Title: NJOY 99/2001: New Capabilities in Data Processing

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SUMMARY
The NJOY Nuclear Data Processing System is used all over the world to process evaluated nuclear data in the ENDF format into libraries for applications. Over the last few years, a number of new capabilities have been added to the system to provide advanced features for MCNP, MCNPX, and other applications codes. These include probability tables for unresolved range self shielding, capabilities optimized for high-energy libraries (typically to 150 MeV for accelerator applications), options for detailed treatments of incident and outgoing charged particles, and a capability to handle photonuclear reactions. These new features and recent experience using NJOY99 for library production will be discussed, along with possible future work, such as delayed-neutron processing and capabilities to handle the new generation of photo-atomic, electro-atomic, and atomic-relaxation data, and the processing methods must be upgraded appropriately. Finally, increased accuracy requirements and improvements in applications codes (such as the provision of probability tables for self shielding and delayed neutrons for time dependent calculations in MCNP) have led to other needs for improvements in processing methods.

II. NJOY 99
The current version of the NJOY code is NJOY 99.64, which supports a number of new capabilities.

A. Unresolved-Range Probability Tables
Recent versions of the MCNP3 continuous-energy Monte Carlo code support the use of probability tables for handling the effects of self shielding in the unresolved energy range. These tables are generated using the PURR module of NJOY and recast into the ACE format for MCNP using the ACER module. The tables are generated by randomly sampling in a number of different "ladders" of resonances, each of which satisfies the distributions of resonance spacings and widths specified in the ENDF evaluations. The result is a table of the probability of seeing a total cross section in a given cross section range for an event and tables of conditional cross sections for the partial reactions. A special feature of our approach is that it also provides a conditional cross section for estimating the self shielding of nuclear heating. The effects of unresolved self shielding are expected to be of interest for the fast-reactor type cores proposed for the accelerator-driven burning of waste.

B. High-Energy Cross Sections
Accelerator-driven concepts for the transmutation of wastes or production of energy rely on the copious numbers of high-energy neutrons produced by the spallation process. At higher
energies, these neutrons can be transported adequately using intranuclear cascade methods in codes like MCNPX, but at lower energies (say below 150 MeV), nuclear structure effects begin to become important, and better results are obtained using actual evaluated cross sections processed with NJOY. Elastic scattering at these energies is very sharply peaked in the forward direction, and new methods for handling them in MCNP and MCNPX had to be devised (i.e., the cumulative angular distribution). These evaluations depend heavily on the "File 6" representation introduced with the ENDF-6 format. In the 20-150 MeV range, a single inclusive reaction is given that describes the yield and energy-angle distribution for the various reaction products (neutrons, charged particles, photons, and residual nuclei). New methods had to be implemented to handle the wide range of options allowed with File 6, including using systematics to describe angle-energy distributions and the new "Law 61" representation. All these new features in NJOY and the MCNP and MCNPX codes allow for very good results up to 150 MeV, including nuclear heating based on solid predictions of the nuclear reaction paths.

C. Charged-Particle Capabilities
Accelerator-driven concepts use proton beams to drive spallation. Protons are also produced in high-energy nuclear reactions. Thus, it is necessary to develop evaluated data for incident protons and proton production in the 20-150 MeV range and to process these data for codes like MCNPX that can handle them. Proton production from reactions is handled using the "File 6" representation, which provides for full energy-angle correlated distributions for emitted protons. Incident protons also have the complication of charged-particle elastic scattering with its extremely forward-peaked Coulomb component. There is also a complication related to nuclear heating: the proton component that is usually included in tabulated heating values has to be subtracted off of the normal heating value when a coupled neutron-proton transport problem is executed; that energy is deposited directly as the protons are slowed down. NJOY methods have been developed to handle all of these aspects of charged-particle data.

In addition to the high-energy regime, charged-particle reactions are also of interest at low energies for fusion calculations and astrophysics. NJOY now contains capabilities to treat important compound systems like d+D and d+T in full detail, including the complex representation of nuclear + Coulomb interference in the elastic channel.

D. Delayed Neutrons
Recent versions of MCNP contain the ability to work with delayed neutron data given using the classical six time groups, and NJOY has been updated to produce ACE libraries containing these data. For static cases, these data can be used to improve the fission spectrum. This is of interest because the delayed neutrons are emitted with lower energies than the prompt fission neutrons, and the resulting change in shape of the effective fission spectrum can lead to small changes in criticality for some systems. The new data are even more interesting for doing time-dependent calculations.

E. Photoneutron Data
It is now possible to use MCNP to do photoneutron calculations. An IAEA Coordinated Research Project running over the last few years has resulted in the creation of a large number of new photonuclear evaluations in ENDF format (with contributions from LANL in the US, KAERI in Korea, CNDC in China, JENDL in Japan, and the BOFOD collaboration in Russia). NJOY has been upgraded to process these new evaluations and to produce the appropriate MCNP libraries, and 188 of the new evaluations have now been processed successfully. An example of a plot made during processing for MCNP is given in Figure 1. This work provides a new area for nuclear calculations that is currently being explored by several laboratories around the world. Work to implement a multigroup photoneutron capability is in progress.

![Figure 1. Example of photonuclear data.](image-url)
F. Atomic Data
Another area of work in progress relates to atomic data, which are of some interest to the medical community. New highly detailed evaluations of photo-atomic, electro-atomic, and atomic-relaxation data are now available in ENDF format, and NJOY is gradually being updated to take advantage of them. An example of an area where these new data can be effective is the fluorescence treatment in MCNP. It is now quite old and uses a simplified representation of the X-ray emission from atomic transitions resulting from photoionization that was appropriate for the time. The new data will require a new format for the MCNP library and new sampling schemes to follow the X-ray and Auger electron cascades. But with these improvements in place, MCNP will be able to generate highly detailed X-ray and electron spectra from surfaces in addition to being able to track photon transmission and energy deposition. As an interim measure, work is underway to develop and qualify a new photo-atomic library for MCNP that does not require a new version of the code; it will give users access to more accurate cross sections while still providing the older fluorescence representation. Further down the line, additional improvements in NJOY, MCNP, and MCNPX will introduce a more accurate and detailed representation of the additional X-rays and Auger electrons resulting from the ionization produced by electrons.

III. NJOY 2001
The next version of NJOY has the same computational capabilities as NJOY99, but it has been converted to use a modern subset of Fortran-90/95 that should improve portability and maintainability. NJOY2001 makes extensive use of formal modules to package the different NJOY processing modules, to eliminate Fortran COMMON blocks, to provide common physics constants, and to provide libraries of routines used throughout the code. Examples of these libraries include the set of routines used to handle ENDF-type data, the mathematics routines, and the set of routines that NJOY uses to make color Postscript plots of cross sections and distributions. Old problems of precision have been eliminated using the KIND capability. Memory allocation is now done with native Fortran features that replace NJOY's old storage system, thus making for more readable coding. More regions of the code have been converted into block structures, although some statement numbers still remain! A new report is in progress.

IV. CONCLUSIONS
The combination of new evaluated evaluated nuclear data with updated NJOY processing and improved transport methods promises to improve the accuracy of classical nuclear calculations and to extend our ability to do good simulations into a number of new areas.

REFERENCES
2. For current information on the various versions of NJOY, see http://t2.lanl.gov/codes/.
5. See http://t2.lanl.gov/data/photonuclear.html.
6. See the paper in this conference, Dermott E. Cullen and Robert E. MacFarlane, "ENDF/B-VI Coupled Photon-Electron Data for Use in Radiation Shielding Applications."