

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)

mat9228

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

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	0
0	0	0	0	0	0	0	0
1	820286	820377	820424	820471	820518	82056	82056
1306975	1513550	1513595	1703760	1867817	1867862	1867907	1868801
1868846	1868846	1868891	2023403	820675	2023448	1689	1689
1692768	1692834	1692840	0	0	0	0	0
1.000000000000e-11	1.000001000000e-11	1.000123000000e-11					
1.000367000000e-11	1.000489000000e-11	1.000611000000e-11					
1.000855000000e-11	1.000978000000e-11	1.001100000000e-11					1.001222000000e-11

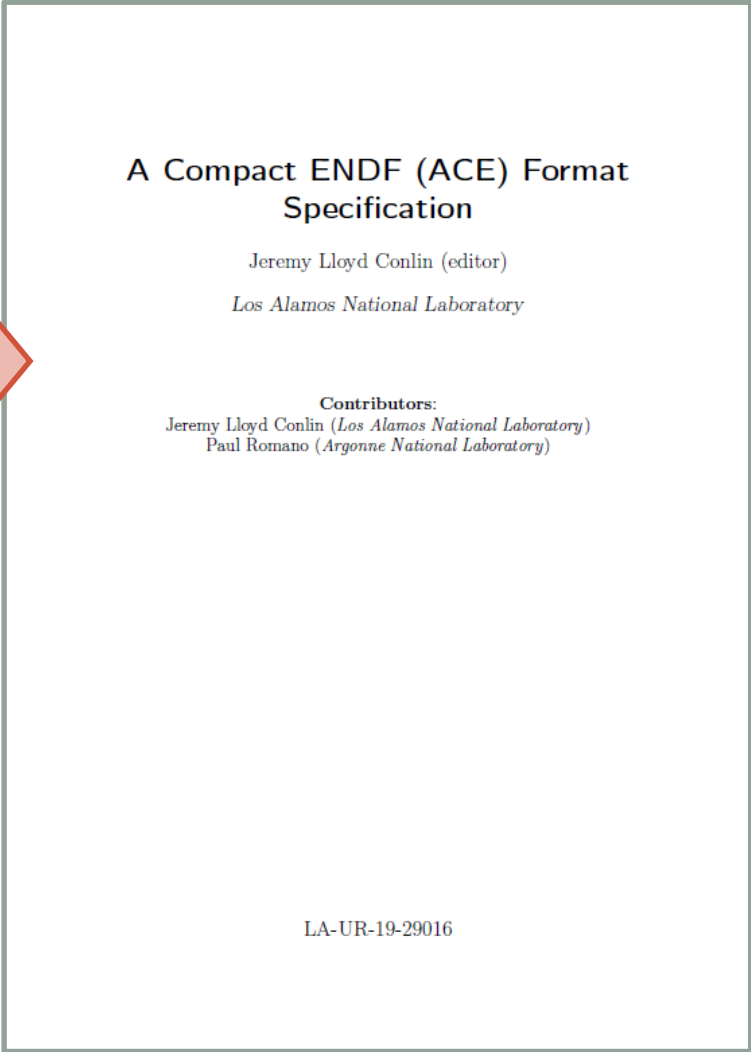
General information (NXS array)

Data position (JXS array)

Energy grids and XS data (ESZ block)

Format Manual of ACE file

- Two types of ACE format manual are prepared.
 - (1) MCNP manual, Volume III: Developer's Guide
 - (2) A Compact ENDF (ACE) Format Specification, LA-UR-19-29016
 - <https://github.com/NuclearData/ACEFormat>
 - <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.

[Example of data array of ACE]

Energy grids [MeV]

Total XS [barn]

1.7000000000e+01	1.7500000000e+01	1.8000000000e+01	1.8500000000e+01
1.9000000000e+01	1.9500000000e+01	2.0000000000e+01	1.17726171500e+03
1.15929185200e+03	1.14212078270e+03	1.12569106010e+03	1.10995080730e+03

- Transport code uses data position list to find desired data.

[Example of data position list]

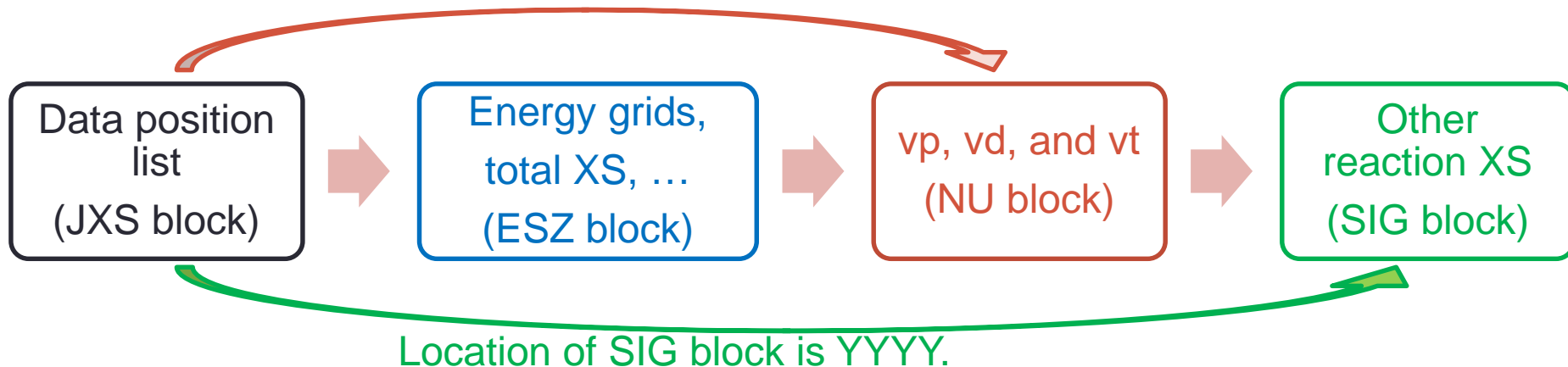
-1	-1	-1	0
0	1	76	111
164170	164179	237838	238294
238687	239073	239424	239763
240088	240405	240716	241026

First data: 1-75
 Second data: 76-110
 Third data: 111-164169
 Forth data: 164170-164179

How to access desired data?

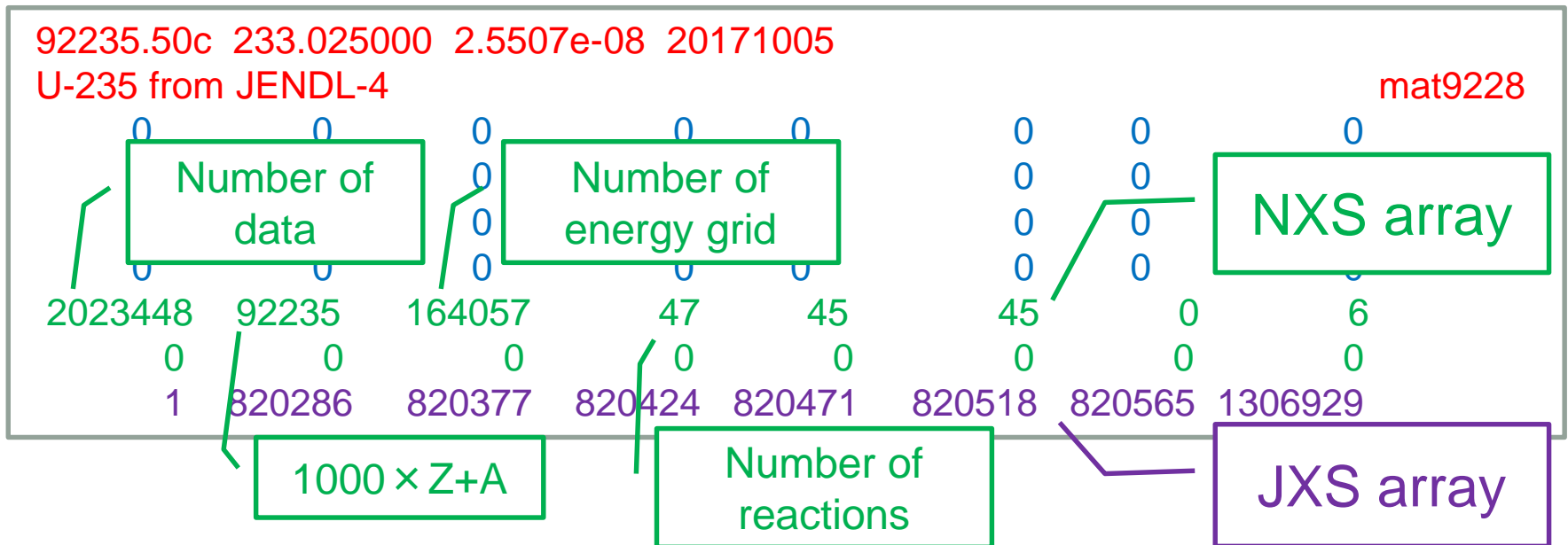
- General information is set in head of ACE file (NXS array).
 - Number of energies, number of reactions, ...
- First data position list (JXS block) shows location of each data block.
 - ESZ block: energy grids, total XS, ...
 - NU block: number of neutron per fission
- Data position lists are also prepared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

Location of NU block is XXXX.



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>
- Comment line of old header format is only one.
 - New header format allows multiline for comment line.

[Example of new header format]

The diagram illustrates the new header format with the following components:

- Version number of header format:** 2.0.0
- Number of comment line:** 3
- Old header format (Written as comment lines):**

```

92235.710nc 233.024800 2.5301E-08 12/19/12 ENDFB-VII.1
92235.80c 233.024800 2.5301E-08 12/19/12
U235 ENDF71x (jlconlin) Ref. see jlconlin (ref 09/10/2012 10:00:53) mat9228
                
```
- Comment lines:** The three lines of the old header format are grouped as 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 5: ESZ Block.

Location in XSS	Parameter	Description
S_{ESZ}	$E(l), l = 1, \dots, N_E$	Energies
$S_{ESZ} + N_E$	$\sigma_t(l), l = 1, \dots, N_E$	Total cross section (MT=1)
$S_{ESZ} + 2N_E$	$\sigma_a(l), l = 1, \dots, N_E$	Total neutron disappearance cross section [†] (MT=101)
$S_{ESZ} + 3N_E$	$\sigma_{el}(l), l = 1, \dots, N_E$	Elastic cross section (MT=2)
$S_{ESZ} + 4N_E$	$H_{ave}(l), l = 1, \dots, N_E$	Average Heating numbers

[†] 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 14: SIG Block.

Location in XSS	Description
$LXS+LOCA_1-1$	Cross section array for reaction MT_1
$LXS+LOCA_2-1$	Cross section array for reaction MT_2
...	
$LXS+LOCA_{NMT}-1$	Cross section array for reaction MT_{NMT}

Read ACE file (SIG block 2/2)

- Each reaction data contains three data
 - IE_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.
 - IE_i and $N_{E,i}$ are important to reduce data size.

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

Location in XSS	Parameter	Description
LXS + LOCA _{i} -1	IE_i	Energy grid index for reaction MT _{i}
LXS + LOCA _{i}	$N_{E,i}$	Number of consecutive entries for MT _{i}
LXS + LOCA _{i} +1	$\sigma_i[E(l)]$ for $l = IE_i, \dots, IE_i + N_{E,i} - 1$	Cross section for reaction MT _{i}

Edit ACE file using FRENDY module (1/2)

- FRENDY 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