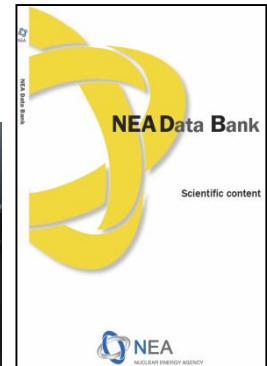
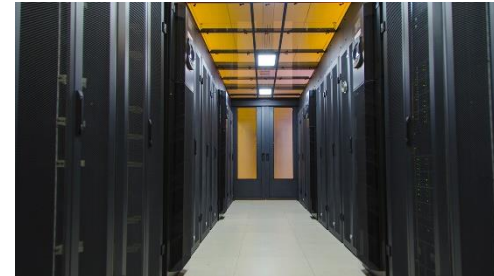


Automated, Reproducible Data Processing, Verification, and Validation at the NEA

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Nuclear Data Scientists

CSEWG 2022
Virtual Participation
November 11, 2022

- ☐ Automation
- ☐ Reproducibility
- ☐ Verification
- ☐ Validation



Automation

- ☐ Use GitLab CI/CD infrastructure to
 - ☐ Perform consistency checks
 - ☐ Process to different formats (with inputs auto-generated)
 - ☐ NJOY
 - ☐ AMPX
 - ☐ ...
 - ☐ Run verification suites
 - ☐ Auto-generated test files
 - ☐ Run validation suites
 - ☐ ICSBEP, ...

Reproducibility

- ☐ Integrated with our Computer Program Services team
 - ☐ Source code distributed by CPS is same source CPS uses to build docker image
- ☐ Docker
 - ☐ Uniquely defined build process through a docker file
 - ☐ Starts with identical, versioned base image (e.g. Ubuntu-20.04)
 - ☐ Identical environments and software versions
 - ☐ Identical build process
 - ☐ Execution is identical
- ☐ Automatically generated, version controlled inputs
 - ☐ Identical inputs + Identical software environment = Identical results

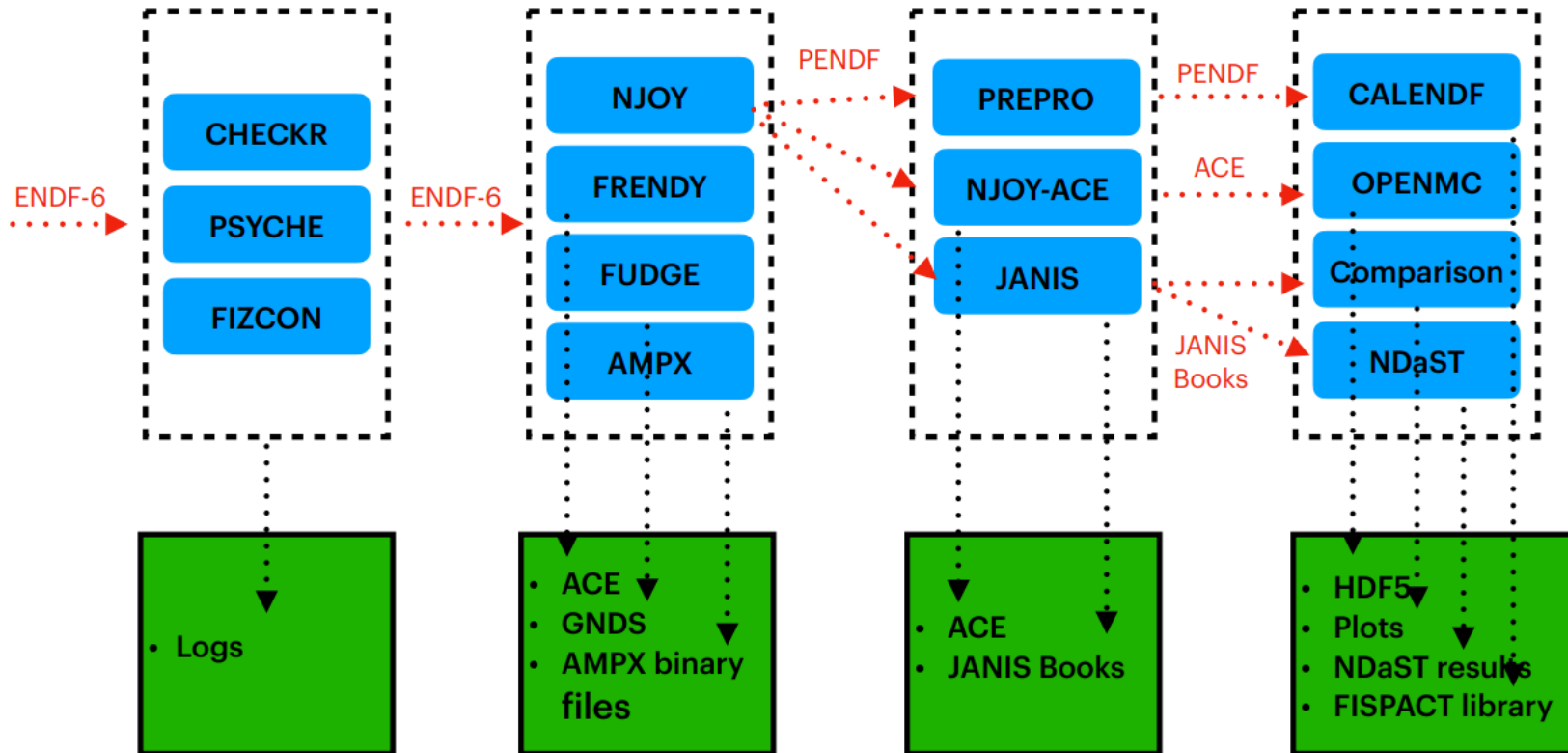
Verification

- ☐ Auto-generated inputs test that data is well formed (no measure of quality or performance)
 - ☐ For SCALE/AMPX, use **exsite** to generate tests
 - ☐ KENO infinite homogenous inputs to test thermal/epithermal
 - ☐ H-H₂O + U-235 + material of interest (TSL or isotope)
 - ☐ MAVRIC leakage tests for fast region
 - ☐ Cf-252 neutron source, test leakage through sphere of material of interest (isotopes)
- ☐ Plan to expand to other codes

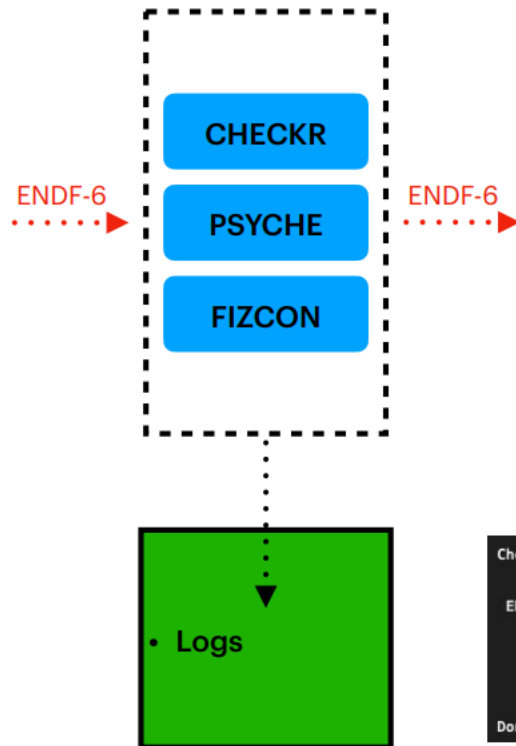
Validation

- ☐ Leverage NEA hosted repositories to perform data testing
 - ☐ ICSBEP
 - ☐ SCALE
 - ☐ Serpent
 - ☐ Others 😊
 - ☐ IRPhE? Others?
- ☐ Automated, Reproducible, Verified...
 - ☐ Codes
 - ☐ Execution
 - ☐ Results

The pipeline Phase I



The pipeline Phase I



```
Check material 92-U -235 MAT 9228

ERROR(S) FOUND IN MAT=9228, MF=40, MT= 4
FIRST SUB-SUBSECTION MUST BE MAT1=0, MF1=10,
MT1=MT AND LFS1=LFS                               SEQUENCE NUMBER 3
FIRST SUB-SUBSECTION MUST BE MAT1=0, MF1=10,
MT1=MT AND LFS1=LFS                               SEQUENCE NUMBER 924

Encountered 2 errors, 0 warnings
Done CHECKR
```

```
Check material 92-U -235 MAT 9228

ERROR(S) FOUND IN MAT=9228, MF= 1, MT=455
SECTION DOES NOT SPAN THE SAME ENERGY RANGE AS FILE 1, MT= 452

ERROR(S) FOUND IN MAT=9228, MF= 2, MT=151
NEGATIVE WIDTHS FOR RESONANCE-7.54054E+01      SEQUENCE NUMBER 6
NEGATIVE WIDTHS FOR RESONANCE-7.54054E+01      SEQUENCE NUMBER 6

WARNING(S) IN MAT=9228, MF= 3, MT= 4
ELEVEL= 7.70000E+01 MIGHT BE UNREASONABLE      SEQUENCE NUMBER 1

ERROR(S) FOUND IN MAT=9228, MF= 3, MT= 18
Q VALUE NOT COMPATIBLE WITH MF=1, MT=458      SEQUENCE NUMBER 2
Q= 1.93405E+08 ENERGY RELEASE= 1.93865E+08

ERROR(S) FOUND IN MAT=9228, MF= 3, MT= 22
THE MINIMUM INCIDENT ENERGY OF 1.00000E+03(EV)
SHOULD BE 1.00000E-05(EV) FOR Q= 4.67827E+06(EV)

WARNING(S) IN MAT=9228, MF= 3, MT= 51
ELEVEL= 7.70000E+01 MIGHT BE UNREASONABLE      SEQUENCE NUMBER 1

ERROR(S) FOUND IN MAT=9228, MF= 3, MT=107
THE MINIMUM INCIDENT ENERGY OF 1.00000E+03(EV)
SHOULD BE 1.00000E-05(EV) FOR Q= 1.11186E+07(EV)

ERROR(S) FOUND IN MAT=9228, MF= 5, MT=455
NO FISSION SPECTRUM FOR A FISSION REACTION      SEQUENCE NUMBER 1

ERROR(S) FOUND IN MAT=9228, MF=12, MT= 70
LIST OUT OF ORDER NEAR N= 2                     SEQUENCE NUMBER 3

ERROR(S) FOUND IN MAT=9228, MF=12, MT= 76
LIST OUT OF ORDER NEAR N= 2                     SEQUENCE NUMBER 3

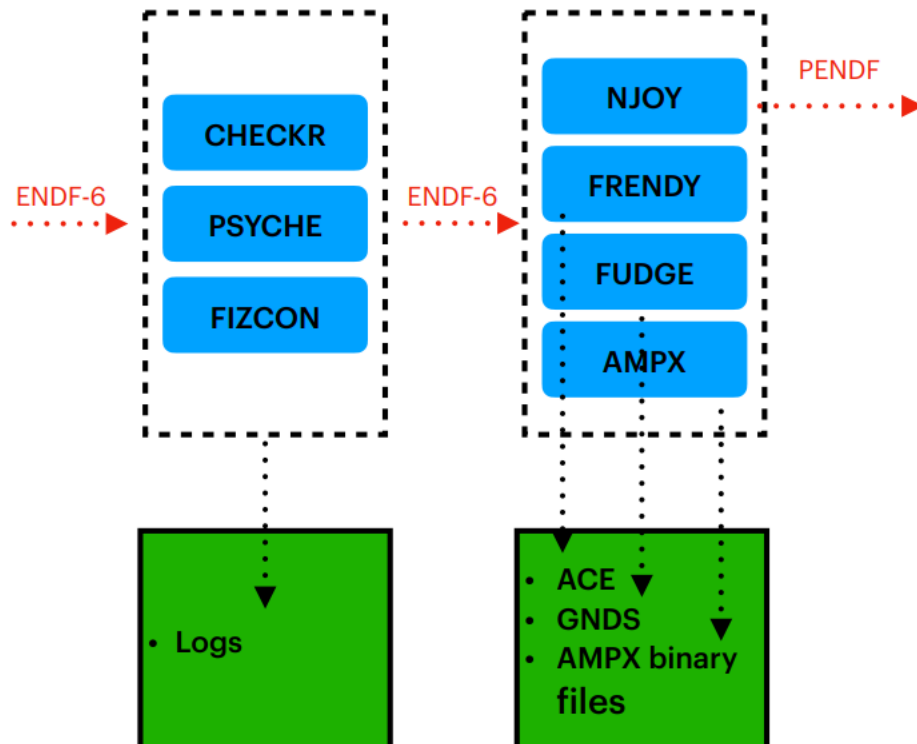
ERROR(S) FOUND IN MAT=9228, MF=12, MT= 77
LIST OUT OF ORDER NEAR N= 2                     SEQUENCE NUMBER 3

ERROR(S) FOUND IN MAT=9228, MF=12, MT= 79
LIST OUT OF ORDER NEAR N= 2                     SEQUENCE NUMBER 3

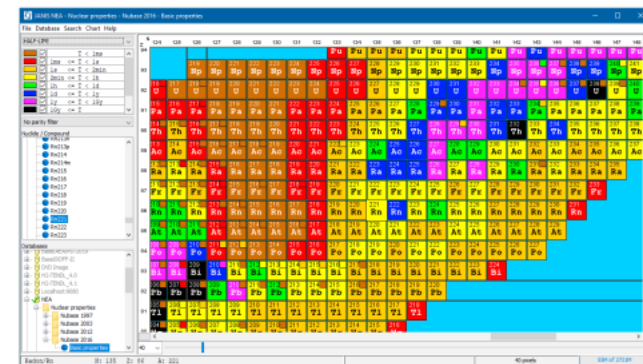
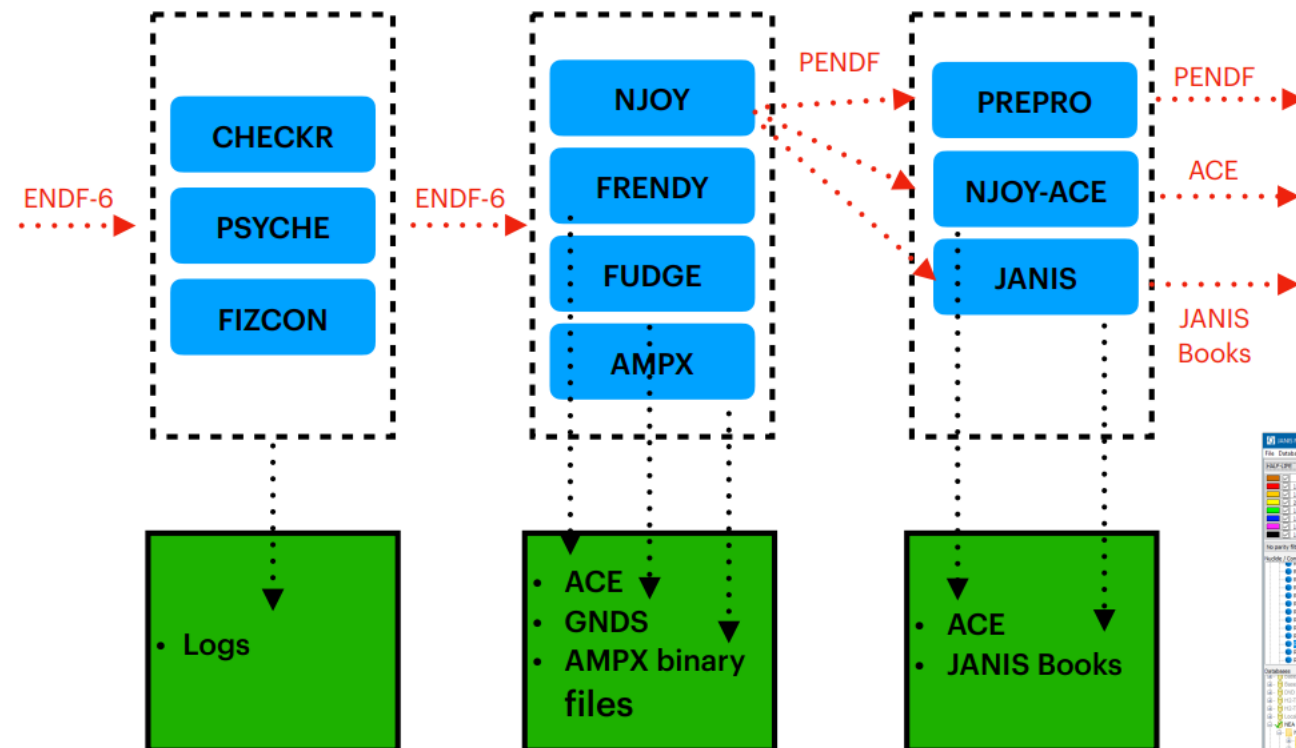
ERROR(S) FOUND IN MAT=9228, MF=40, MT= 4
IZAP 0 NOT IN RANGE 3000 TO 120000              SEQUENCE NUMBER 2

Encountered 12 errors, 2 warnings
Done FIZCON
```


The pipeline Phase I

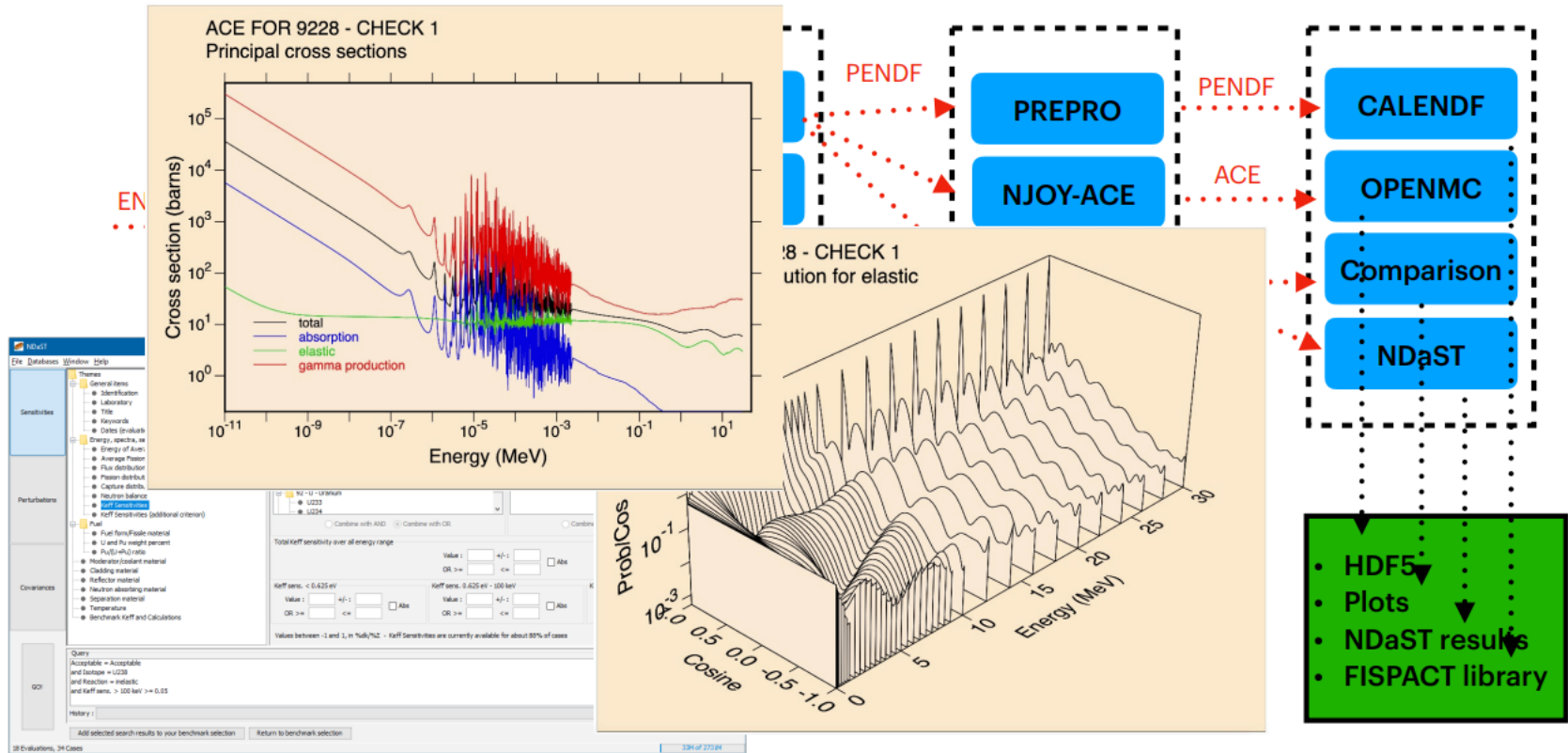


The pipeline Phase I

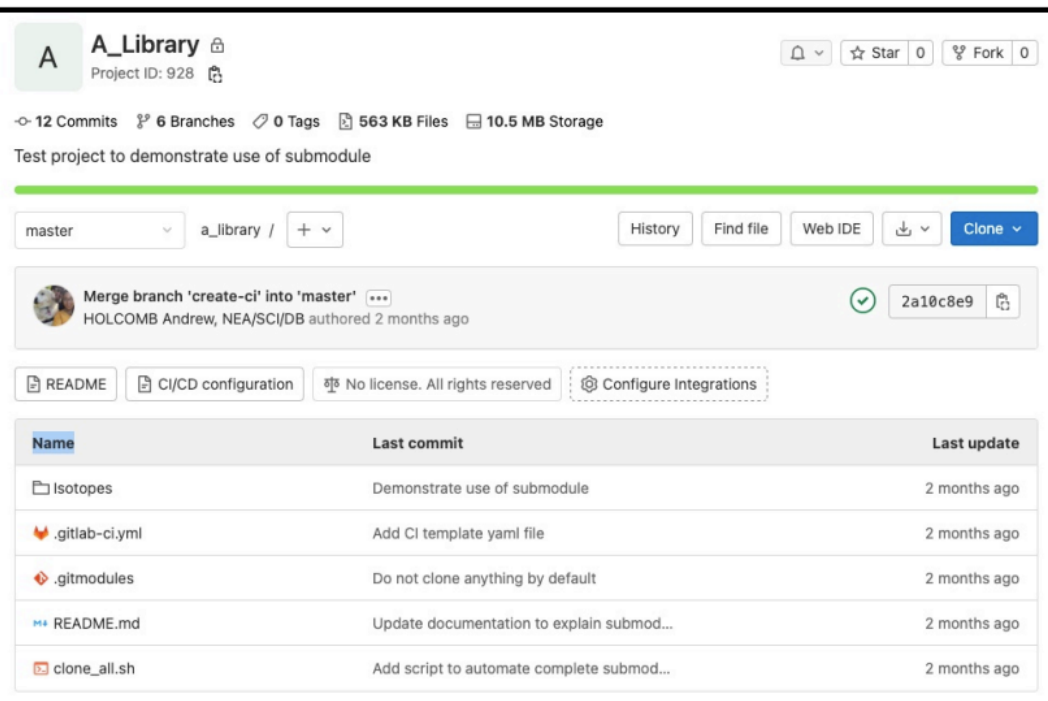




The pipeline

Phase I



JEFF-4Tx Phase II










A_Library 
Project ID: 928 





🔗 12 Commits 6 Branches 0 Tags 563 KB Files 10.5 MB Storage

Test project to demonstrate use of submodule

master a_library / + History Find file Web IDE Clone

 Merge branch 'create-ci' into 'master'  2a10c8e9 
HOLCOMB Andrew, NEA/SCI/DB authored 2 months ago

 README  CI/CD configuration  No license. All rights reserved  Configure Integrations

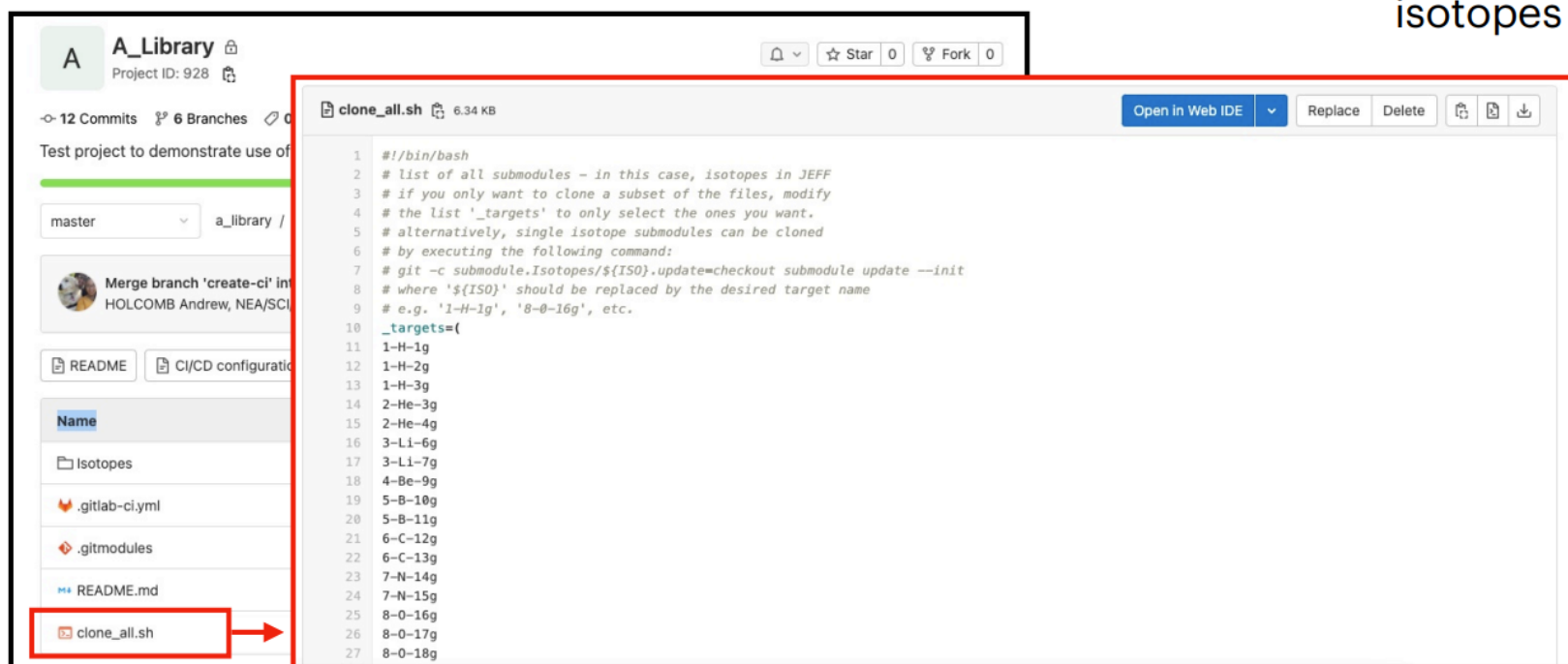
Name	Last commit	Last update
Isotopes	Demonstrate use of submodule	2 months ago
 .gitlab-ci.yml	Add CI template yaml file	2 months ago
 .gitmodules	Do not clone anything by default	2 months ago
 README.md	Update documentation to explain submod...	2 months ago
 clone_all.sh	Add script to automate complete submod...	2 months ago

The project contains:

- a Readme
- a yaml
- a script to clone the isotopes
- a folder containing the submodules
- a .gitmodules file

JEFF-4Tx Phase II

This script is used to clone all isotopes at once



The screenshot shows a GitLab repository for 'A_Library' (Project ID: 928). The left sidebar contains a file tree with 'Isotopes' and 'clone_all.sh' highlighted. The main area displays the content of 'clone_all.sh', a 6.34 KB script. The script is a bash script that clones all submodules in the 'JEFF' library. It includes comments explaining its purpose and usage, and a list of targets to be cloned.


```
1  #!/bin/bash
2  # list of all submodules - in this case, isotopes in JEFF
3  # if you only want to clone a subset of the files, modify
4  # the list '_targets' to only select the ones you want.
5  # alternatively, single isotope submodules can be cloned
6  # by executing the following command:
7  # git -c submodule.Isotopes/${ISO}.update=checkout submodule update --init
8  # where '${ISO}' should be replaced by the desired target name
9  # e.g. '1-H-1g', '8-0-16g', etc.
10 _targets=(
11 1-H-1g
12 1-H-2g
13 1-H-3g
14 2-He-3g
15 2-He-4g
16 3-Li-6g
17 3-Li-7g
18 4-Be-9g
19 5-B-10g
20 5-B-11g
21 6-C-12g
22 6-C-13g
23 7-N-14g
24 7-N-15g
25 8-O-16g
26 8-O-17g
27 8-O-18g
```


JEFF-4Tx

Phase II

Each submodule is associated
with a commit

A

A_Library


Project ID: 928 

12 Commits


6 Branches

0 Forks

Test project to demonstrate use of submodules

master

a_library /



Merge branch 'create-ci' in
HOLCOMB Andrew, NEA/SC

README

CI/CD configurati

Name

Isotopes

.gitlab-ci.yml

.gitmodules

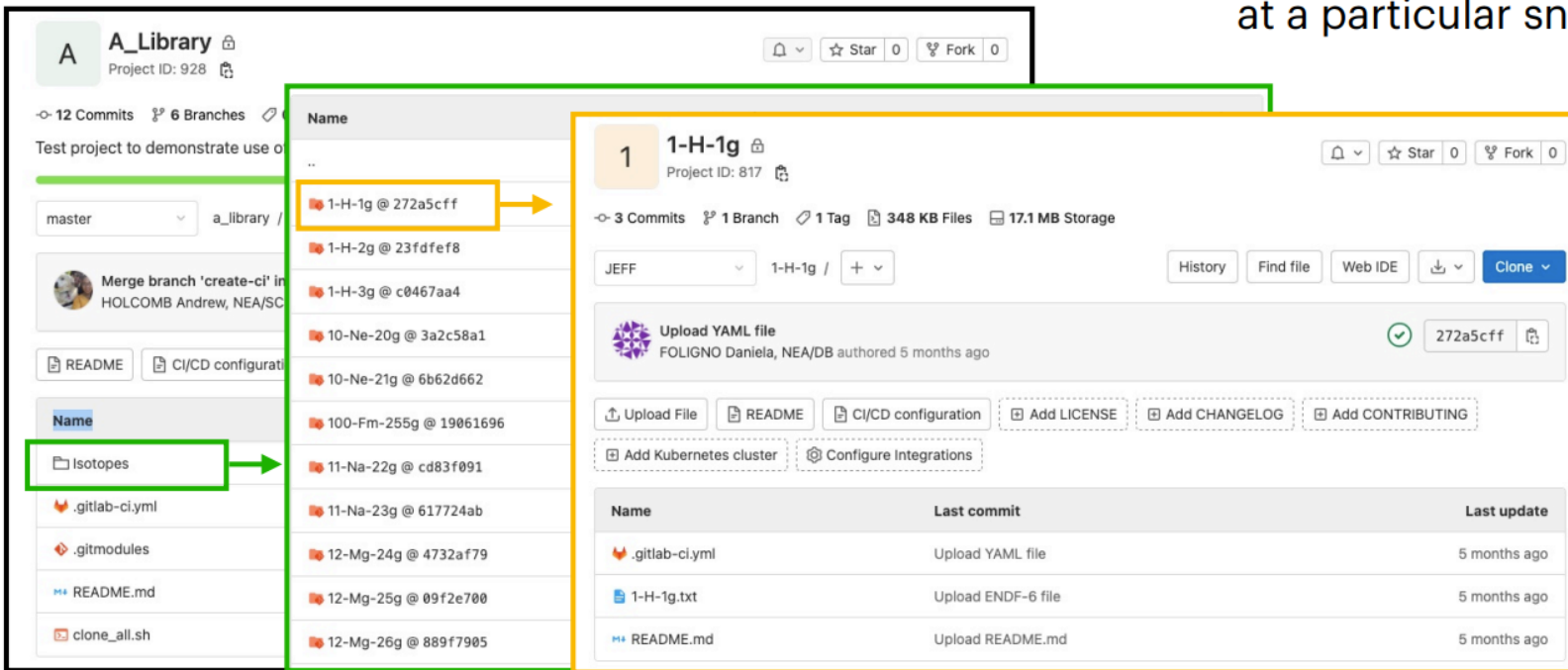
README.md

clone_all.sh

Name	Last commit	Last update
1-H-1g @ 272a5cff	Demonstrate use of submodule	2 months ago
1-H-2g @ 23fddef8	Demonstrate use of submodule	2 months ago
1-H-3g @ c0467aa4	Demonstrate use of submodule	2 months ago
10-Ne-20g @ 3a2c58a1	Demonstrate use of submodule	2 months ago
10-Ne-21g @ 6b62d662	Demonstrate use of submodule	2 months ago
100-Fm-255g @ 19061696	Demonstrate use of submodule	2 months ago
11-Na-22g @ cd83f091	Demonstrate use of submodule	2 months ago
11-Na-23g @ 617724ab	Demonstrate use of submodule	2 months ago
12-Mg-24g @ 4732af79	Demonstrate use of submodule	2 months ago
12-Mg-25g @ 09f2e700	Demonstrate use of submodule	2 months ago
12-Mg-26g @ 889f7905	Demonstrate use of submodule	2 months ago

JEFF-4Tx Phase II

Git submodules are simply a reference to another repository at a particular snapshot in time.



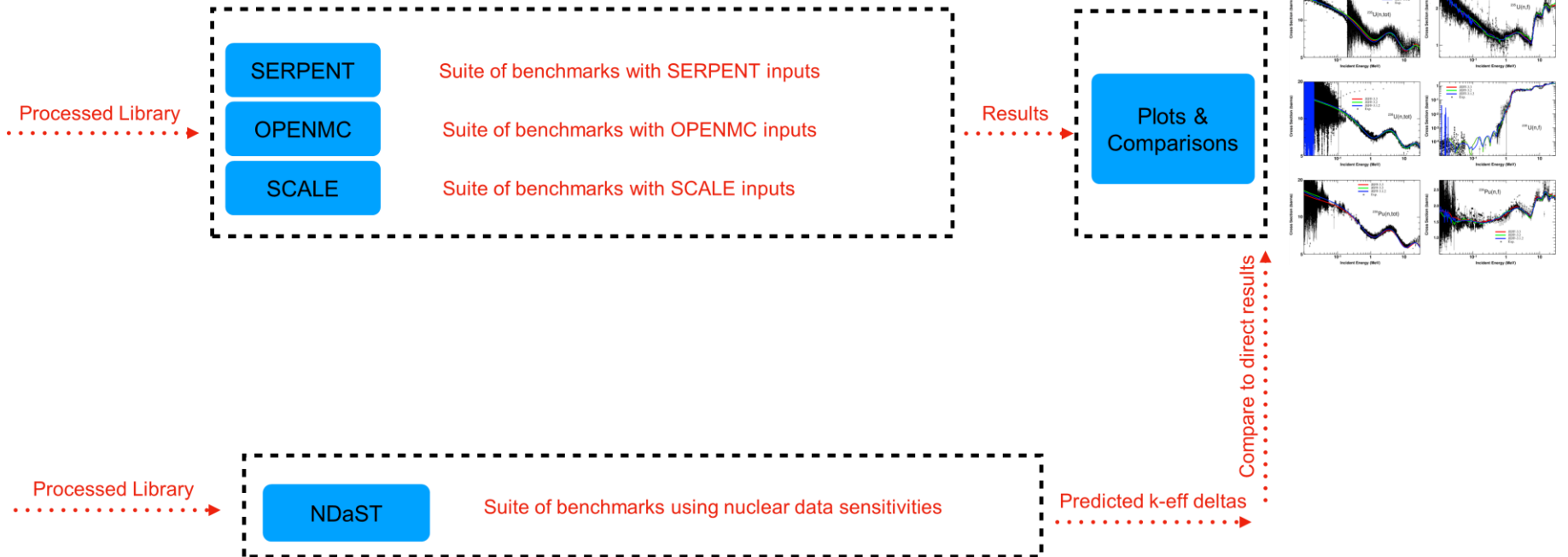
The screenshot illustrates a Git repository setup for the JEFF-4Tx Phase II project. It shows a main repository, **A_Library** (Project ID: 928), which contains a submodule named **1-H-1g** (Project ID: 817). The submodule is referenced to a specific commit, **272a5cff**.

Repository Structure:

- A_Library** (Project ID: 928)
 - 12 Commits, 6 Branches
 - Test project to demonstrate use of
 - master branch
 - Merge branch 'create-ci' in HOLCOMB Andrew, NEA/SC
 - README, CI/CD configuration
 - Isotopes (highlighted with a green box and arrow pointing to the submodule list)
 - .gitlab-ci.yml
 - .gitmodules
 - README.md
 - clone_all.sh
- 1-H-1g** (Project ID: 817) (highlighted with an orange box)
 - 3 Commits, 1 Branch, 1 Tag, 348 KB Files, 17.1 MB Storage
 - JEFF repository
 - 1-H-1g / +
 - History, Find file, Web IDE, Clone
 - Upload YAML file (FOLIGNO Daniela, NEA/DB authored 5 months ago) - 272a5cff
 - Upload File, README, CI/CD configuration, Add LICENSE, Add CHANGELOG, Add CONTRIBUTING
 - Add Kubernetes cluster, Configure Integrations
 - Commit history table:

Name	Last commit	Last update
.gitlab-ci.yml	Upload YAML file	5 months ago
1-H-1g.txt	Upload ENDF-6 file	5 months ago
README.md	Upload README.md	5 months ago

Phase II



Example: AMPX

- ☐ Templates created for CE data processing and verification
 - ☐ One-time human effort, version controlled
- ☐ Metadata files (XML) created for specific libraries (used to expand templates into working inputs)
 - ☐ ENDF-7.1, ENDF-8.0, JEFF-4T1 (easy to replicate for other libraries)
 - ☐ Automatically populated, minor human tweaking required for TSL data (one-time human effort, version controlled)
- ☐ Exsite expands template + metadata, launches jobs (automated)
 - ☐ Working AMPX inputs (version controlled)
 - ☐ Working SCALE inputs (version controlled)
 - ☐ Library files (output from AMPX)
- ☐ All “tweaking” documented, scripted

Processed Files

JEFF-4T1	ACE, XSDIR, NJOY inputs	NJOY	CE, 293K	563	1 GB	Download
JEFF-4T1	ACE, XSDIR, PENDF, NJOY input	NJOY	H in H2O 293K	1	40 MB	Download
JEFF-4T1	H5	OPENMC	CE, 293K	563	1 GB	Download
JEFF-4T1	Binaries for SCALE	AMPX	CE, 293K, 565K, 600K, 900K, 1200K, 2000K (TSL data is at the temperature specified in the file)	563 + 20 TSL (PuO2, UO2, Mesi-PhII, Tolue-PhII have not been processed)	21 GB	Download
JEFF-4T1	Binaries for SCALE (split to make downloading easier on slow connections)	AMPX	CE, 293K, 565K, 600K, 900K, 1200K, 2000K (TSL data is at the temperature specified in the file)	563 + 20 TSL (PuO2, UO2, Mesi-PhII, Tolue-PhII have not been processed)	21 GB, max 2 GB per file. Extract with 7-Zip by selecting all files	split.zip split.z01 split.z02 split.z03 split.z04 split.z05 split.z06 split.z07 split.z08 split.z09 split.z10

<https://www.oecd-neo.org/dbdata/jeff/jeff40/t1/>

Next steps

- ☐ Automatic processing for JANIS
 - ☐ Nicolas' processing system already implemented into GitLab CI (still need to work on JANIS import)
- ☐ Fully integrate AMPX processing and SCALE testing
 - ☐ Input generation automated and version controlled (data processing and verification inputs)
 - ☐ working SCALE/AMPX docker images (including MPI enabled for SCALE)
 - ☐ Use exsite in GitLab CI to launch library processing
 - ☐ Test processed files with benchmark suites
- ☐ Continue to expand data processing and validation suites

**Thank you for
your attention**

