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Author(s): Kahler, Albert C. III

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NJOY – Where We Are and Directions for Future Work

A. C. (Skip) Kahler
Theoretical Division
Los Alamos National Laboratory

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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, lets 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;
  - Additional releases in 1978, 1983, 1987, 1989, 1991, 1994, 1997 and 1999;
    - 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.
      - See http://www.oecd-nea.org/dbprog/njoy-links.html.
  - NJOY99.384 will be released this week.
    - See 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);
      - …

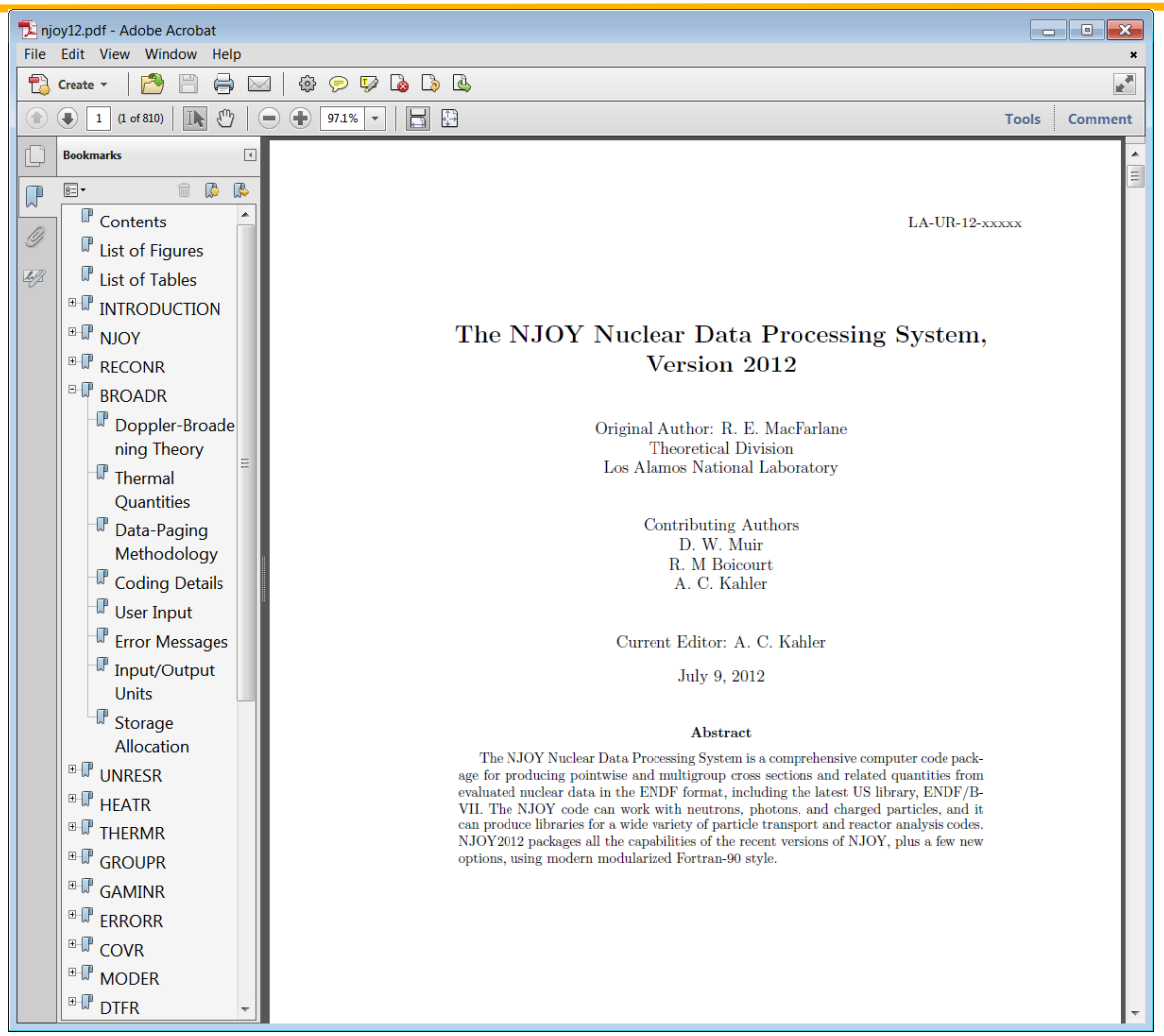
NJOY99 to NJOY2012

- **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, 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 σ_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) σ_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.

NJOY2012 … going forward …

- **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 (^{nat}C,^{14}N,^{16}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 …

- **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 …**