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

Author(s): Haeck, Wim

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Processing files with NJOY
Reading and manipulating ACE files with ACEtk

W. Haeck

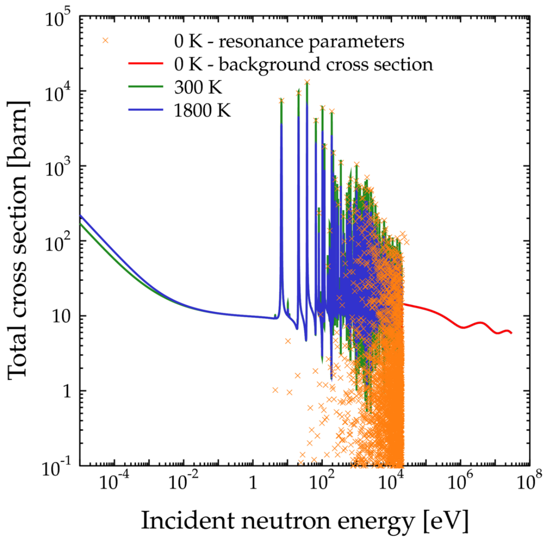
2022 MCNP User Symposium, October 17-21, 2022

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

```
M + 1 = N
I + 1 = J
N + 1 = O
X + 1 = Y
```

Which version of NJOY should you use?

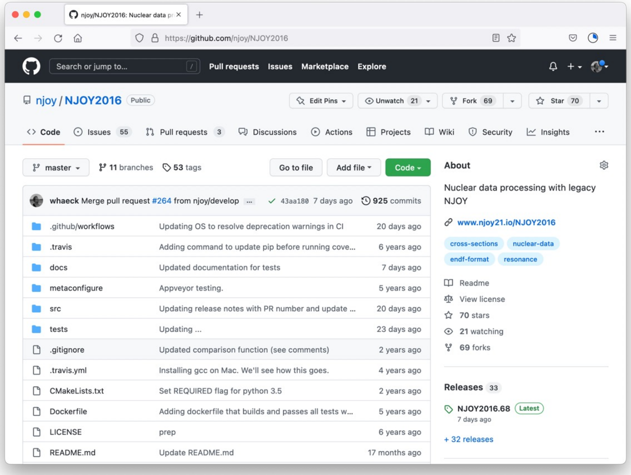
- NJOY has been around for over 40 years now
  - Major versions: NJOY99, NJOY2012, NJOY2016, NJOY21

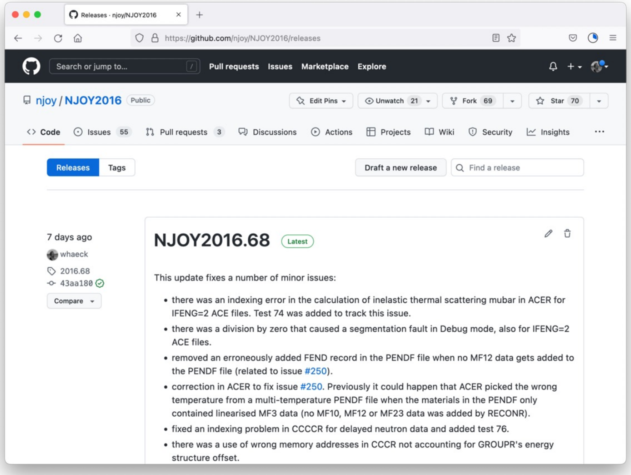
- NJOY2016 is the production version in use at LANL
  - The MCNP ENDF/B-VIII.0 library was produced using NJOY2016
  - Latest version is NJOY2016.68 (September 2022)

- NJOY21 is in essence a NJOY2016 wrapper
  - It provides additional input verification
  - Latest version is NJOY21 v1.2.2 (January 2021)
  - <u>We advice you to use NJOY2016 instead</u>

NJOY processing for MCNP libraries

- Get it at 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

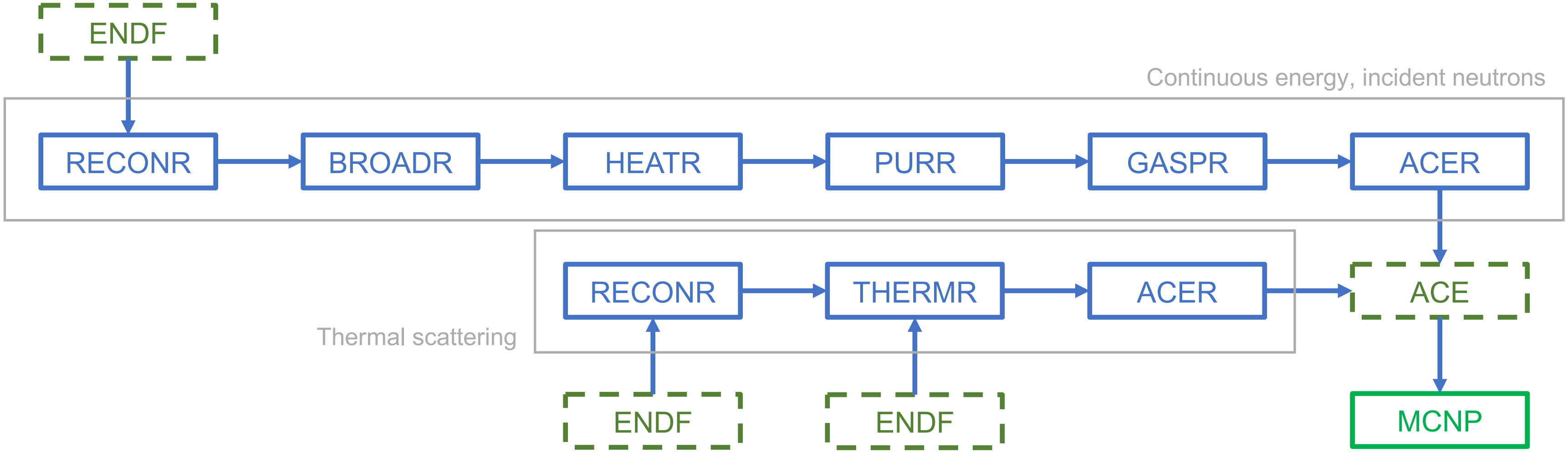
- Prerequisites:
  - git
  - cmake 3.15 or higher
  - a Fortran 2003 compliant compiler such as gcc-7 or higher

- 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

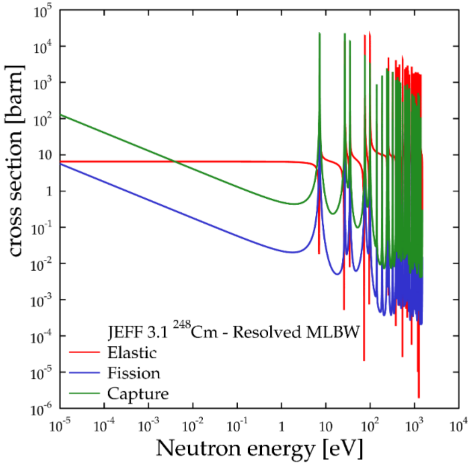
- NJOY provides a set of data processing modules that are called sequentially
  - Different processing paths for different library types and applications
  - Incident neutron, incident charged particles, thermal scattering, photonuclear, etc.

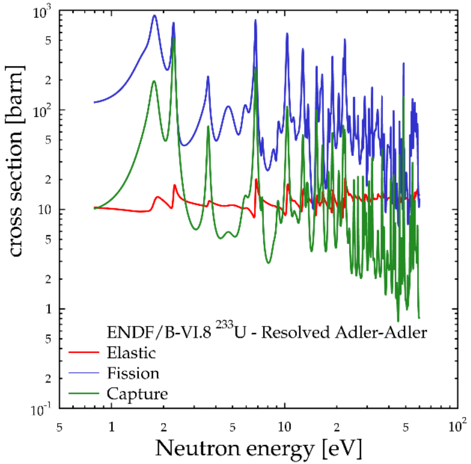


Module example: RECONR

- 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
```

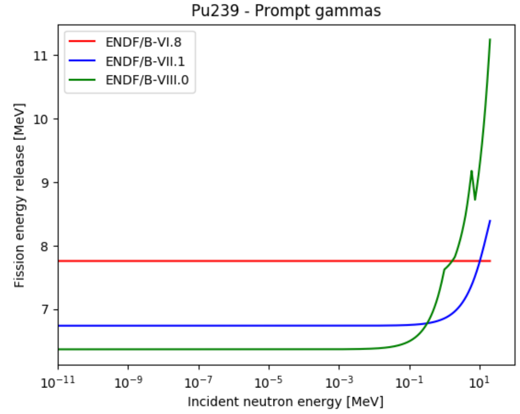


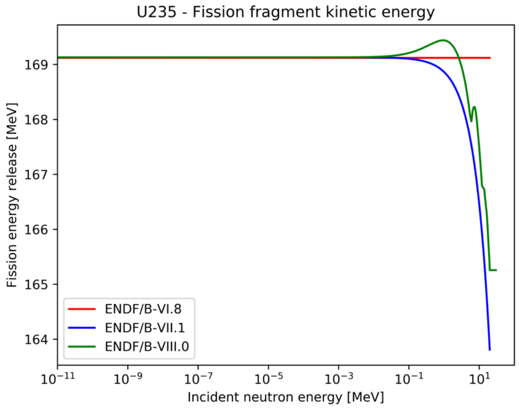


Other notable NJOY modules

- 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

```
estimated maximum error due to
resonance integral check (errmax,errint)
```

upper energy	elastic integral	percent error	capture integral	percent error	fission integral	percent error
1.00E-05						
1.00E-04	2.26E+00	0.000	3.58E+01	0.000	1.24E-01	0.000
1.00E-03	2.26E+00	0.000	1.13E+01	0.000	3.92E-02	0.000
1.00E-02	2.26E+00	0.000	3.58E+00	0.000	1.24E-02	0.000
1.00E-01	2.26E+00	0.000	1.13E+00	0.000	3.92E-03	0.000
...						
1.00E+05	1.10E+00	0.003	1.53E-03	0.038	2.01E-03	1.743
2.00E+05	5.86E+00	0.001	2.04E-03	0.247	1.30E-03	1.077
5.00E+05	2.48E+00	0.010	1.22E-03	0.866	6.59E-04	1.765
1.00E+06	1.52E+00	0.018	5.29E-04	1.057	2.69E-05	2.025

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


A Compact ENDF (ACE) Format Specification

Jeremy Lloyd Conlin (editor)

Los Alamos National Laboratory

Contributors:
Jeremy Lloyd Conlin (*Los Alamos National Laboratory*)
Wim Haeck (*Los Alamos National Laboratory*)
Paul Romano (*Argonne National Laboratory*)

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- 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

header

```
92235.00c  233.024800  2.5301E-08   05/01/18
U235 Lib80x (jlconlin)  Reference LA-UR-18-24034 by Conlin, J.L., et al. mat9228
```

`izaw` array

```
          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.
```

`nxs` array

```
    7168374      92235      76027         91         44        583          5          6
          0         92        235          0          0          0          0          0
```

`jxs` array

```
          1     380136     380483     380574     380665     380756     380847    4018427
    4018472    4157159    4157203    5083731    5159758    5160341    5160924    5166428
    5167011    5167011    5167594    5351569     456964    5351650    5070901    5072750
    5072763    5072805    5072811          0          0    5351651    5351656    5351661
```

`xss` array

```
 1.00000000000E-11   1.03125000000E-11   1.06250000000E-11   1.09375000000E-11
 1.12500000000E-11   1.15625000000E-11   1.18750000000E-11   1.21875000000E-11
 1.25000000000E-11   1.28125000000E-11   1.31250000000E-11   1.34375000000E-11
 ...
```

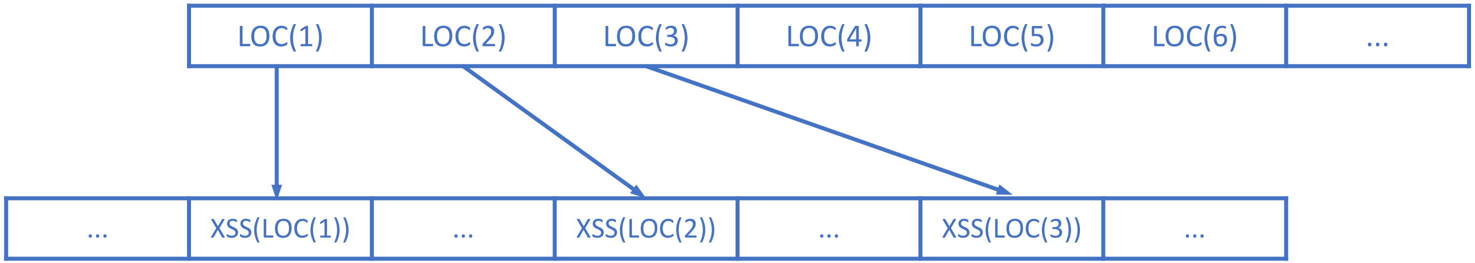
Overview of the ACE format and structure

- 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 <u>always 1-based</u> 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

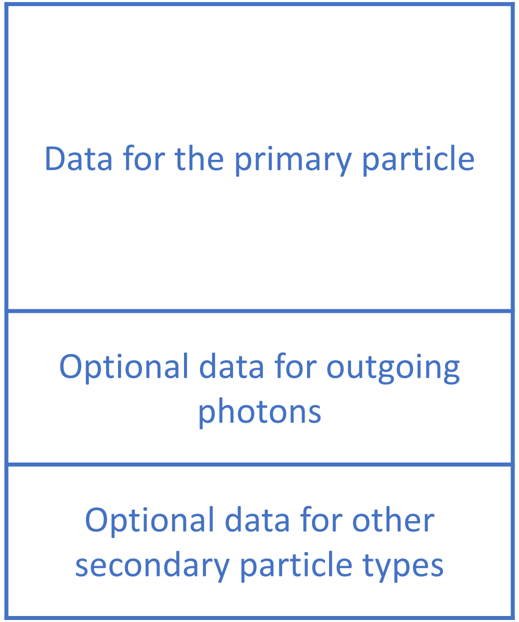
- The `xss` array is a flat array of real values interpreted through locators
  - The `jxs` array contains the locators for an ACE table's main data blocks
  - The `xss` array can contain locators to secondary data blocks
  - All locators are 1-based absolute or relative indices because Fortran
  - Locators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



Overview of the ACE format and structure

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

- The `xss` 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

- 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

- Data for the primary particle
- Optional data for outgoing photons
- Optional data for other secondary particle types

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)
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- Optional unresolved ptable block (UNR)
- Optional delayed neutron data blocks (DNU, BDD and DEND)

These last 2 blocks often appear after the photon data

Principal cross section block (ESZ):

- 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

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

Reaction (MT) numbers
Q-values
Frame and multiplicity values

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)

These last 2 blocks often appear after the photon data

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

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

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

Locators for each reaction

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

Elastic scattering is always the first reaction given

Overview of the ACE format and structure

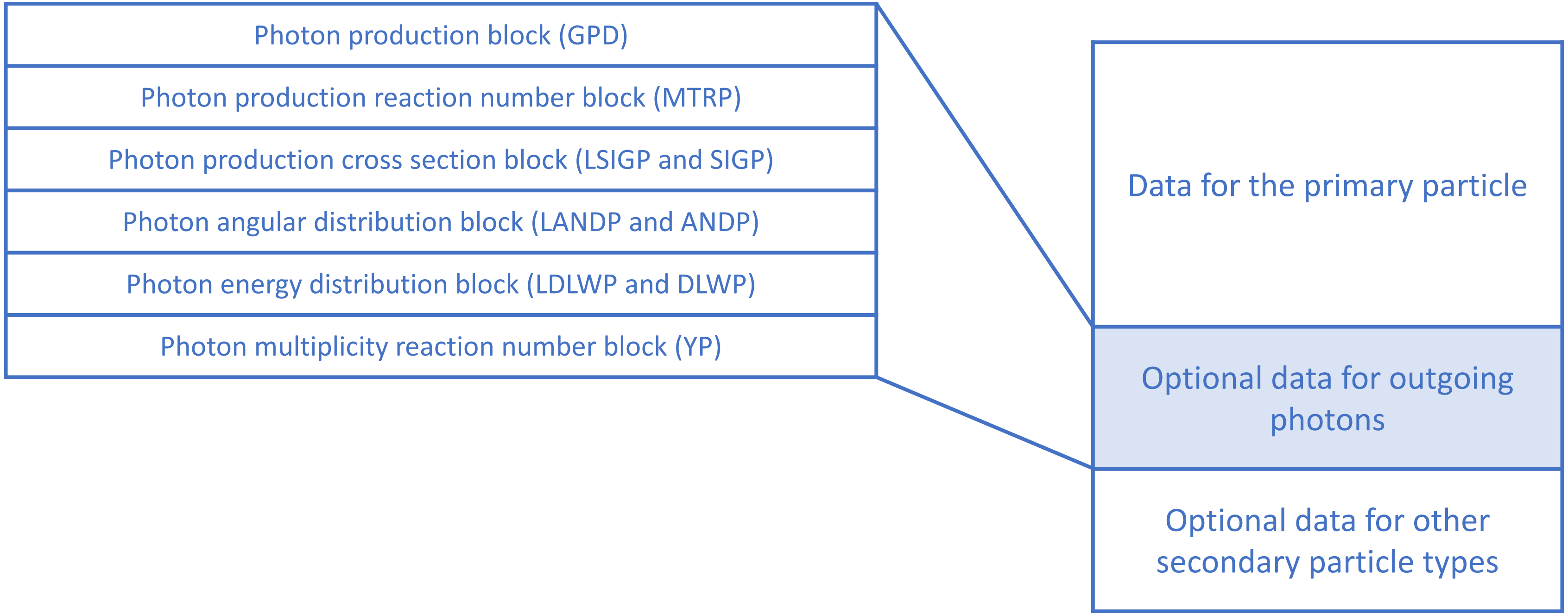
- Principal cross section block (ESZ)
- Optional fission multiplicity block (NU)
- Reaction number block (MTR)
- Reaction Q-value block (LQR)
- Frame and multiplicity block (TYR)
- Cross section block (LSIG and SIG)
- Angular distribution block (LAND and AND)
- Energy distribution block (LDLW and DLW)

- Optional unresolved ptable block (UNR)
- Optional delayed neutron data blocks (DNU, BDD and DEND)

These last 2 blocks often appear after the photon data

- Data for the primary particle
- Optional data for outgoing photons
- Optional data for other secondary particle types

Overview of the ACE format and structure



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)

These last 7 blocks are repeated for each secondary particle type in PTYPE

- Data for the primary particle
- Optional data for outgoing photons
- Optional data for other secondary particle types

Overview of the ACE format and structure

- And this is only the top of the iceberg

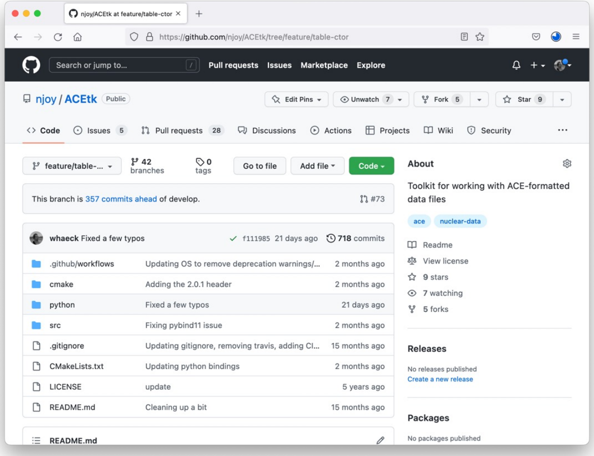
- The ACE format has certain idiosyncrasies
  - Locator logic is not consistent
  - Storing multiple pieces of data in a single field (e.g. TYR)
  - Subtle differences depending on where a block appears (e.g. SIG, SIGP, SIGH)
  - And many more …

- 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
  - 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
```