Title: NJOY - Where We Are and Directions for Future Work

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Intended for: MCNP/NJOY/ENDF Workshop, 2012-10-30/2012-11-01 (Los Alamos, New Mexico, United States)
NJOY – Where We Are and Directions for Future Work

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presented at the
MCNP/NJOY/ENDF Workshop

held at
Los Alamos National Laboratory
October 30 – November 1, 2012
Abstract

We provide an update on the current status of the NJOY Nuclear Data Processing System and discuss several areas for future development.
NJOY – brief history

- Before we can say where we’re going, let’s remember where we came from …
  - NJOY is a LANL developed code, started in mid-1970s;
  - First release to RSIC (no second “C” yet!) in 1977;
    - See “Methods for Processing ENDF/B-VII with NJOY,” by MacFarlane & Kahler, *Nuclear Data Sheets* 111, 2739 (2010) for details;
    - International distribution coordinated through the OECD Nuclear Energy Agency.
  - Primary developer throughout has been Bob MacFarlane.
NJOY99 – latest updates

Some recent changes …

- NJOY99.364 was released in the Spring, 2011;

- A number of NEA generated updates have been created;
  - Thanks to Andre Trkov for coordinating this work.

- NJOY99.384 will be released this week.
  - See [http://t2.lanl.gov/codes/njoy99](http://t2.lanl.gov/codes/njoy99) for a complete description;
  - Updates include
    - Larger fixed arrays (a never-ending issue with f77 codes);
    - Fix lingering 32-bit/64-bit inconsistencies (will not be an NJOY2012 issue);
    - Recognize the many new reaction MT values defined by CSEWG2010;
      - Was partially implemented in 99.364.
    - New User plotting options in COVR for correlation matrix scaling;
    - Implement the polynomial fission energy release format (mf1/mt458);
NJOY99 to NJOY2012

- **NJOY99.x to NJOY2012**
  - The long overdue release of NJOY2012 is imminent!
  - Preliminary versions have already been released to selected users via NDAs with LANL’s Technology Transfer Division;
    - ANL, AWE, BNL, Bettis, KAPL, ORNL, Sandia.
  - A new, hyperlinked, pdf-formatted manual has been written;
    - Largely done by Bob … but also thanks for Jeremy Conlin, XCP-5, for LaTeX assistance!

- Distribution of NJOY2012 will be handled through LANL’s Technology Transfer Division.
  - Contact Kathleen McDonald, [kathleen_m@lanl.gov](mailto:kathleen_m@lanl.gov), for licensing information … BUT NOT BEFORE 11/30!!!
  - Earlier requests will be held pending completion of internal release paperwork.
NJOY99 to NJOY2012

The new NJOY Nuclear Data Processing System Manual

- Now a pdf file;

- Table of Contents and Index are hyperlinked;

- Chapter headings, Section headings, Figures, Tables, Equations and References are hyperlinked.
NJOY99 to NJOY2012

- NJOY99.x to NJOY2012
  - New capability, which will *NOT* appear in NJOY99.x, includes
    - Process the “Limited Reich-Moore” resolved resonance format;
      - MF2/MT151 LRF=7 (for those who speak ENDFese);
      - Can also calculate elastic scattering angular distributions.
    - No limit on number of temperatures (BROADR, UNRESR, HEATR, GROUPR, PURR);
    - No limit on the number of $\sigma_0$’s (UNRESR, PURR, GROUPR);
    - Revised input for THERMR;
      - See Card 2 description; use of NJOY99 format will abort.
    - Revised input for ERRORR;
      - ERRORR will internally condense any GROUPR file to only contain data for one temperature, one (infinitely dilute) $\sigma_0$, no more than $P_1$ for all mat’s.
      - Makes Card 3 mandatory (to know the User temperature of interest).

No input changes for standard ACE file creation.
NJOY2012 … going forward ...

➢ Future work

➢ ENDF-6 Format → Generalized Nuclear Data (GND) Format;
  ➢ Initial effort led by LLNL (Mattoon/Beck) and BNL (Brown);
  ➢ This work the subject of a new WPEC Sub-Group;
  ➢ NDS article (December 2012) has been accepted for publication.

➢ Revised ACE format;
  ➢ This work led by Jeremy Conlin (LANL, XCP-5);
  ➢ Initial ideas outlined in LA-UR-12-22033 & LA-UR-12-25177;
  ➢ To be further discussed at 2012 CSEWG and Winter ANS meetings.

➢ Covariance data into MCNP;
  ➢ This work led by Brian Kiedrowski (LANL, XCP-3);
  ➢ Initial work discussed earlier in this Workshop;
  ➢ NS&E article (LA-UR-12-22089) has been accepted for publication;
  ➢ Three year funding proposal has been accepted by DOE/NCSP.
NJOY2012 … going forward …

- Generalized Nuclear Data
  - The existing ENDF format has served the nuclear data community well for nearly 50 years!
    - … but it is rooted in a technology that is now obsolete;
    - Data are constrained to an 80 character per record (card image) format;
    - Individual items are constrained to fit into an 11 character format.
      - Too few digits for some “real” numbers; too many digits for integer flags;
      - Shows up in resolved resonance energy grid degeneracies, or in small but negative eigenvalues for truncated covariance matrices.

- The underlying “MF”/”MT” set of identifiers requires that all data must fit into pre-defined slots.
  - Use of a generic reaction type, MT=5, and/or “LR” flags can be awkward and is neither intuitive nor easy to read.
NJOY2012 … going forward …

- Generalized Nuclear Data (con’t)
  - Further details of GND will be presented later this week;
  - Current work is led by LLNL/BNL, but broad participation of the international nuclear data community is expected (and needed!) as the GND Project moves forward;
    - Future work will be performed under the auspices of a WPEC Subgroup.
      - Initial meeting will occur following the Fall JEFF meeting in late November.
  - NJOY will require significant modification of its “ENDF” I/O routines and its data search routines which are currently MF/MT centric;
    - Data in ENDF file 6 requires knowledge of incident and outgoing ZA’s.
      - Coding developed to process these data will be more amenable to a new format that no longer uses MF/MT flags.

LANL/NJOY will be active participants in the development of GND.
NJOY2012 … going forward …

- Revised ACE Format (Conlin)
  - A new format is required to overcome the limitations of the current 10-character ZAID + suffix notation …
  - ZZZAAA.ddx
    - ZZZ = Atomic number; AAA=Atomic mass number; dd=library identifier; x=data class (c=continuous energy; t=thermal; …).

- Define a new, 24-character, variable …
  - SSSZZZAAA.dddxx
    - SSS = excited state (use ENDF “LIS” from mf1/mt451);
    - ZZZ = atomic number (as before);
    - AAA = atomic mass number (as before);
    - ddd = library identifier;
      - Three digits allows for additional data files for a given ZA.
    - xx = data class (use ENDF “NSUB”, “IPART”, “ITYPE”).
      - Defined in the ENDF format manual; but allow NJOY/ACER input to override.
NJOY2012 … going forward …

- Revised ACE Format (con’t)
  - New data in the revised ACE file include
    - New line 1 with ACE format version #, new ZAID+suffix and more;
    - New line 2 with basic nuclear data;
      - Default action is to obtain as much information from the original ENDF-formatted input file as possible;
      - Allow NJOY/ACER input to override;
      - Final ACE file is a text-based file which can be further modified.
  - N comment lines (N may be zero);
    - Similar to User comment lines in RECONR that appear on the PENDF tape.
  - Remainder of ACE file conforms to current format.
    - User *may* have to create a unique ZZZAAA.ccx name.
NJOY2012 … going forward …

- Revised ACE Format (con’t)
  - Revised xsdir info:
    - Item 6 in an xsdir directory entry identifies the line number where the ACE file data for a given material start.
      - For standalone files this is typically 1 (and will remain so for the new format data);
      - For backward compatibility it can be set to (3+N).
        - Allows for use of new ACE file data in old MCNP versions.
  - NJOY2012 and NJOY99 patches implementing these changes will be made available.
Covariance Data for MCNP (Kiedrowski)

- The appearance of nuclear cross section covariance data in evaluated nuclear data files is becoming increasingly common.
  - ENDF/B-III & earlier – no format available;
    - Information may be mentioned in MF1/MT451 comments.
  - ENDF/B-IV (mid-1970s) – 3 files \((\text{natC},^{14}\text{N},^{16}\text{O})\) with limited data;
  - ENDF/B-V (early-1980s) – 24 materials/reactions;
  - ENDF/B-VI (1990s & early 2000s) – 48 materials/reactions;
  - ENDF/B-VII.0 (2006) – 26 materials / 142 reactions;
  - ENDF/B-VII.1 (2011) – 190 of 423 files contain covariance data.
- Said to be “complete” for most materials, meaning that “… the full energy range is covered and that data are provided for essentially all major reaction channels”.

NJOY2012 … going forward …
NJOY2012 … going forward …

- Covariance Data for MCNP (con’t)
  - A method is under development allowing MCNP to compute $k$-eigenvalue sensitivity coefficients with respect to nuclear data;
  - We plan to expand the ACE format to include ENDF covariance data to support this new capability.
  - Coordinated effort involving the MCNP team (XCP-3), the Nuclear Data team (XCP-5) and the NJOY team (T-2);
    - Is a multi-year development project with initial funding provided by the DOE/NCSP;
    - Steps in this process include
      - Develop specifications for a revised ACE file containing ENDF covariance data;
      - Develop coding in NJOY and MCNP to implement these specifications and propagate ENDF covariance data into MCNP;
      - Create new ACE files with covariance data;
      - Iterate as needed.
NJOY … Final Thoughts

- The **NJOY Nuclear Data Processing System** has been the preferred code for creating continuous energy and multi-group application libraries for decades.
  - LANL remains committed to maintaining and extending NJOY’s capabilities.
  - The previous pages illustrate a variety of on-going tasks that demonstrate this commitment.

- NJOY funding comes from the DOE/NCSP and /ASC/PEM/Nuclear Physics Programs.
  - Funding has been stable for many years, and is expected to remain so going forward, 😊.

- Now let’s hear from our European friends …