How to read ACE file

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ACE file (A Compact ENDF)

- Cross section (XS) library for continuous Monte Carlo calculation codes
  - Ex) MCNP, PHITS, OpenMC and Serpent.
- It is difficult to read comparing to ENDF file.

Overview of ACE file
(Opening)

General information
(NXS array)

Data position
(JXS array)

Energy grids and
XS data
(ESZ block)

92235.50c 233.025000 2.5507e-08 20171005
U-235 from JENDL-4

mat9228

0   0      0   0     0   0      0         0
0   0      0    0     0          0      0         0
0   0  0    0     0          0      0        0
0   0  0    0  0          0      0         0
2023448    92235   164057   47    45     45   0       6
1   820286   820377   820424   820471   820518   820565  1306929
1306975  1513550  1513595  1703760  1867817  1867862  1867907  1868801
1868846  1868846  1868891  2023403   820675  2023448  1689111  1692747
1692768  1692834  1692840        0  0  0  0    0

1.00000000000e-11   1.00000100000e-11   1.00012300000e-11   1.00024500000e-11
1.00036700000e-11   1.00048900000e-11   1.00061100000e-11   1.00073300000e-11
1.00085500000e-11   1.00097800000e-11   1.00110000000e-11   1.00122200000e-11
Format Manual of ACE file

- Two types of ACE format manual are prepared.
  - (1) MCNP manual, Volume III: Developer’s Guide
    - [https://github.com/NuclearData/ACEFormat](https://github.com/NuclearData/ACEFormat)
    - [https://github.com/NuclearData/ACEFormat/blob/master/ACEFormat.pdf](https://github.com/NuclearData/ACEFormat/blob/master/ACEFormat.pdf)
  - (1) is only available for US users.
  - Current version of (2) is only for continuous neutron and thermal scattering law (TSL) data
    - (2) is not complete.
Note on reading ACE file

- Unit of energy is MeV (1.0E6 eV).
  - Evaluated nuclear data file uses eV.
- It is difficult to find the end of each data.
  - Four data is set in each line.

Transport code uses data position list to find desired data.

Example of data array of ACE:

<table>
<thead>
<tr>
<th>Energy grids [MeV]</th>
<th>Total XS [barn]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.70000000000e+01</td>
<td>1.17726171500e+03</td>
</tr>
<tr>
<td>1.90000000000e+01</td>
<td>1.85000000000e+01</td>
</tr>
<tr>
<td>1.15929185200e+03</td>
<td>1.10995080730e+03</td>
</tr>
</tbody>
</table>

Example of data position list:

<table>
<thead>
<tr>
<th>-1</th>
<th>-1</th>
<th>-1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>76</td>
<td>111</td>
</tr>
<tr>
<td>164170</td>
<td>164179</td>
<td>237838</td>
<td>238294</td>
</tr>
<tr>
<td>238687</td>
<td>239073</td>
<td>239424</td>
<td>239763</td>
</tr>
<tr>
<td>240088</td>
<td>240405</td>
<td>240716</td>
<td>241026</td>
</tr>
</tbody>
</table>

First data: 1-75
Second data: 76-110
Third data: 111-164169
Forth data: 164170-164179
How to access desired data?

- General information is set in head of ACE file (NXS array).
  - Number of energies, number of reactions, …
- First data position list (JXS block) shows location of each data block.
  - ESZ block: energy grids, total XS, …
  - NU block: number of neutron per fission
- Data position lists are also prepared in each data block.
  - Transport code accesses desired data using general information and data position lists.

Location of NU block is XXXX.

Location of SIG block is YYYY.
Read ACE file (Header region)

- **NXS array** contains general information of ACE file.
  - NXS array is located lines 7-8.
- **JXS array** contains data position to access each data.
  - JXS array is located lines 9-12.
  - Containing data in NXS and JXS arrays are written in ACE format manual.
    - ACE format manual must be required to read ACE file.
Introduction of new header format (2.0.X)

- Official ACE file of ENDF/B-VII.1 and B-VIII.0 uses new header format.
  - [https://nucleardata.lanl.gov/ACE/index.html](https://nucleardata.lanl.gov/ACE/index.html)
- Comment line of old header format is only one.
- New header format allows multiline for comment line.

[Example of new header format]

<table>
<thead>
<tr>
<th>Version number of header format</th>
<th>Number of comment line</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0.0 92235.710nc ENDFB-VII.1</td>
<td>3</td>
</tr>
<tr>
<td>233.024800 2.5301E-08 12/19/12</td>
<td></td>
</tr>
</tbody>
</table>

The next two lines are the first two lines of 'old-style' ACE.

```
92235.80c  233.024800  2.5301E-08   12/19/12   3
U235 ENDF71x (jiconlin) Ref. see jiconlin (ref 09/10/2012  10:00:53)   mat9228
```

Old header format (Written as comment lines)

Comment lines
Read ACE file (ESZ block)

- ESZ Block is the first block of ACE file.
  - ESZ block contains energy grids, several XS data, and heating number.
    - Total, disappearance, and elastic scattering XS
    - Total neutron disappearance XS (MT=101) is sum of XSs of MT=102-117, 155, 182, 191-193, and 193.
  - Number of energy $N_E$ is found in NXS array of header.

<table>
<thead>
<tr>
<th>Location in XSS</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_{ESZ}$</td>
<td>$E(l), l = 1, \ldots, N_E$</td>
<td>Energies</td>
</tr>
<tr>
<td>$S_{ESZ} + N_E$</td>
<td>$\sigma_t(l), l = 1, \ldots, N_E$</td>
<td>Total cross section (MT=1)</td>
</tr>
<tr>
<td>$S_{ESZ} + 2N_E$</td>
<td>$\sigma_a(l), l = 1, \ldots, N_E$</td>
<td>Total neutron disappearance cross section† (MT=101)</td>
</tr>
<tr>
<td>$S_{ESZ} + 3N_E$</td>
<td>$\sigma_{el}(l), l = 1, \ldots, N_E$</td>
<td>Elastic cross section (MT=2)</td>
</tr>
<tr>
<td>$S_{ESZ} + 4N_E$</td>
<td>$H_{ave}(l), l = 1, \ldots, N_E$</td>
<td>Average Heating numbers</td>
</tr>
</tbody>
</table>

† The disappearance cross section is defined in [2, Appendix B] as MT101

Read ACE file (SIG block 1/2)

- SIG block contains XS of other reactions.
  - Without total, disappearance, and elastic scattering XSs
- LXS is 6th data of JXS array in header region.
- $LOCA_1 \sim LOCA_{NMT}$ indicate data position.
  - These location data are found in LSIG block (one block before SIG block).
  - $LOCA_N$ shows location from head of SIG block.

<table>
<thead>
<tr>
<th>Location in XSS</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LXS+LOCA$_1$-1</td>
<td>Cross section array for reaction $MT_1$</td>
</tr>
<tr>
<td>LXS+LOCA$_2$-1</td>
<td>Cross section array for reaction $MT_2$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>LXS+LOCA$_{NMT}$-1</td>
<td>Cross section array for reaction $MT_{NMT}$</td>
</tr>
</tbody>
</table>

Read ACE file (SIG block 2/2)

- Each reaction data contains three data
  - $I_E_i$: Energy grid point of the first XS data
  - $N_{E,i}$: Number of XS data
  - $\sigma_i[E(l)]$: XS data
- ACE file uses unique energy grid point shown in ESZ block.
  - Threshold reaction does not need all energy grid data.
  - $I_E_i$ and $N_{E,i}$ are important to reduce data size.

<table>
<thead>
<tr>
<th>Location in XSS</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LXS + LOCA$_{i-1}$</td>
<td>$I_E_i$</td>
<td>Energy grid index for reaction $MT_i$</td>
</tr>
<tr>
<td>LXS + LOCA$_i$</td>
<td>$N_{E,i}$</td>
<td>Number of consecutive entries for $MT_i$</td>
</tr>
<tr>
<td>LXS + LOCA$_{i+1}$</td>
<td>$\sigma_i[E(l)]$ for $l = I_E_i, \ldots, I_E_i + N_{E,i} - 1$</td>
<td>Cross section for reaction $MT_i$</td>
</tr>
</tbody>
</table>

Table 15: Cross section array for the $i$-th reaction.

Edit ACE file using FRENODY module (1/2)

- FRENODY prepares read/write classes.
  - "frendy/ContinuousEnergyXSUtils/AceDataParser"
  - "frendy/ContinuousEnergyXSUtils/AceDataWriter"
  - AceDataWriter class automatically modifies data position (location).
  - User does not need to consider modification of data position.

- AceDataObject handles all data in ACE file.
  - frendy/ContinuousEnergyXSUtils/AceDataObject
  - A corresponding table between data name of AceDataObject and that of ACE format manual has not been prepar…
  - Source file of AceDataParser class will helpful to understand what data is read in each block.
Edit ACE file using FRENDY modules (2/2)

- ACE file perturbation tool will be a good sample to develop ACE file editing tool.
  - tools/perturbation_ace_file/PerturbMain.cpp
  - frendy/ContinuousEnergyXSUtils/PerturbUtils

- Procedure of editing ACE file using FRENDY modules
  - Read ACE file using AceDataParser module
    - All data in ACE file is copy to AceDataObject
  - Modify AceDataObject
    - XS, number of neutrons per fission, energy and angular distribution, …
  - Write ACE file using AceDataWriter module