Title: Processing files with NJOY - Reading and manipulating ACE files with ACEtk

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Processing files with NJOY
Reading and manipulating ACE files with ACEtk

W. Haeck

2022 MCNP User Symposium, October 17-21, 2022
Outline

• So you have the evaluated data, now what?
• NJOY processing for MCNP libraries
• Overview of the ACE format and structure
• The ACEtk toolkit
So, you have the evaluated data - now what?

• What we have: evaluated nuclear data libraries
  – Not necessarily in a “simple” format and processing might be needed before use
  – Incident neutron and charged particle data
  – Covariance data
  – Fission yield data, radioactive decay data
  – Photoatomic and photonuclear data
  – Thermal scattering data

• What we need: nuclear data application libraries
  – A subset of the data for the particular application
  – Provides derived data not available in evaluated data:
    ▪ Temperature dependent data
    ▪ Energy deposition data, etc.
So, you have the evaluated data - now what?

• This is where the XCP-5 Nuclear Data Team at LANL comes into play:
  – Produce and maintain nuclear data libraries for LANL simulation codes
  – Verify and validate new data libraries when they become available

• NJOY is the nuclear data processing software developed at Los Alamos
  – Initially developed in the ‘70s as a single package to replace individual programs
  – Originally written in Fortran-77
  – Known as MINX-II prior to a printer malfunction

\[
\begin{align*}
M + 1 &= N \\
I + 1 &= J \\
N + 1 &= O \\
X + 1 &= Y
\end{align*}
\]
Which version of NJOY should you use?

• NJOY has been around for over 40 years now
  – Major versions: NJOY99, NJOY2012, NJOY2016, NJOY21

• NJOY2016 is the production version in use at LANL
  – The MCNP ENDF/B-VIII.0 library was produced using NJOY2016
  – Latest version is NJOY2016.68 (September 2022)

• NJOY21 is in essence a NJOY2016 wrapper
  – It provides additional input verification
  – Latest version is NJOY21 v1.2.2 (January 2021)
  – We advice you to use NJOY2016 instead
NJOY processing for MCNP libraries

• Get it at [https://github.com/njoy/NJOY2016](https://github.com/njoy/NJOY2016)

• Latest version is NJOY2016.68 (September 2022)
  - We aim to release updates every three months – even if the changes are minor
  - This coincides with quarterly reports that we give to our funding sources
NJOY processing for MCNP libraries

• Prerequisites:
  − git
  − cmake 3.15 or higher
  − a Fortran 2003 compliant compiler such as gcc-7 or higher

• Installation instructions:

  ```
  git clone https://github.com/njoy/NJOY2016.git
  cd NJOY2016
  mkdir build
  cd build
  cmake -DCMAKE_BUILD_TYPE=Release ..
  make -j8
  ```
NJOY processing for MCNP libraries

• NJOY provides a set of data processing modules that are called sequentially
  - Different processing paths for different library types and applications
  - Incident neutron, incident charged particles, thermal scattering, photonuclear, etc.
Module example: RECONR

• Reconstruction and linearisation of cross sections
  - Takes the resonances parameters and computes cross sections for total, elastic, fission and capture
  - Takes the other cross sections and linearises them
  - Puts all reactions on the same energy grid

• Important input parameters
  - Fractional reconstruction tolerances
  - Maximum integral error

• Input: reconr
  20 21
  ‘A fancy title for the new tape’
  9228 0 0
  0.001 /
  0
Other notable NJOY modules

- BROADR: temperature dependent cross sections
- GROUPR: multi-group cross sections
- HEATR: calculate KERMA and DPA cross sections
- THERMR: thermal scattering data
- GASPR: charged particle production cross sections
- PURR: unresolved resonance probability tables
- ACER: produce ACE libraries for MCNP
- PLOTR & VIEWR: visualisation of nuclear data

- And many more …
NJOY processing for MCNP libraries

moder
20 -25
reconr
-25 -21
'AM241 - 293.6 K - ENDF/B-VIII.0 (NJOY2016.68)'
9543 0 0
0.001 0 0.01 5e-08
0 /
broadr
-25 -21 -22
9543 1 0 0 0
0.001 1e+06 0.01 5e-08
293.6
0 /
heatr
-25 -22 -21 /
9543 5 0 0 0 0 /
302 318 402 442 444 /
thermr
0 -21 -22 /
0 9543 16 1 1 0 1 221 2 /
293.6
0.001 5.0
gaspr
-25 -22 -21 /

unresr
-25 -21 -22
9543 1 9 1
293.6
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
0 /
purr
-25 -22 -21
9543 1 9 20 64 1 0
293.6
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
0 /
acer
-25 -21 0 40 41
1 0 1 .02 /
'AM241 - 293.6 K - ENDF/B-VIII.0 (NJOY2016.68)'
9543 293.6
1 1 /
acer
0 40 42 40 41
7 1 1 -1 /
'AM241 - 293.6 K - ENDF/B-VIII.0 (NJOY2016.68)'
stop
NJOY output is worth looking at ...

- Something is wrong with this output for elemental sulphur
  - Can you guess what it is?
  - The original evaluation dates back to 1979, as old as I am

<table>
<thead>
<tr>
<th>upper energy</th>
<th>elastic integral</th>
<th>percent error</th>
<th>capture integral</th>
<th>percent error</th>
<th>fission integral</th>
<th>percent error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00E-05</td>
<td>2.26E+00</td>
<td>0.000</td>
<td>3.58E+01</td>
<td>0.000</td>
<td>1.24E-01</td>
<td>0.000</td>
</tr>
<tr>
<td>1.00E-04</td>
<td>2.26E+00</td>
<td>0.000</td>
<td>1.13E+01</td>
<td>0.000</td>
<td>3.92E-02</td>
<td>0.000</td>
</tr>
<tr>
<td>1.00E-03</td>
<td>2.26E+00</td>
<td>0.000</td>
<td>3.58E+00</td>
<td>0.000</td>
<td>1.24E-02</td>
<td>0.000</td>
</tr>
<tr>
<td>1.00E-02</td>
<td>2.26E+00</td>
<td>0.000</td>
<td>1.13E+00</td>
<td>0.000</td>
<td>3.92E-03</td>
<td>0.000</td>
</tr>
<tr>
<td>...</td>
<td>1.10E+00</td>
<td>0.003</td>
<td>1.53E-03</td>
<td>0.038</td>
<td>2.01E-03</td>
<td>1.743</td>
</tr>
<tr>
<td>1.00E+05</td>
<td>5.86E+00</td>
<td>0.001</td>
<td>2.04E-03</td>
<td>0.247</td>
<td>1.30E-03</td>
<td>1.077</td>
</tr>
<tr>
<td>5.00E+05</td>
<td>2.48E+00</td>
<td>0.010</td>
<td>1.22E-03</td>
<td>0.866</td>
<td>6.59E-04</td>
<td>1.765</td>
</tr>
<tr>
<td>1.00E+06</td>
<td>1.52E+00</td>
<td>0.018</td>
<td>5.29E-04</td>
<td>1.057</td>
<td>2.69E-05</td>
<td>2.025</td>
</tr>
</tbody>
</table>
Overview of the ACE format and structure

• The nuclear data application library files for MCNP are referred to as ACE files
  – Each ACE file contains one or more ACE tables
  – Specifications: https://github.com/NuclearData/ACEFormat

• There are multiple ACE table types:
  – Incident neutron and charged particle ACE tables
  – Photonuclear ACE tables
  – Thermal scattering ACE tables
  – Photoatomic ACE tables
  – Dosimetry ACE tables
  – Multigroup ACE tables

• Each ACE table type has its own structure but some pieces are shared
Overview of the ACE format and structure

- Each ACE table has 5 basic components: a header and 4 arrays

<table>
<thead>
<tr>
<th>header</th>
<th>izaw array</th>
<th>nxs array</th>
<th>jxs array</th>
<th>xss array</th>
</tr>
</thead>
<tbody>
<tr>
<td>92235.00c 233.024800 2.5301E-08 05/01/18</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 92 235 0 0 0 0 0</td>
<td>1 380136 380483 380574 380665 380756 380847 4018427</td>
</tr>
<tr>
<td>U235 Lib80x (jlconlin) Reference LA-UR-18-24034 by Conlin, J.L., et al. mat9228</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>1 4018472 4157159 4157203 5083731 5159758 5160341 5160924 5166428</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
</tr>
<tr>
<td></td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
</tr>
<tr>
<td></td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
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<tr>
<td></td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>5167011 5167011 5167011 5167594 4018472 4157159 4157203 5083731</td>
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</tr>
<tr>
<td></td>
<td>0 0. 0 0. 0. 0 0 0</td>
<td>0 0. 0 0. 0. 0 0 0</td>
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</tr>
</tbody>
</table>
Overview of the ACE format and structure

• The header information (multiple header types are available)
  - The most important information: the ZAID, the atomic weight ratio and the temperature
• The izaw array: 16 pairs of ZA and atomic weight ratio values
  - Essentially only used in thermal scattering files
• The nxs array: 16 integers with table related information
  - Things like number of reactions, number of secondary particle types, etc. go here
• The jxs array: 32 integers that function as locators to specific ACE blocks
  - Locators are always 1-based indices into the xss array
• The xss array: a single array of real values containing blocks of data

• The interpretation of the nxs, jxs and xss array differs by ACE table type
Overview of the ACE format and structure

- The $\textit{xss}$ array is a flat array of real values interpreted through locators
  - The $\textit{jxs}$ array contains the locators for an ACE table’s main data blocks
  - The $\textit{xss}$ array can contain locators to secondary data blocks
  - All locators are 1-based absolute or relative indices because Fortran
  - Locators only point to the beginning of a data block (there can be “gaps”)

```
LOC(1)  LOC(2)  LOC(3)  LOC(4)  LOC(5)  LOC(6)  ...
...
...
XSS(LOC(1))  ...
...
...
XSS(LOC(2))  ...
...
...
XSS(LOC(3))  ...
...```
Overview of the ACE format and structure

• Let’s take a look at the incident neutron and charged particle ACE tables

• The $x_{SS}$ array can be subdivided into 3 main pieces
  - Primary particle data
    ▪ Everything MCNP needs to transport the primary particle
    ▪ Additional data such as heating data
  - Distribution data for outgoing photons
    ▪ Only used when transporting photons
  - Distribution data for other secondary particle types
    ▪ Only used when transporting those particle types
Overview of the ACE format and structure

<table>
<thead>
<tr>
<th>Data for the primary particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Principal cross section block (ESZ)</td>
</tr>
<tr>
<td>Optional fission multiplicity block (NU)</td>
</tr>
<tr>
<td>Reaction number block (MTR)</td>
</tr>
<tr>
<td>Reaction Q-value block (LQR)</td>
</tr>
<tr>
<td>Frame and multiplicity block (TYR)</td>
</tr>
<tr>
<td>Cross section block (LSIG and SIG)</td>
</tr>
<tr>
<td>Angular distribution block (LAND and AND)</td>
</tr>
<tr>
<td>Energy distribution block (LDLW and DLW)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional data for outgoing photons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional unresolved ptable block (UNR)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional data for other secondary particle types</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional delayed neutron data blocks (DNU, BDD and DEND)</td>
</tr>
</tbody>
</table>

These last 2 blocks often appear after the photon data
Overview of the ACE format and structure

- Principal cross section block (ESZ)
- Optional fission multiplicity block (NU)
- Reaction number block (MTR)
- Reaction Q-value block (LQR)
- Frame and multiplicity block (TYR)
- Cross section block (LSIG and SIG)
- Angular distribution block (LAND and AND)
- Energy distribution block (LDLW and DLW)
- Optional unresolved ptable block (UNR)
- Optional delayed neutron data blocks (DNU, BDD and DEND)

These last 2 blocks often appear after the photon data

- Common energy grid
- Total cross section values
- Elastic cross section values
- Disappearance cross section values
- Heating numbers

Each one of these arrays have the same size, as given by NES = NXS(3)
Overview of the ACE format and structure

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These last 2 blocks often appear after the photon data

<table>
<thead>
<tr>
<th>Reaction (MT) numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q-values</td>
</tr>
<tr>
<td>Frame and multiplicity values</td>
</tr>
</tbody>
</table>

Each one of these arrays have the same size, as given by NTR = NXS(4)

This one is a great example of how not to do things:
- Sign indicates LAB or CM reference frame
- Absolute value indicates integer multiplicity if the value is less than 100 or not equal to 19
- An absolute value of 19 means fission
- An absolute value above 100 indicates an energy dependent multiplicity (located in the DLW block)
Overview of the ACE format and structure

- Principal cross section block (ESZ)
- Optional fission multiplicity block (NU)
- Reaction number block (MTR)
- Reaction Q-value block (LQR)
- Frame and multiplicity block (TYR)
- Cross section block (LSIG and SIG)
- Angular distribution block (LAND and AND)
- Energy distribution block (LDLW and DLW)
- Optional unresolved ptable block (UNR)
- Optional delayed neutron data blocks (DNU, BDD and DEND)

Locators for each reaction
Common energy grid index
Number of cross section values
Cross section values

These last 3 blocks are repeated for each reaction in MTR

These last 2 blocks often appear after the photon data
### Overview of the ACE format and structure

- **Principal cross section block (ESZ)**
- **Optional fission multiplicity block (NU)**
- **Reaction number block (MTR)**
- **Reaction Q-value block (LQR)**
- **Frame and multiplicity block (TYR)**
- **Cross section block (LSIG and SIG)**
- **Angular distribution block (LAND and AND)**
- **Energy distribution block (LDLW and DLW)**
- **Optional unresolved ptable block (UNR)**
- **Optional delayed neutron data blocks (DNU, BDD and DEND)**

**Locators for each reaction**

**Locators indicate types of angular distribution data**
- Locator = -1: energy-angle data given in DLW
- Locator = 0: fully isotropic data
- Any other positive value is a tabulated angular distribution

**Angular distribution data for each reaction that gives a locator value different from -1 or 0**

**Elastic scattering is always the first reaction given**

These last 2 blocks often appear after the photon data
### Overview of the ACE format and structure

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<tbody>
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<td>Optional delayed neutron data blocks (DNU, BDD and DEND)</td>
</tr>
</tbody>
</table>

These last 2 blocks often appear after the photon data
Overview of the ACE format and structure

Data for the primary particle

- Photon production block (GPD)
- Photon production reaction number block (MTRP)
- Photon production cross section block (LSIGP and SIGP)
- Photon angular distribution block (LANDP and ANDP)
- Photon energy distribution block (LDLWP and DLWP)
- Photon multiplicity reaction number block (YP)

Optional data for outgoing photons

Optional data for other secondary particle types
Overview of the ACE format and structure

- Secondary particle information block (PTYPE)
- Secondary particle locator block (IXS)
- Secondary particle production block (HPD)
- Secondary particle reaction number block (MTRH)
- Secondary particle frame block (TYRH)
- Secondary particle cross section block (LSIGH and SIGH)
- Secondary particle distribution block (LANDP and ANDP)
- Secondary particle energy distribution block (LDLWH and DLWH)
- Secondary particle multiplicity reaction number block (YH)

Data for the primary particle

Optional data for outgoing photons

Optional data for other secondary particle types

These last 7 blocks are repeated for each secondary particle type in PTYPE.
Overview of the ACE format and structure

• And this is only the top of the iceberg

• The ACE format has certain idiosyncrasies
  - Locator logic is not consistent
  - Storing multiple pieces of data in a single field (e.g. TYR)
  - Subtle differences depending on where a block appears (e.g. SIG, SIGP, SIGH)
  - And many more …

• Solution: do not interact with the ACE file directly, use an interface instead
  - ACEtk: this interface abstracts away some of the ACE idiosyncrasies
The ACEtk toolkit

- **ACEtk**: [https://github.com/njoy/ACEtk](https://github.com/njoy/ACEtk)
  - A format component developed in the NJOY modernisation project
  - Reading, writing and manipulate ACE files
  - Using a C++ and Python API at the same time

- ACEtk support for the following ACE file types:
  - Incident neutron and charged particle ACE files
  - Photoatomic and photonuclear ACE files
  - Thermal scattering ACE files
The ACEtk toolkit

• Prerequisites:
  − git
  − cmake 3.15 or higher
  − a C++-17 compliant compiler such as gcc-7 or higher
  − Python 3.5 or higher

• Installation instructions:
  
git clone https://github.com/njoy/ACEtk
cd ACEtk
git checkout feature/table-ctor
mkdir build
cd build
cmake -DCMAKE_BUILD_TYPE=Release ../
make ACEtk.python -j8