

# Tools and data management in the FENDL project

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CM on Further Development of FENDL

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### **Outline**

- Data management at the isotope level
- Data management at the library level
- Proof-of-concept user interaction

Data management at isotope level

## Some types of tasks at the isotope level

#### **Checking**

- Is the file in the library indeed numerically equivalent to the version in the indicated source library?
- How is an updated file different from a previous version?
- Does the file conform to the ENDF-6 format specification?

#### **Maintenance**

- Updating meta information in the ENDF header (MF1/MT451)
- Cleaning up (removing evaluator auxiliary info not part of ENDF-6 standard)

#### In the future (potentially):

- Consistently merge IRDFF-II and other useful data into transport files
- Remove bumps at transition energy from explicit to lumped representation (i.e. MT5)
- Upgrading files with covariance matrix information

### **ENDF-6** file interaction

Several publicly available packages and databases for reading and interpreting nuclear data in ENDF-6 format, e.g.\*

- IAEA NDS web interface (https://nds.iaea.org/exfor/endf.htm)
- ENDFtk (https://github.com/njoy/ENDFtk)
- Endf-python (https://github.com/paulromano/endf-python)
- ENDFtables (https://www-nds.iaea.org/talys/)
- PyNE (http://pyne.io/)
  - → Data consumers are well served

### **ENDF-6** file interaction

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- PyNE (http://pyne.io/)
  - → Data consumers are well served

**But what about data producers?** 

### **ENDF-6** file creation/updating

**SANDY** (https://github.com/luca-fiorito-11/sandy)

Contains functions to update an important subset of the information stored in an ENDF-6 formatted file

**ENDFtk** (https://github.com/njoy/ENDFtk)

Core functionality to write ENDF-6 files probably there but it's not obvious to me from the GitHub website how to use it in Python

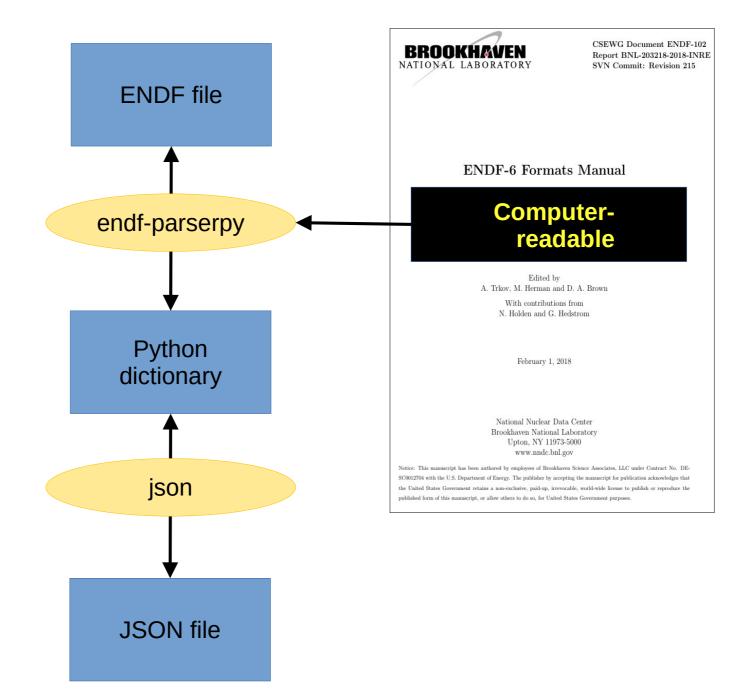
**FUDGE** (https://github.com/LLNL/fudge)

- Translate ENDF-6 file to GNDS format (e.g. in xml format)
- Manipulate the xml file using Python or similar
- Translate the xml file to ENDF-6 format

### endf-parserpy

- Python package developed\* at the IAEA to read and write ENDF-6 formatted files
- Implements the full\*\* ENDF-6 format specification given in the ENDF-6 formats manual (as released in 2018)
- Verified on all major libraries for incident neutrons (other library types presumably also should work)
- At present, only low-level functionality (i.e. no R-matrix reconstruction, self-shielding, covariance matrix reconstruction)
- Implementation approach is unique, greatly reducing the probability for bugs in the package
- Hosted at https://github.com/iaea-nds/endf-parserpy

### **Basic design**



## **Using ENDF-6 recipe files**

endf-

parserpy

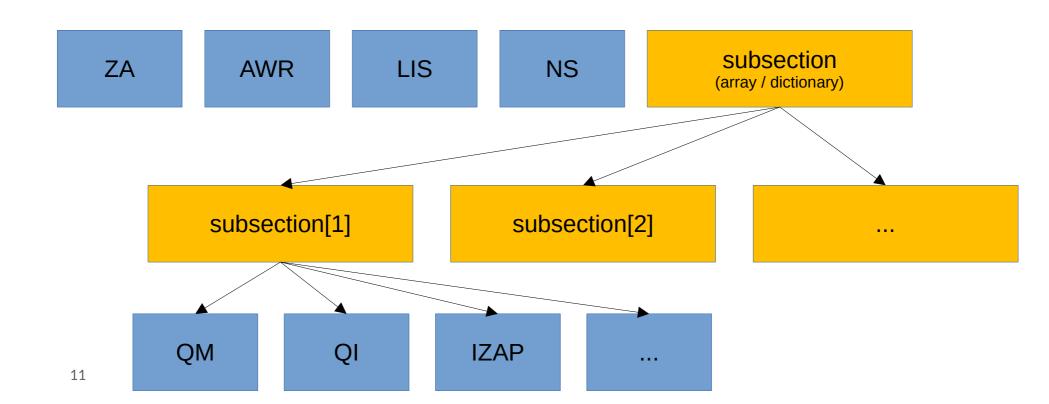
```
[MAT, 1,451/ ZA, AWR, LRP, LFI, NLIB, NMOD]HEAD
[MAT, 1,451/ ELIS, STA, LIS, LISO, 0, NFOR]CONT
[MAT, 1,451/ AWI, EMAX, LREL, 0, NSUB, NVER]CONT
[MAT, 1,451/ TEMP, 0.0, LDRV, 0, NWD, NXC]CONT
for i=1 to NWD:
    [MAT, 1,451/ DESCRIPTION[i]]TEXT
endfor
```



2.906300+4 6.238900+2	l 1	0	0	52925	1451
0.000000+0 0.000000+0	0	0	0	62925	1451
1.000000+0 1.500000+8	8	0	10	72925	1451
0.000000+0 0.000000+0	0	0	481	1152925	1451
29-Cu- 63 LANL,ORNL	EVAL-FEB98 A.Koni	ng , M . Chad	wick,Hetrick	2925	1451
CH98,CH99	DIST-DEC06 REV4-		20011	.108 2925	1451
ENDF/B-VII	MATERIAL 2925	REVI	SION 4	2925	1451
INCIDENT NEUTRON	DATA			2925	1451
ENDF-6 FORMAT				2925	1451

### **Hierarchical representation**

```
[MAT, 10, MT/ ZA, AWR, LIS, 0, NS, 0]HEAD
for k=1 to NS:
(subsection[k])
    [MAT, 10, MT/ QM, QI, IZAP, LFS, NR, NP/ E / sigma ]TAB1
(/subsection[k])
endfor
SEND
```



# Detailed debug output on failure (here: inconsistent variable assignment)

```
Failed: BasicEndfParser failed on file 18-Ar-40g.endf with exception
Here is the parser record log until failure:

------ Line 0 ------

Template: [ MAT , 4 , MT / ZA AWR , 0 , LTT , 0 , 0 ] HEAD
Line: " 1.804000+ 3.961910+1 0 1 0 01837 4 2 1"

------ Line 1 ------

Template: [ MAT , 4 , MT / 0 0 , AWR , LI , LCT , 0 , 0 ] CONT
Line: " 0.000000+ 3.965640+1 0 2 0 01837 4 2 2"

Error message: Expected 39.6191 in the ENDF file but got 39.6564. The value was encountered
```

### 4.2.1 Legendre Polynomial Coefficients (LTT=1, LI=0)

When LTT=1 (angular distributions given in terms of Legendre polynomial coefficients), the structure of the section is:

```
[MAT, 4, MT/ ZA, AWR, 0, LTT, 0, 0] HEAD (LTT=1) [MAT, 4, MT/ 0.0, AWR, LI, LCT, 0, 0] CONT (LI=0) [MAT, 4, MT/ 0.0, 0.0, 0, 0, NR, NE/ E_{int}] TAB2 [MAT, 4, MT/ T, E_1, LT, 0, NL, 0/ a_l(E_1)] LIST [MAT, 4, MT/ T, E_2, LT, 0, NL, 0/ a_l(E_2)] LIST
```

Take a New Screensho

## **Example of use:**Changing (n,tot) cross section

from endf\_parserpy import ExtEndfParser

parser = ExtEndfParser()
endf\_dict = parser.parsefile("input.endf")

parser.writefile("output.endf", endf\_dict)

## **Example of use:**Changing (n,tot) cross section

```
parser = ExtEndfParser()
endf_dict = parser.parsefile("input.endf")

updated_energies = np.linspace(1e6, 1e8, 100)

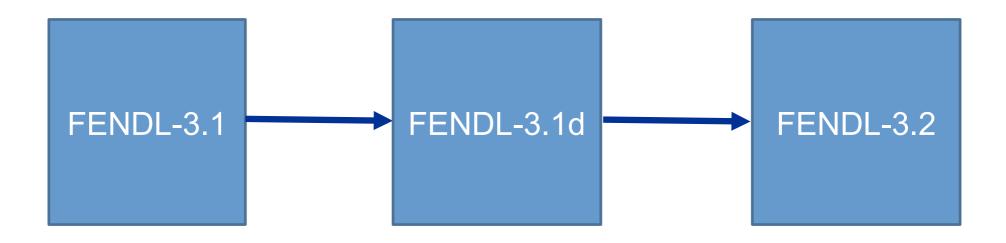
endf_dict[3][1]['xstable']['E'] = updated_energies
endf_dict[3][1]['xstable']['xs'] = np.sin(updated_energies) + 2

endf_dict[3][1]['xstable']['NBT'] = [len(updated_energies)]
endf_dict[3][1]['xstable']['INT'] = [2]

parser.writefile("output.endf", endf_dict)
```

## Data management at library level

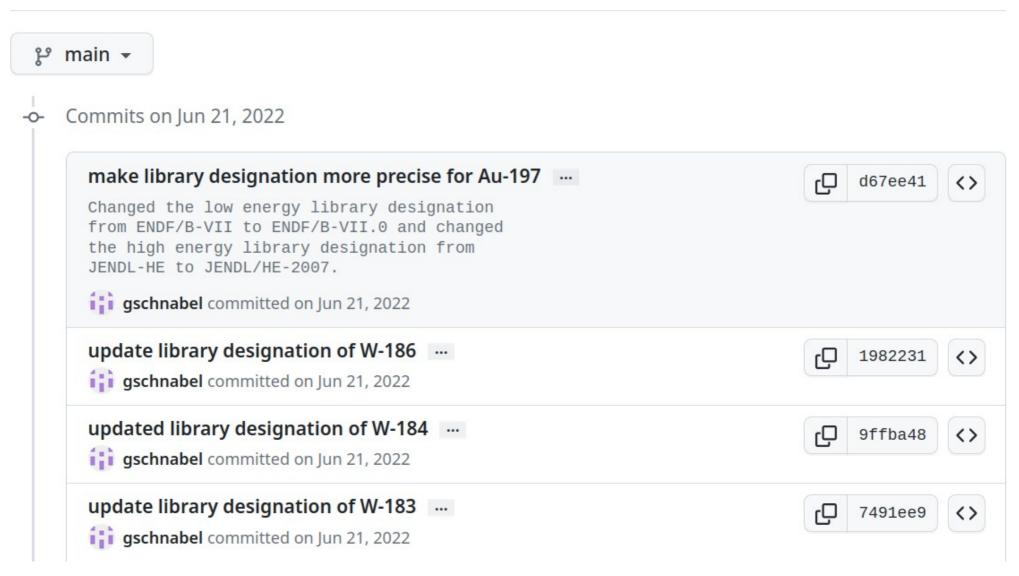
# Keeping track of ENDF files (evaluated data)



Which ENDF files changed?
When were the files changed?
Why were the changes effected?
What are the exact differences?

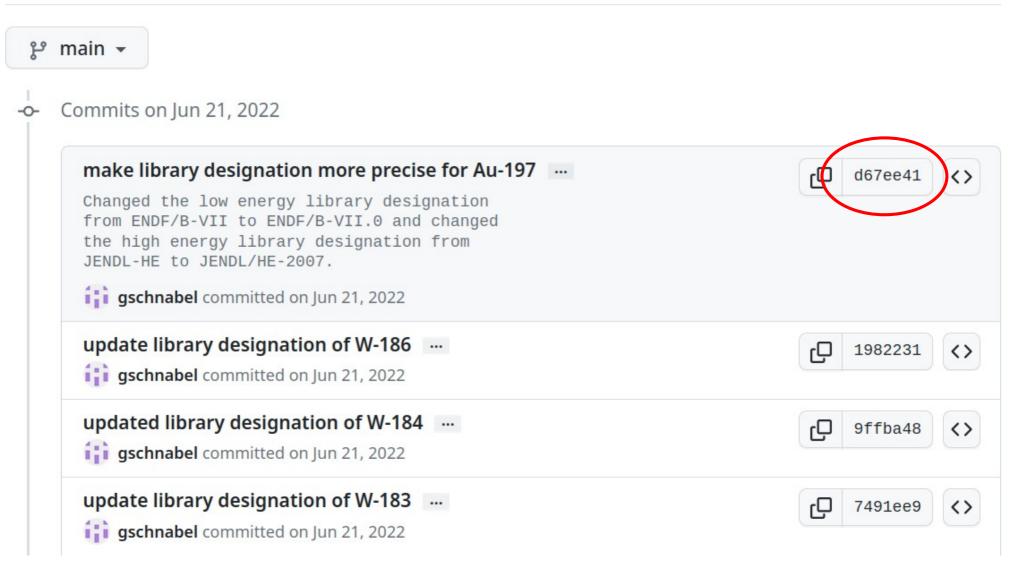
## Version tracking with git

#### Commits

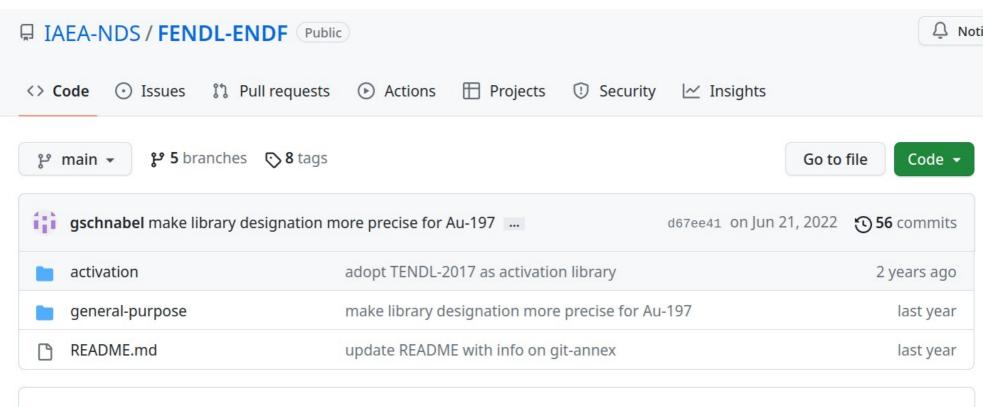


## Version tracking with git

#### Commits



### Hosted on IAEA-NDS GitHub account



README.md

### Fusion Evaluated Nuclear Data Library @

This repository keeps track of updates to the ENDF files of the Fusion Evaluated Nuclear Data Library (FENDL) whose different versions are published on the IAEA-NDS website at https://www-nds.iaea.org/fendl/.

## Git is not enough for FENDL

- Git was designed for the tracking of code projects
- It is not suited for tracking tens of thousands of files with a total size of hundreds of gigabytes with numerical data

→ Decouple version tracking and content storage

## **Use fingerprints**





### **Use fingerprints**

#### File

\$Rev:: 257	2011-03-08			_	0 0	0
7.418400+4 1.823710+2	1	0	0	17437	1451	1
0.000000+0 0.000000+0	0	0	0	67437	1451	2
1.000000+0 1.500000+8	1	0	10	77437	1451	3
0.000000+0 0.000000+0	0	0	567	1407437	1451	4
74-W -184 IAEA Eval0	90806			7437	1451	5
				7437	1451	6
ENDF/B-VII.1 MATER	IAL 7437			7437	1451	7
INCIDENT NEUTRON DATA				7437	1451	8
ENDF-6 FORMAT				7437	1451	9
				7437	1451	10
*******	*****	*****	*****	*** 7437	1451	11
				7437	1451	12
Comment in June 2022 by	G. Schnabe	l:		7437	1451	13
				7437	1451	14
This IAEA evaluation	with the or	iginal lib	rary	7437	1451	15
designation INDL/V-3				. 7437	1451	16
The library designati					1451	17
updated to ENDF/B-VII					1451	18
				7437	1451	19
				7437	1451	20
******	*****	*****	***	7437	1451	21
FAST ENERGY REGION				7437	1451	22
Authors: R. Capote, A. Trk	ov. E. Souk	hovitskii		7437	1451	23
				7437	1451	24
CROSS-SECTION EVALUATION P	ROCEDURE			7437	1451	25
				7437	1451	26
Adopted procedure is based	on careful	theoretic	al	7437	1451	27
analysis utilizing availab				7437	1451	28
nuclear reaction model cal				7437	1451	29
				7/137	1/151	30



cce8ef57d8837cf23e87f7 7f34834dc90d0a607b7ec 8a9a89cac8ba3f536c458

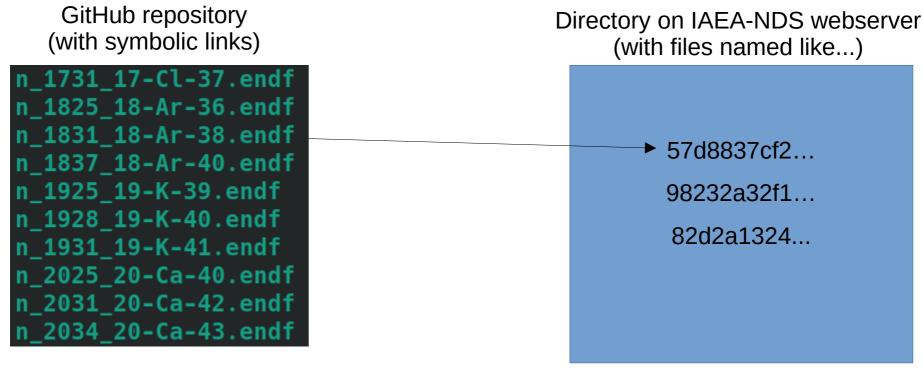
Compress file content into a world-wide unique number (64 digits hexadecimal number) (SHA256 hash)

### **Decoupling**

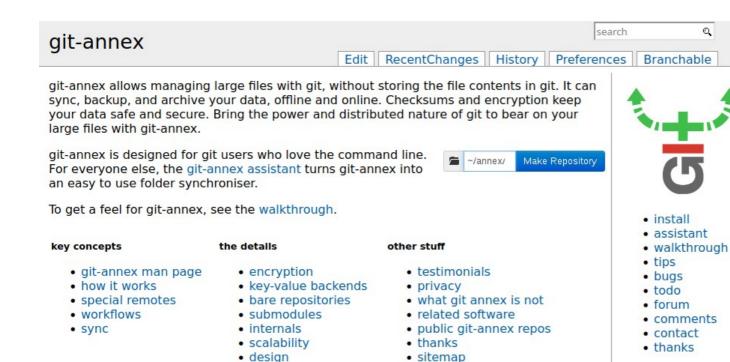
- Git repository contains symbolic links pointing to a file containing the unique number in the filename
- Store the content elsewhere using the unique number as filename

## **Decoupling**

- Git repository contains symbolic links pointing to a file containing the unique number in the filename
- Store the content elsewhere using the unique number as filename



## git-annex





Joey Hess

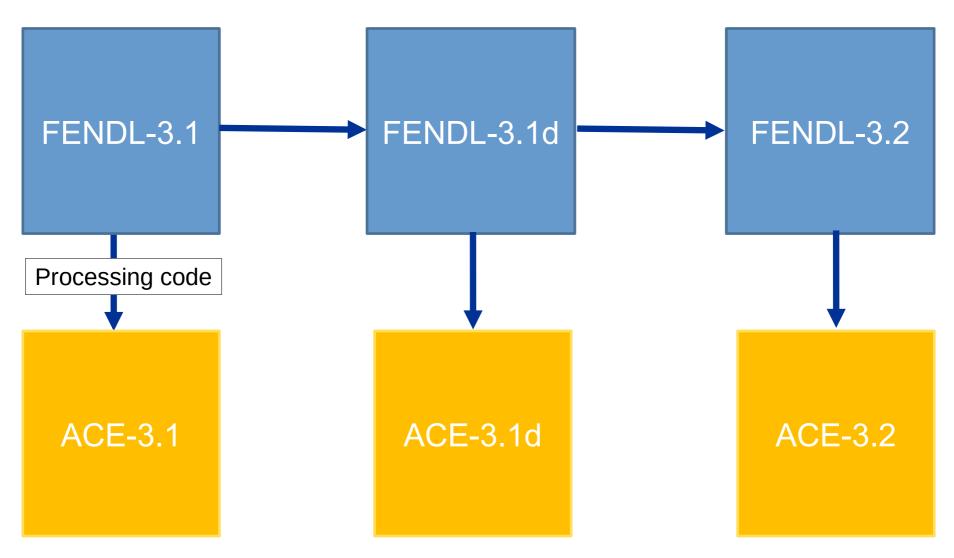
https://git-annex.branchable.com/

## How does it work from the git user point of view?

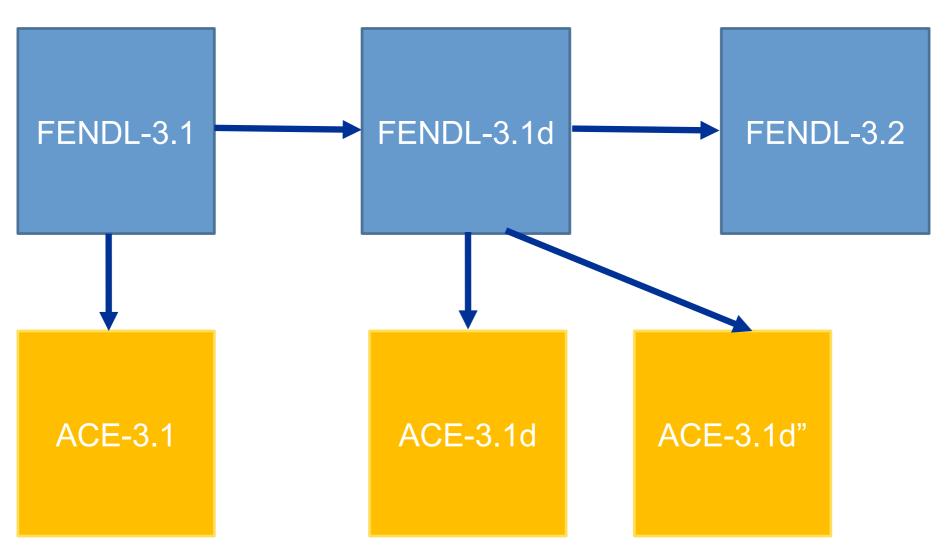
git clone https://github.com/iaea-nds/fendl-endf.git

cd fendl-endf/activation/neutron-activ/endf git annex get .

## **Keeping track of (derived) ACE files**



# Changes in processing (e.g. bugs fixed in NJOY16)



## Some inspiring resources

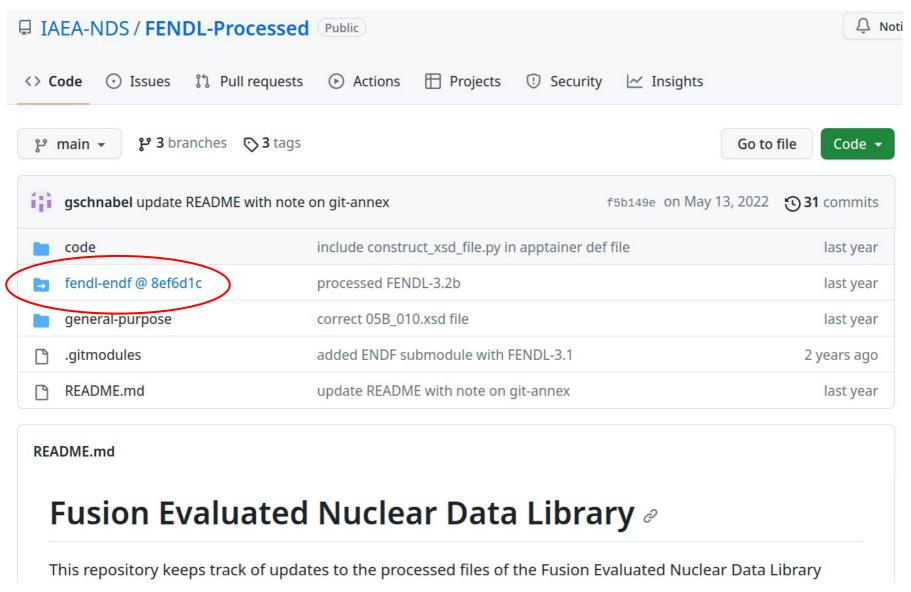
- DataLad: https://www.datalad.org/
- YODA principles\*
- YODAs Organigram on Data Analysis
- How to organize data, processing codes and processed data



### Using git submodules

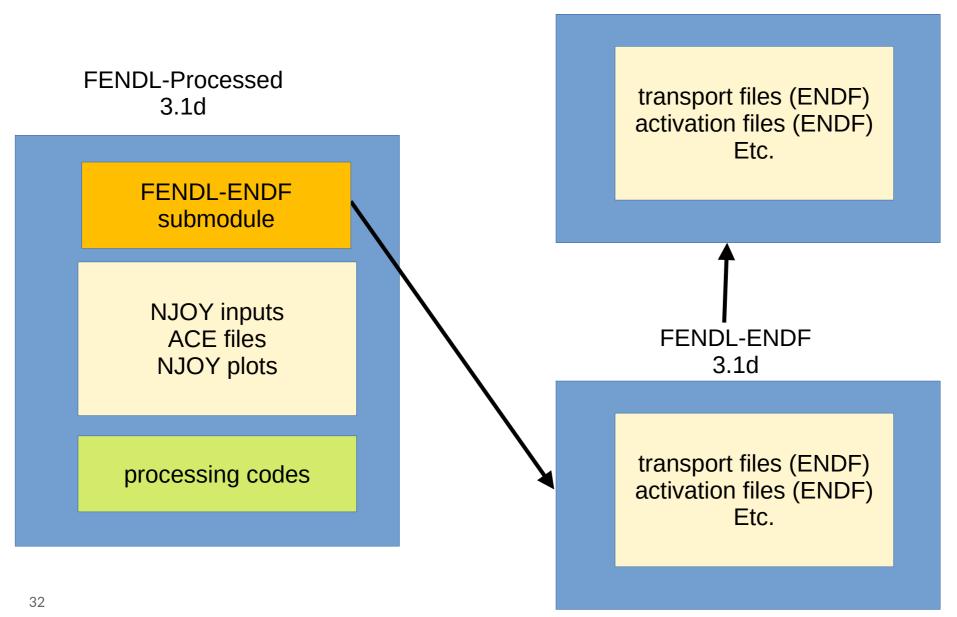
## **FENDL-Processed git repository FENDL-ENDF** repository FENDL-ENDF transport files (ENDF) submodule activation files (ENDF) Etc. NJOY inputs **ACE files** NJOY plots processing codes

### **FENDL-Processed GitHub repository**



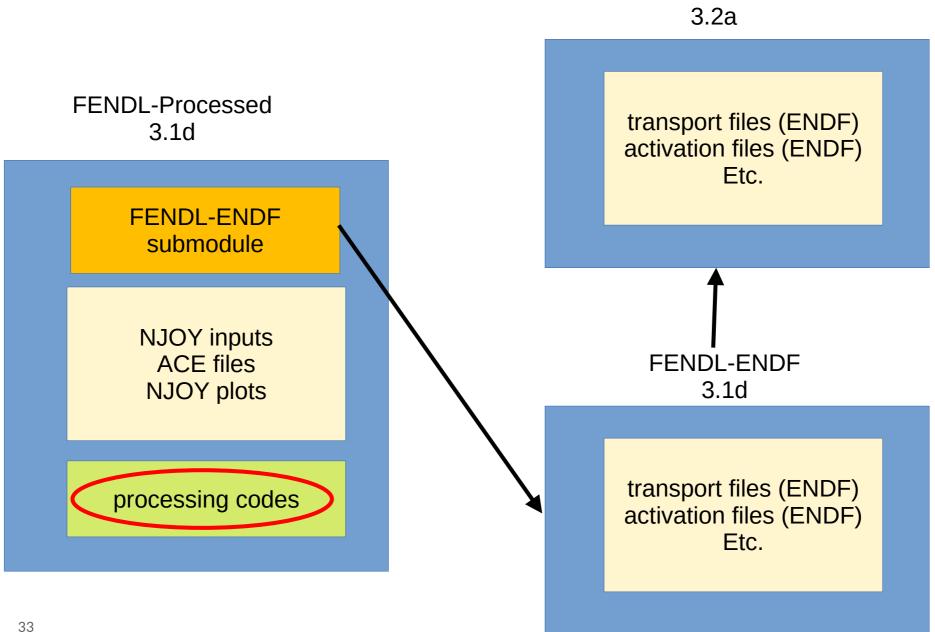
### Version of submodule is pinned

FENDL-ENDF 3.2a

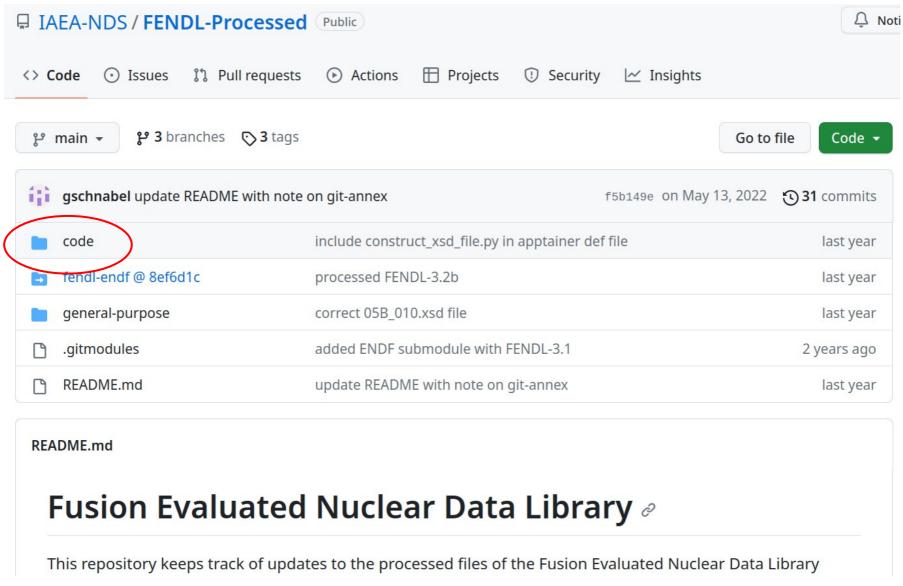


### Reproducible processing

FENDL-ENDF



### Codes in FENDL-Processed repo



### Codes in FENDL-Processed repo

#### FENDL-Processed / code / 「□ gschnabel include construct\_xsd\_file.py in apptainer def file 788eb96 · last year Last commit message Name Las comparison-tools add code and trackdb trackdb update trackdb with new hash of B-10 construct\_xsd\_file.py make construct\_xsd\_file.py usable as module process-fendl.def include construct\_xsd\_file.py in apptainer def file process-fendl.py process-fendl.py now also creates xsd file process-fendl.sif include construct\_xsd\_file.py in apptainer def file Apptainer image Apptainer definition file

## **Apptainer**



## **Apptainer**

#### THE CONTAINER SYSTEM FOR SECURE HIGH PERFORMANCE COMPUTING

Apptainer/Singularity is the most widely used container system for HPC. It is designed to execute applications at bare-metal performance while being secure, portable, and 100% reproducible. Apptainer is an open-source project with a friendly community of developers and users. The user base continues to expand, with Apptainer/Singularity now used across industry and academia in many areas of work.

**Get Started** 

Need help?

# Apptainer definition file (for NJOY2016 in FENDL)

#### FENDL-Processed / code / process-fendl.def

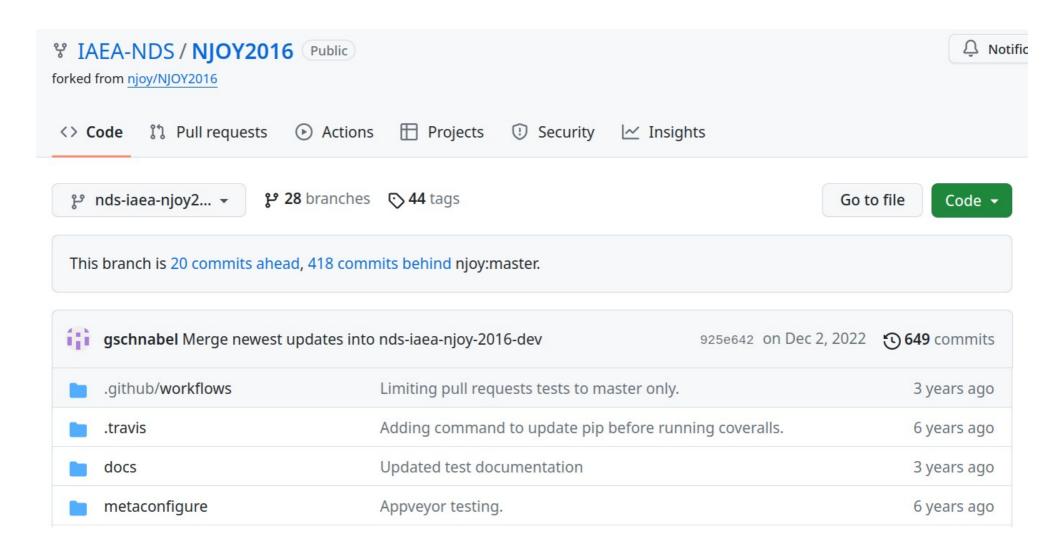
```
%post
 9
10
11
           apt update &&
           apt install -y git=1:2.17.1-1ubuntu0.9 &&
12
           apt install -y cmake=3.10.2-1ubuntu2.18.04.2 &&
13
14
           apt install -y gfortran=4:7.4.0-1ubuntu2.3 &&
           apt install -y python3.7=3.7.5-2ubuntu1~18.04.2 &&
15
           apt install -y ghostscript=9.26~dfsg+0-0ubuntu0.18.04.15 &&
16
           cd /opt &&
17
           git clone https://github.com/IAEA-NDS/NJOY2016.git &&
18
           cd NJ0Y2016 &&
19
           git checkout 304a3e92bc037982126b6c7ab3cea4baabf597b1 &&
20
           mkdir bin && cd bin &&
21
22
           cmake -D CMAKE_BUILD_TYPE=Release .. &&
23
           make &&
           cd /usr/local/bin &&
24
25
           ln -s /opt/NJOY2016/bin
```

# Apptainer definition file (for NJOY2016 in FENDL)

#### FENDL-Processed / code / process-fendl.def

```
9
       %post
10
11
           apt update &&
           apt install -y git=1:2.17.1-1ubuntu0.9 &&
12
           apt install -y cmake=3.10.2-1ubuntu2.18.04.2 &&
13
           apt install -y gfortran=4:7.4.0-1ubuntu2.3 &&
14
           apt install -y python3.7=3.7.5-2ubuntu1~18.04.2 &&
15
           apt install -y ghostscript=9.26~dfsg+0-0ubuntu0.18.04.15 &&
16
           cd /opt &&
17
           git clone https://github.com/IAEA-NDS/NJOY2016.git &&
18
           cd NJ0Y2016 &&
19
           git checkout 304a3e92bc037982126b6c7ab3cea4baabf597b1
20
           mkdir bin && cd bin &&
21
22
           cmake -D CMAKE_BUILD_TYPE=Release .. &&
23
           make &&
           cd /usr/local/bin &&
24
           ln -s /opt/NJOY2016/bin
25
```

## **Local NJOY2016 repository**



https://github.com/iaea-nds/njoy2016

### Recreate all processed files

```
git clone –recurse-submodules https://github.com/iaea-nds/fendl-processed.git cd fendl-processed/fendl-endf/general-purpose git annex get .
```

cd ../..

git annex get code/ general-purpose/neutron/njoy/\*.nji

apptainer run code/process-fendl.sif

Proof-of-concept user interaction

## Without git & git-annex: Viewing in web browser

#### FENDL/7fef6b6[FENDL-3.2]/fendl-endf/data/general-purpose/ [up]

atom/ imported photo-atomic ENDF files of FENDL-3.2

deuteron/ imported ENDF files of FENDL-3.1

<u>neutron/</u> imported neutron ENDF files of FENDL-3.2

<u>neutron-shadow/</u> imported ENDF files of FENDL-3.1 <u>proton/</u> imported ENDF files of FENDL-3.1

#### FENDL/7fef6b6[FENDL-3.2]/fendl-endf/data/general-purpose/neutron/[up]

#### Default-View

Meaning of row colors:

green current version in library

red current version in library (newly added) blue superseded version

FENDL version	Mat	Material	Lab.	Date	Authors	Source	Emax (eV)	Header	File	short-diff	full-diff
FENDL-3.2	125	1-H-1	LANL	EVAL-OCT05	G.M.Hale	FENDL-3.0	1.50E+08	[header]	[endf]		
FENDL-3.2	128	1-H-2	LANL	EVAL-FEB97	P.G.Young,G.M.Hale,M.B.Chadwick	ENDF/B-VII	1.50E+08	[header]	[endf]		
FENDL-3.2	131	1-H-3	LANL	EVAL-NOV01	G.M.Hale	ENDF/B-VII	6.00E+07	[header]	[endf]		
FENDL-3.2	225	2-He-3	JAERI	EVAL-JUN87	K.SHIBATA	JENDL-4	6.00E+07	[header]	[endf]		
FENDL-3.2	228	2-He-4	LANL	EVAL-SEP10	Hale	ENDF/B-VII	6.00E+07	[header]	[endf]		
FENDL-3.2	325	3-Li-6	LANL	EVAL-APR06	G.M.Hale, P.G.Young	FENDL-3.0	2.00E+08	[header]	[endf]		
FENDL-3.2	328	3-Li-7	LANL	EVAL-AUG88	P.G.Young	FENDL-3.0	2.00E+08	[header]	[endf]		
FENDL-3.2	425	4-Be-9	LLNL,LANL	EVAL-OCT09	G.HALE,PERKINS ET AL,FRANKLE	FENDL-3.0	2.00E+08	[header]	[endf]		
FENDL-3.2	525	5-B-10	LANL	EVAL-APR06	G.M.Hale,P.G.Young	FENDL-3.0	2.00E+08	[header]	[endf]		
FENDL-3.1d	525	5-B-10	LANL	EVAL-APR06	G.M.Hale,P.G.Young	FENDL-3.0	2.00E+08	[header]	[endf]	[short-diff]	[full-diff]
FENDL-3.2	528	5-B-11	LANL	EVAL-MAY89	P.G. Young	FENDL-3.0	2.00E+08	[header]	[endf]		

#	Material	Source	Emax
			[MeV]
1	1-H-1	JENDL-1	3000
2	1-H-2	ENDF/B-VII	150
3	1-H-3	ENDF/B-VII	20
4	$2 ext{-He-}3$	ENDF/B-VII	20
5	3-Li-6	JENDL-4.0/HE	200
6	3-Li-7	JENDL-4.0/HE	200
7	4-Be-9	ENDF/B-VII	113
8	5-B-10	ENDF/B-VII	3
9	5-B-11	ENDF/B-?????	200

```
from endf_parserpy.endf_parser import BasicEndfParser
from endf_parserpy.debugging_utils import compare_objects
parser = BasicEndfParser()
fendl_endf = parser.parsefile(fendl_filename)
other_endf = parser.parsefile(other_endffile)
del fendl_endf[1][451]
del other_endf[1][451]
compare_objects(fendl_endf, other_endf, fail_on_diff=False)
```

```
---- difference for MAT 125 -----
at path .3: only obj2 contains {208, 209, 210}
at path .6: only obj2 contains {208, 209, 210}
```

JENDL-2007/HE

# Advanced diff functionality (Provenance checking in FENDL)

#	Material	Source	Emax [MeV]
1	1-H-1	JENDL-1	3000
2	1-H-2	ENDF/B-VII	150
3	1-H-3	ENDF/B-VII	20
4	2-He-3	ENDF/B-VII	20
5	3-Li-6	JENDL-4.0/HE	200
6	3-Li-7	JENDL-4.0/HE	200
7	4-Be-9	ENDF/B-VII	113
8	5-B-10	ENDF/B-VII	3
9	5-B-11	ENDF/B-?????	200

```
from endf_parserpy.endf_parser import BasicEndfParser
from endf_parserpy.debugging_utils import compare_objects
parser = BasicEndfParser()
fendl_endf = parser.parsefile(fendl_filename)
other_endf = parser.parsefile(other_endffile)
del fendl_endf[1][451]
del other_endf[1][451]
compare_objects(fendl_endf, other_endf, fail_on_diff=False)
```

FENDL 3.2b = ENDF/B.VII.0

```
---- difference for MAT 131 -----
Value mismatch at .3.50.QI (-0.76387 vs -763870.0)
Value mismatch at .3.50.QM (-0.76387 vs -763870.0)
Value mismatch at .3.650.QI (-4.0329 vs -4032900.0)
Value mismatch at .3.650.QM (-4.0329 vs -4032900.0)
```

### **Summary**

- Data management at the isotopic level with endf-parserpy
- Data management at the library level using git and git-annex
- Association between processed files, processing code and endf files achieved via git submodules and Apptainer images (~VM image file)
- Proof-of-concept visualization interface for users
- Update of NDS IAEA website not discussed. Semi-automated, see at https://github.com/iaea-nds/fendl-code