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Updating the Format of ACE Data Tables

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INTRODUCTION

The ACE data format has been around for several decades. The ACE format is a compact version of the Evaluated Nuclear Data File (ENDF) format [1]. ACE files contain the nuclear data used in MCNP [2] Monte Carlo simulations. The ACE files are generated by the Nuclear Data Team at Los Alamos National Laboratory using NJOY [3] and are distributed with the MCNP5, MCNPX, and MCNP6 codes through RSICC.

MCNP currently ships with *many* tables of data processed from several original sources including ENDF/B-V, ENDF/B-VI, and ENDF/B-VII. Because of the many data tables available and a two-digit limit on the suffix, the available suffixes for new data tables are being depleted.

In this summary, we are announcing a change to the ACE data format for continuous energy neutron files. The motivating factors for making this change are three-fold; 1) expansion of the number of tables available for future data; 2) improvement of ZAIDs for excited state evaluations; and 3) backwards compatibility with existing codes (e.g., MCNP5, MCNPX).

Exhaustion of Available ZAID Suffixes

The current ACE data format allows ten characters for a ZAID and a suffix; six digits indicating the ZAID, plus a two-digit and one-character suffix. The ZAID+suffix looks like

$$\text{ZZZAAA.ddC},\qquad(1)$$

where

ZZZ the atomic number,

AAA the atomic mass,

dd the library identifier,

C class of data.

The ZAID can be constructed using the formula

$$\text{ZAID} = Z * 1000 + A,\qquad(2)$$

with the two-digits in the suffix being chosen as needed. For the case of continuous energy data for a neutron incident on ^{235}U, the ZAID+suffix could be 92235.70c.

The MCNP, NJOY and Nuclear Data teams at LANL would like to continue the practice of providing older nuclear data even when new and improved data are available. While the ACE data format is still valuable, it is beginning to show its age and limitations; in particular we are running out of unused ZAID suffixes.

Excited State ZAIDs

In the ZAID/suffix description in Equation (1) there is nothing which specifies the state (ground or excited) of the ACE data table. Because there is no natural way to include the state in a ZAID, unconventional ZAID naming schemes for excited state evaluations were created for previous releases of ACE data.

The ZAID naming scheme used by Trellue et al. [4], used the traditional ZAID naming scheme (given in Equation (1)) for the ground state evaluations. For the excited state evaluations the excited state was indicated by adding a value to the atomic mass number (AAA) portion of the ZAID. The value added was

$$\text{AAA} = A + 300 + m * 100\qquad(3)$$

where A is the atomic mass number of the isotope and m is the metastable state. For example, the ground state of ^{58}Co was given the ZAID, 27058, while the first excited state evaluation was given the ZAID, 27458. This naming scheme gives a ZAID involving unrealistic atomic mass numbers (AAA) and so the excited state evaluations can be distinguished from the ground state evaluations.

Although a ZAID such as 27458 does work, it is unnatural and may cause confusion. We do not imply that the scheme chosen for this release of data was a poor choice, only that it was the best available option given the current definition of a ZAID and its suffix.

NEW ACE DATA FORMAT

To address the near exhaustion of ZAID suffixes and to provide a natural method of indicating excited state evaluations, the Nuclear Data Team along with the MCNP and NJOY teams from Los Alamos National Laboratory have agreed to a new format for ACE data tables and future releases of nuclear data will use this new format.

Expanded SZA and Suffix

The new SZA (ZAID) and suffix looks like

$$\text{SSSZZZAAA.dddCC},\qquad(4)$$

where

SSS the excited state,

ZZZ the atomic number,

AAA the atomic mass,

ddd the library identifier,

CC class of data.

The new SZA can be constructed using the formula

$$ZAID = S * 1\,000\,000 + Z * 1000 + A, \tag{5}$$

With this formula, the ground state evaluation keeps the traditional ZAID and only the excited state evaluations have a new identifier. Note that since the excited state is now included the name "ZAID" is incomplete; we will refer to the new identifier as the SZA of the data table.

In addition to including the excited state as part of the SZA, multiple characters can now be used to indicate the class of data. For incident neutron, continuous energy data, the characters nc will be used.

Continuing to use ^{58}Co as an example, the new SZA and suffix could be

27058.710nc	ground state
1027058.710nc	excited state

Modified ACE Table Header

In the current ACE format, only 10 characters are allowed for the ZAID. Since the SZA will be longer than 10 characters, a change in the ACE table header was necessary. The current format is described in Appendix F of the MCNP manual [2] and will not be described here. Note that only the header of the ACE table has been modified in the new ACE format, the JXS and XSS arrays remain unchanged.

The new/modified ACE table header looks like

```
FMTVERSION SZAS                    SOURCE
ATWGTR    TEMP  DATE  NCOMMENTS
N lines of comments
```

where

FMTVERSION format version number, 10-character limit, no spaces;

SZAS SZA+suffix, 24-character limit, no spaces;

SOURCE the source of the data, e.g., ENDF/B-VII.1, 24-character limit, no spaces;

ATWGTR atomic weight ratio;

TEMP temperature (in MeV) of processed data;

DATE the date when the data table was created;

NCOMMENTS the number of comment lines.

The above lines and comments replace the first two lines of the current ACE format data. Note that the SZA and suffix (SZAS) as described in Equation (4) only utilizes up to 15 characters

while the SZAS entry in the ACE header allows for 24 characters. There is room to expand the SZAS as needs change, however the SZAS cannot contain any spaces.

In addition to the changes described above, we have begun to utilize elements 9–11 of the NXS array to hold integers representing the excited state (element 9), atomic number (element 10), and atomic mass (element 11). Elements 9–11 are unused in the current ACE format.

Maintaining Backwards Compatibility

We have designed the new ACE header to be able to support backwards compatibility with codes that don't understand the new format; e.g., MCNP5, MCNPX. In the xsdir file, each ZAID listed has a number corresponding to the line number of the file where the data table begins. In the new ACE format, the two header lines of the traditional ACE format can be included in the comment lines; the entry in the xsdir file can point to the comment line as the first line of the ACE data table and the code can read the file as before without any changes.

By including the traditional header files in the comment lines of the new format we can remain backwards compatible with codes that can't parse the new format. This provides code developers some time to implement new ACE data table readers without losing the ability to use the newest ENDF data.

We raise a warning concerning two items which may cause some problems. As mentioned above, elements 9–11 of the NXS array in the ACE data table are unused in the current ACE format. If a particular code has modified those elements and use them for a specific purpose, that code will need to reconsider how to use their custom data.

In previous ACE data releases from Los Alamos National Laboratory, every entry on the xsdir file fit on one line (less than 80 characters). There was no requirement that this be the case, but it was done that way. Future releases of ACE data may include xsdir entries that are longer than 80 characters and therefore must be continued on the next line. Line continuation is part of the xsdir format as described in Appendix F of the MCNP manual. If a code (other than MCNP) utilizes the xsdir file and data files provided with MCNP, the code will need to make sure it can parse xsdir entries that extend to multiple lines.

DOCUMENTATION

Currently, the documentation for the xsdir file and ACE data tables are included in Appendix F of the MCNP manual. This appendix is currently being updated and separated from the MCNP manual so it can be distributed separately. The new ACE format specification will be included as a major part of this updated document.

CONCLUSIONS

A new ACE format has been created which addresses limitations of the old format. The limitations include a near exhaustion of available ZAID suffixes and an unnatural scheme for specifying ZAIDs for evaluations of excited states. The new ACE format remains backwards compatible with existing codes due to the free-format of the comment lines. This summary announces the new ACE format and briefly describes the coming changes. Full documentation will be released as a formal document.

ACKNOWLEDGEMENTS

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