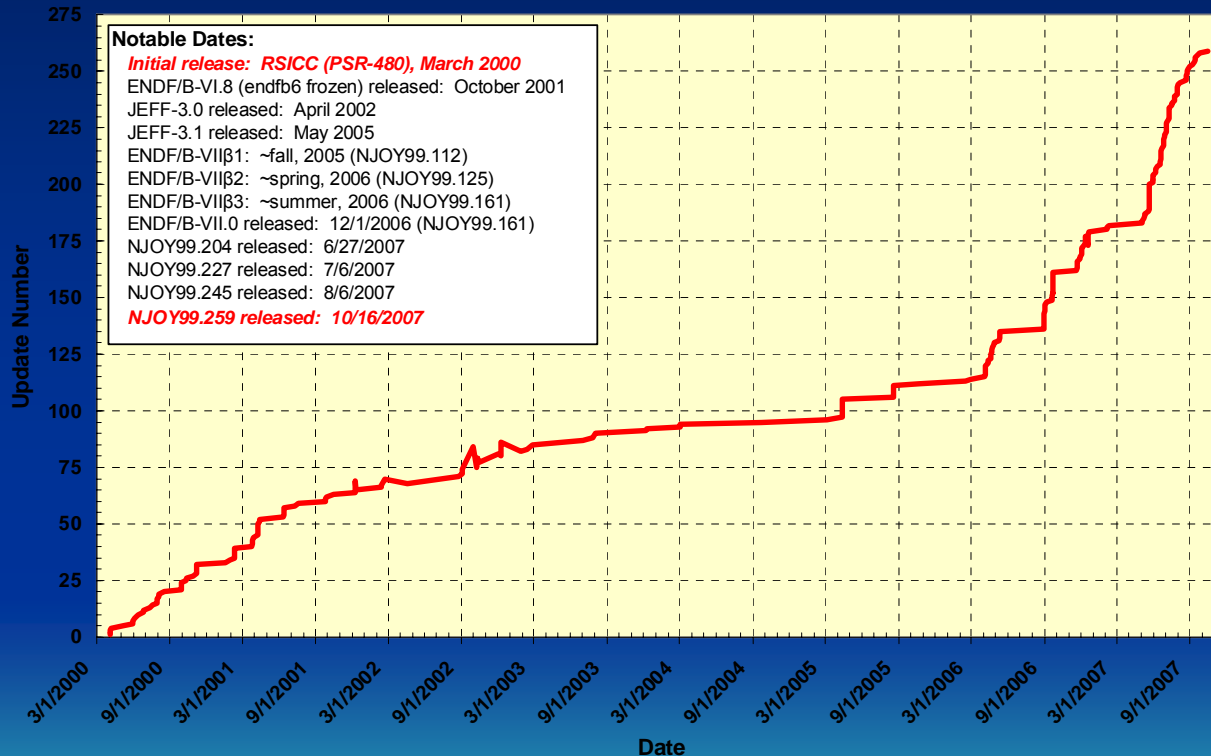
NJOY – Open Discussion

- We make no promises, but let's start a dialogue.
 - We hope to continue doing what Bob has done well in the past and I hope to improve in areas where Users feel we could do better.
 - Future Update Strategies.
 - Issue Tracker.
 - Transition from NJOY99 to NJOY2008.
 - Training & LANL/User Interaction.
 - Test Problem Suite.
 - File Checking.
 - Other issues?



NJOY – Update Strategy

NJOY99 Update Progression with Time



- Frequent (too many?) Updates in Recent Years.

- Are Preliminary Updates Useful?

- Are Users who Report Problems Willing to Test Proposed Updates Before General Public Release?

NJOY – Issue Tracker

- How Should Developers (Bob & I) and Users Keep Track of Current Issues and Future Plans?
 - “Issue Tracking System” at <http://t2.lanl.gov/codes/njoy99/Issues.html>.
 - Has not been used for years!
 - Was its implementation useful? Should it be resurrected? What would be better?
 - NJOY Listserver at <http://www.nea.fr/lists/njoy.html>.



NJOY – Issue Tracker

- For LANL “Issue Tracking System”.
 - Issues are submitted directly to the developers.
 - But, if not posted, others Users are not kept up to date.
- For the NEA NJOY Listserver, an Independent Third Party Filters Issues.
 - All users can see outstanding problems.
 - If the developer doesn’t keep up, no central “official” solution will become available.



NJOY – Issue Tracker

- Other Options?
 - Create a New Locally or Third Party Maintained Web Site?
 - A comprehensive table of outstanding issues, perhaps modeled after the JEFF-3.1 Feedback Tables.
 - Columns for “Date”, “NJOY Module”, “Evaluated File being Processed”, “User”, “User Comment & Relevant Error Messages”, “Status/Resolution”.
 - Develop a “forum” web site, such as exists for MCNP?
- Maybe nothing new is needed?



NJOY – NJOY2008/NJOY99

- The Next Major Release Should Occur in 2008.
 - What is missing from NJOY99 that should be in NJOY2008?
- Once Available Via RSICC and the NEA, how Quickly will/should Users Switch?
 - Must be a Local Institutional Decision.
 - How Long Should LANL be Expected to Maintain NJOY99?



NJOY - Training

- How Should LANL (me!) Interact with Current and Future Users?
 - On-line Tutorial (“Understanding NJOY”).
 - Developed during NJOY97.
 - Not well publicized (and incomplete).
 - Available at <http://t2.lanl.gov/njoy/title.html>.
 - Workshops
 - Hands on workshops are planned for ICRS-11 (April 2008) and the ANS Annual Meeting (June 2008).
 - Some good, but password protected, JEF-DOCs.
 - JEF-DOC-1099 and 1125 (Haeck & Verboomen).
 - JEF-DOC-1127 (draft).



NJOY – Test Problem Suite

- Historical Test Suite includes 14 Jobs:
 - Test 1: moder/reconr/broadr/heatr/thermr/groupr with endf/b-v C.
 - Test 2: moder/reconr/broadr/unresr/groupr/ccccr with endf/b-iv ^{238}Pu .
 - Test 3: reconr/gaminr/dtfr/matxsr/viewr with “DLC7E” photon data.
 - Test 4: moder/reconr/errorr/groupr with endf/b-v ^{235}U .
 - Test 5: moder/errorr/covr/viewr with endf/b-v C.
 - Test 6: plotr/viewr with endf/b-v C.
 - Test 7: moder/reconr/broadr/heatr/groupr/acer with endf/b-v C.
 - Test 8: moder/reconr/broadr/heatr/groupr/acer with endf/b-vi.1 ^{61}Ni .
 - Test 9: moder/reconr/broadr/leapr/thermr with endf/b-v ^1H .
 - Test 10: moder/reconr/broadr/unresr/purr/acer with endf/b-iv ^{238}Pu .
 - Test 11: moder/reconr/broadr/unresr/thermr/groupr/wimsr with endf/b-iv ^{238}Pu .
 - Test 12: reconr/gaspr/plotr/viewr with endf/b-vi.1 ^{61}Ni .
 - Test 13: moder/reconr/broadr/heatr/gasrp/acer/viewr with endf/b-vi.1 ^{61}Ni .
 - Test 14: acer/viewr with endf/b-vi p+ ^{14}N .

NJOY – Test Problem Suite

- Recently added three new jobs for ERRORJ (contributed by Go Chiba).
 - “ej1”: moder/reconr/broadr/groupr/errorr, JENDL-3.3 ²³⁸U.
 - “ej2”: moder/reconr/broadr/errorr, JENDL-3.3 ²³⁸U.
 - “ej3”: reconr/broadr/groupr/errorr, JENDL-3.3 ^{235,238}U & ²³⁹Pu.
- No changes to existing test jobs are planned while NJOY99 remains active.
- Upgrading to NJOY2008 provides an opportunity to revise the test suite.
 - Suggestions?



NJOY – File Checking

- ENDF Checking Codes are Incomplete.
- Output from One Module may be Physically Unrealistic, but Numerically Acceptable when Passed to another Module.
 - Negative cross sections from UNRESR.
- User Options from One Module may not be Supported by another Module.
 - LEAPR/THERMR with isabt=1.
- What Checking and Warning or Abort Conditions Should be Added to NJOY?



NJOY – other issues?

- ???

- Send email to akahler@lanl.gov.

