

How to read and modify XSDIR file

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Contents

- Overview of XSDIR file
- Data in XSDIR file
- Modification of XSDIR file when user add new ACE file
- Automated XSDIR generation tool

What is XSDIR file?

- XSDIR: Information list of ACE files
 - XSDIR contains information, *e.g.*, nuclide/material ID, path of ACE file, and numbers of data, to handle ACE file.
- Nuclear calculation codes, *e.g.*, MCNP and PHITS, required nuclide ID and material ID for their input files.
 - For example, 1001.50c for H-001, 92235.10c for U-235, and lwtr.10t for HinH2O.

Example of XSDIR

Ratio of mass of material to that of neutron (AWR)

atomic weight ratios

0001	1.000000	0001	1.000000		
1000	0.99931697	1001	0.99916733	1002	1.99679968
2000	3.96821760	2003	2.99012018	2004	3.96821897
3000	6.88131188	3004	3.99259010	3005	4.96947769
		3006	5.96345000	3007	6.95573370

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directory

ACE file directory path information

1001.80c	0.999167	j40/H001.ace	0	1	4	17969	0	0	2.5301E-8	
2003.80c	2.989032	j40/He003.ace	0	1	4	10004	0	0	2.5301E-8	
92235.80c	233.0248	j40/U235.ace	0	1	4	837481	0	0	2.5301E-8	ptable
92235.70c	233.0248	j40f01j	0	1	1238702	832644	0	0	2.5301E-08	ptable
92235.71c	233.0248	j40f01j	0	1	1446875	689688	0	0	5.1704E-08	ptable
lwtr.20t	0.999167	j40tsl/lwtr.20t	0	1	1	1228849	0	0	2.530E-08	
lwtr.21t	0.999167	j40tsl/lwtr.21t	0	1	1	1201502	0	0	3.016E-08	
lwtr.22t	0.999167	j40tsl/lwtr.22t	0	1	1	1165553	0	0	3.447E-08	



nuclide/material ID, .suffix number, ACE data class, AWR, File name and path, 0, 1, Data position (Start data position/Total data number), 0, 0, Temperature [MeV], Use probability table

Features of XSDIR

- XSDIR contains several temperature data and several library data with one file.
 - Transport codes distinguish these different data by suffix number.
 - Available suffix number: .00~.99
 - The last character of nuclide/material name means ACE data class.
 - c: continuous-energy neutron data, t: thermal scattering law data

HinH2O U-235	{	92235.80c 233.0248 j40/U235.ace 0 1 1 837481 0 0 2.5301E-8 ptable
		92235.70c 233.0248 j40f01j 0 1 1238702 832644 0 0 2.5301E-08 ptable
		92235.71c 233.0248 j40f01j 0 1 1446875 689688 0 0 5.1704E-08 ptable
	{	lwtr.20t 0.999167 j40tsl/lwtr.20t 0 1 1 1228849 0 0 2.530E-08
		lwtr.21t 0.999167 j40tsl/lwtr.21t 0 1 1 1201502 0 0 3.016E-08
		lwtr.22t 0.999167 j40tsl/lwtr.22t 0 1 1 1165553 0 0 3.447E-08

ACE data class list

ZAIID suffix	ACE Data Class
c	continuous-energy neutron data
t	thermal $S(\alpha, \beta)$ data
y	dosimetry data
p	photo-atomic data
u	Photonuclear data
h	continuous-energy proton data
o	continuous-energy deuteron data
r	continuous-energy triton data
s	continuous-energy ^3He data
a	continuous-energy alpha data

Notes on Nuclide/Material name (1/2)

- Suffix number **must be different** if user adds other ACE file to a XSDIR file.
 - Suffix number depends on ACE file generator.
 - Transport code user has to read the ACE file manual and check the suffix number.

Transport code reads first 92235.80c data if identical suffix number is found.

```

92235.80c 233.0248 j40/U235.ace 0 1 1 837481 0 0 2.5301E-8 ptable
92235.80c 233.0248 j40f01j 0 1 1238702 832644 0 0 2.5301E-08 ptable
92235.80c 233.0248 j40f01j 0 1 1446875 689688 0 0 5.1704E-08 ptable
    
```

Transport code cannot read these ACE files

Notes on Nuclide/Material name (2/2)

- Transport codes do not need suffix number in their input file.
 - With suffix number: 92235.80c, lwtr.20t, ...
 - Transport code checks suffix number in XSDIR file and **reads corresponding nuclide/material data.**
 - Without suffix number: 92235, lwtr, ...
 - Transport code does not check suffix number and **read first nuclide/material data.**
 - User has to check whether this nuclide/material data is chosen temperature and evaluated data library or not.

Transport code reads 92235.80c if user sets 92235 (without suffix number).

92235.80c	233.0248	j40/U235.ace	0	1	1	837481	0	0	2.5301E-8	ptable
92235.70c	233.0248	j40f01j	0	1	1238702	832644	0	0	2.5301E-08	ptable
92235.71c	233.0248	j40f01j	0	1	1446875	689688	0	0	5.1704E-08	ptable

How to modify nuclide/material name?

- Transport code users sometimes wants to modify **material name** and **suffix number**.
 - **Suffix number** is overlapped.
 - **Material name** of transport code is different to that of ACE file.
- User only modifies XSDIR file and first line of ACE file
 - **Number of characters in each data must not be changed.**
 - User has to add blank character if number of characters is changed.
 - “HinH2O.20t” -> “lwtr.20t ” (Add two blank characters)

```
92235.71c 233.0248 j40f01j 0 1 1446875 689688 0 0 5.1704E-08 ptable
lwtr.20t 0.999167 j40tsl/lwtr.20t 0 1 1 1228849 0 0 2.530E-08
```

```
92235.71c 233.024800 5.1704e-08 20171005
U235 from JENDL-4 mat9228
0 0 0 0 0 0 0 0
```

```
lwtr.20t 0.999167 2.5300e-08 20161017
01_h_in_h2o from JENDL-4 mat 125
1001 0 0 0 0 0 0 0
```

XSDIR file

1st-3rd lines of ACE files



Data in XSDIR file

- XSDIR has two data region, *i.e.*, “atomic weight ratios” and “directory”.
- Atomic weight ratios (AWR)
 - List of ratio of mass of material to that of neutron
 - LANL provides atomic weight ratios list
 - <https://nucleardata.lanl.gov/ACE/install.html#AWR>
 - Released XSDIR files are also useful to make AWR list.
- Directory
 - ACE file directory path information
 - Nuclide/material name, file path, ...

nuclide/material ID, .suffix number, ACE data class, AWR, File name and path, 0, 1, Data position (Start data position/Total data number), 0, 0, Temperature [MeV], Use probability table

ACE file directory path information

- ACE file directory path information consists of 11 data.
 - (1) Nuclide/material name (Maximum: 10 characters)
 - (2) Atomic weight ratio (AWR)
 - (3) File name (Maximum: 60 characters)
 - (4) Directory path (Maximum: 70 characters)
 - (5) ACE file mode (1: ASCII, 2: binary)
 - (6) Start line number of ACE file
 - (7) Total data number of ACE file
 - (8), (9) Used for binary mode
 - (10) Temperature [MeV]
 - (11) Whether probability table is contained or not.

```
92235.70c 233.0248 j40f01j 0 1 1238702 832644 0 0 2.5301E-08 ptable
```

- (1), (2), and (5)-(11) are output in a XSDIR file which is generated with ACE file generation.
 - Data that need to be modified: (1), (3), and (4).

Notes on XSDIR modification

- Maximum number of characters per line: **80**
 - Please add “+” at the end of line and write next line if number of characters is larger than 80.
 - Number of characters per line including “+” must be less than 80.



```
92235.80c 233.0248 j40/rev1/U235.ace 0 1 1 837481 0 0 2.5301E-8 +
ptable
```

- Relative path from XSDIR file is **directory path/file name**”
- “**File name**” is only available when directory path is “**0**”
 - “**j40/rev1/U235.ace**” is relative path from XSDIR file.

Addition of ACE file information

- Nuclear data processing code automatically generates XSDIR file when user generates ACE file.
 - “ace_dif_file_name” for FRENDY (default is “~.ace.dir”)
 - “tapeXX” for NJOY (set in ndir in ACER card 1)
- User has to add the data of generated XSDIR to combined XSDIR file.
 - Combined XSDIR file: Used for transport calculations
 - Suffix number **must not be overlapped**.
 - Material name, e.g., lwtr, **must be identical to input file** of transport code.
 - Modify **filename** and **route**
 - **Number of characters per line must be less than 80.**
 - Add “+” at the end of line and write next line if number of characters is larger than 80.

[Examples of automatically generated XSDIR file using FRENDY and NJOY]

```
92235.80c 233.048 filename route 1 1 837481 0 0 2.585E-8 ptable
lwtr.20t 0.999167 filename route 1 1 2431237 0 0 2.585E-8
```

Example of addition of ACE file information

[Examples of automatically generated XSDIR file using FRENDY and NJOY]

```

92235.80c 233.048 filename route 1 1 837481 0 0 2.585E-8 ptable
lwtr.20t 0.999167 filename route 1 1 2431237 0 0 2.585E-8

```



[Example of addition of ACE file information]

```

92235.80c/23 1 0 0 2.5301E-8 ptable
92235.70c/23 0 0 2.5301E-08 ptable
92235.71c 235.0246 j40tsl 0 1 1446875 069000 0 0 5.1704E-08 ptable
92235.60c 233.048 mod/u235.ace 0 1 1 837481 0 0 2.585E-8 +
ptable
lwtr.20t 0.999167 j40tsl/lwtr.20t 0 1 1 1201502 0 0 3.016E-08
lwtr.21t 0.999167 j40tsl/lwtr.21t 0 1 1 1201502 0 0 3.016E-08
lwtr.22t 0.999167 j40tsl/lwtr.22t 0 1 1 1165553 0 0 3.447E-08
lwtr.60t 0.999167 mod/hinh2o.ace 0 1 1 2431237 0 0 2.585E-8

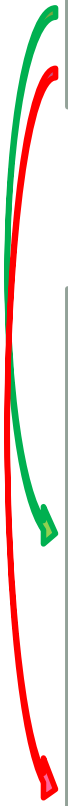
```

1) Modify suffix number of XSDIR and ACE files

2) Modify ACE file name

4) Add "+" at the end of line and write next line if number of characters is larger than 80.

3) Modify directory path from "route" to "0"



Automated XSDIR generation tool

- FRENDY prepares the tool to generate XSDIR file.
 - This tool automatically collect ACE files and modify XSDIR file.
 - **tools/make_xmdir_list**

[Example of generated XSDIR file]

Modified by tool

1001.50c	0.999167	j40/j40f00fa	0	1	1	9751	0	0	2.551e-08
2004.50c	3.968200	j40/j40f00fa	0	1	76161	25308	0	0	2.551e-08
3007.50c	6.955730	j40/j40f00fa	0	1	89852	29277	0	0	2.551e-08

- Input of collection tools (See tools/README_tools)

- **Type of ACE data file**
 - 1: neutron, 2: Thermal scattering law (TSL) data, 3: dosimetry data
- **Modified ACE file name**
- **New XSDIR file name**
- **ACE file directory name that user wants to collect ACE files.**
- **Suffix number**
- **Processing mode (option)**

[Example of neutron induced data]

[Example of TSL data]

1
 ./j40f00f
 ./j40f00f.xsdir
 ./ace/j40
 50c
 individual

2
 ./j40f00t
 ./j40f00t.xsdir
 ./ace/j40/sab
 20t
 individual

Improvement of XSDIR generation tool (1/2)

- XSDIR generation tool is improved in FRENDY Ver.2.
- The old version combined multiple ACE files in to one.
 - The new version can generate XSDIR file without combination of ACE files.

ACE file name is identical to nuclear ID

93235.54c	233.025000	93235.54c	0	1	404551	0	0	2.530e-08	
93236.54c	234.019000	93236.54c	0	1	424289	0	0	2.530e-08	ptable
93237.54c	235.012000	93237.54c	0	1	2905366	0	0	2.530e-08	ptable
93238.54c	236.006000	93238.54c	0	1	618924	0	0	2.530e-08	ptable
93239.54c	236.999000	93239.54c	0	1	467635	0	0	2.530e-08	
94236.54c	234.018000	94236.54c	0	1	312598	0	0	2.530e-08	ptable
94237.54c	235.012000	94237.54c	0	1	461379	0	0	2.530e-08	
94238.54c	236.005000	94238.54c	0	1	1968755	0	0	2.530e-08	ptable
94239.54c	236.999000	94239.54c	0	1	3271302	0	0	2.530e-08	ptable
94240.54c	237.992000	94240.54c	0	1	2575179	0	0	2.530e-08	ptable
94241.54c	238.986000	94241.54c	0	1	2096884	0	0	2.530e-08	ptable
94242.54c	239.979000	94242.54c	0	1	2033244	0	0	2.530e-08	ptable
94244.54c	241.967000	94244.54c	0	1	355532	0	0	2.530e-08	ptable
94246.54c	243.956000	94246.54c	0	1	305188	0	0	2.530e-08	
94247.54c	244.951700	94247.54c	0	1	4955626	0	0	2.530e-08	

Improvement of XSDIR generation tool (2/2)

- Automatically generation of atomic weight ratios (AWR) data at the top of the XSDIR file.
 - AWR values of natural materials e.g., 1000 and 2000, are obtained from XSDIR of ENDF/B-VIII.0.
 - Number of significant digits of this tool is smaller than that of ENDF/B-VIII.0. (12 -> 9)

AWR in ACE file

```
atomic weight ratios
0001 1.00000000 0001 1.00000000
1000 0.99928126 1001 0.99916700 1002 1.99700000 1003 2.98959600
2000 3.96821753 2003 2.99012000 2004 3.96820000
3000 6.88137314 3006 5.96345000 3007 6.95573000
4000 8.93476259 4007 6.95665000 4009 8.93476000 4010 9.92751400
5000 10.71812779 5010 9.92692000 5011 10.91470000
6000 11.90752173 6011 10.91684000 6012 11.89691000 6013 12.89165000
6014 13.88295000
```

Date is also automatically output.

```
100252 249.91700000 100253 250.91110000 100255 252.89900000 100257 254.88650000
06/Dec/2021
directory
1001.54c 0.999167 1001.54c 0 1 1 17714 0 0 2.530e-08
```