NJOY2016 and Modern NJOY

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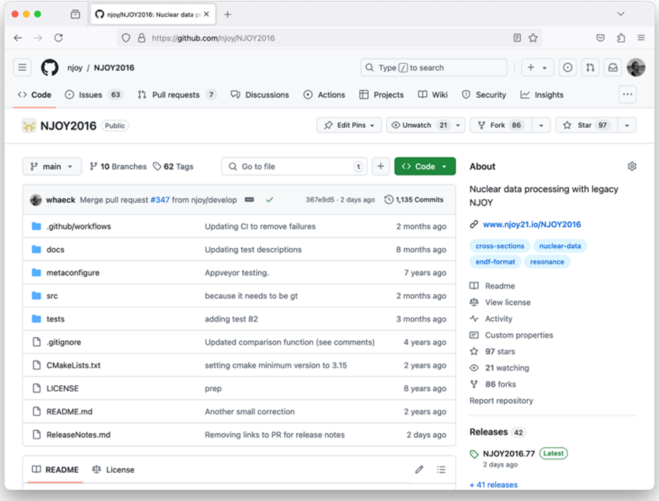
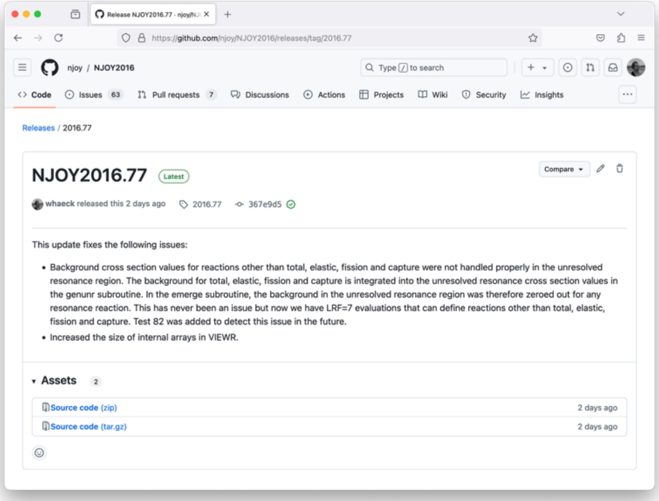
Outline

- NJOY2016 updates
- ENDF/B-VIII.1 libraries for MCNP
  - Lib81 and ENDF81SaB
  - Errata files for Lib81
- A modernization update
  - Bear with us, it’s a long one …
- Conclusions

Maintaining our production version

- Get it at https://github.com/njoy/NJOY2016





- Latest version is NJOY2016.78 (February 2025)
  - Our aim has been to release updates every three months, but our release cadence is probably going to slow down

Noteworthy updates to NJOY2016

- NJOY2016.78:
  - Increase the number of tape numbers from 99 to 999
  - Adding a message to signal malformed resonance data in ENDF files
    - SLBW/MLBW and Reich-Moore can have NRS=0 (no resonances given for this l value)
    - Malformed LIST record with size 0

- We have a large number of user provided updates on GitHub
  - We will look these over and try to merge these (or alternative fixes) into NJOY2016
- We are also aware of other issues but have not gotten to fixing them
  - Covariance data processing sometimes gives abnormally high uncertainties

- LLVM+flang is now a supported compiler

MCNP libraries for ENDF/B-VIII.1

- Lib81 : incident neutron files
  - 557 targets
  - 8 temperatures : 293.6 K, 600 K, 900 K, 1200 K, 2500 K, 0.1 K, *233.15 K, 273.15 K*
  - Extensions : 10c to 17c

- ENDF81SaB : thermal scattering files
  - 103 materials
  - Extensions : 70t to 89t depending on the material
  - 70t will either be room temperature (or close to it) or the lowest available temperature
  - This is a big library at over 40 GB

- Released in September 26, 2025, get them on https://nucleardata.lanl.gov

MCNP libraries for ENDF/B-VIII.1

- Since the release, we have found an issue concerning primary gammas:
  - The new Pt and ^{180m}Ta evaluations cause MCNP to hang (or crash) when `mode p` is on

- This was found by a user and diagnosed by the LANL MCNP team
  - The ACE files for these evaluations have outgoing gamma distributions with >1000 energies (discrete energies and continuum bin edges combined) for capture

- What caused the large distributions?

MCNP libraries for ENDF/B-VIII.1

- These are the first evaluations in ENDF/B with discrete primary gammas in File 6
  - The *emitted* gamma energy is listed in the file
- JENDL has included discrete primary gammas in File 6 for several releases
  - The *binding energy* is listed in the file
- NJOY2016 was modified in 2010 to process the JENDL format
  - The discrete primaries at each incident energy were incorrectly interpreted as different gammas in the union grid created by NJOY2016
- An erratum for Lib81x is being produced

File 6 Format Description

NEP Number of secondary energy points in the distribution.

ND Number of discrete energies given.

The first ND≥0 entries in the list of NEP energies are discrete, and the remaining (NEP-ND)≥ 0 entries are to be used with LEP to describe a continuous distribution. Discrete primary photons should be flagged with negative energies.

File 12 Format Description

EG_k photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, $EG_k \equiv 0.0$ should be used.

LP indicator of whether or not the particular photon is a primary:

LP=0 origin of photons is not designated or not known, and the photon energy is EG_k;

LP=1 for non-primary photons where the photon energy is simply EG_k;

LP=2 for primary photons where in the center-of-mass frame the sum of the photon energy EG'_k and kinetic energy of the residual K_r is

$$EG'_k + K_r = EG_k + \frac{AWR}{AWR+1} E_n$$

and the photon energy EG'_k is given by

$$EG'_k = \left(1 - \frac{EG_k/(m_n c^2)}{2\,(AWR+1)} - \frac{AWR\; E_n/(m_n c^2)}{(AWR+1)^2}\right) EG_k + \left(1 - \frac{AWR\; E_n/(m_n c^2)}{(AWR+1)^2}\right) \frac{AWR}{AWR+1} E_n.$$

MCNP libraries for ENDF/B-VIII.1

- This format divergence needs to be addressed:

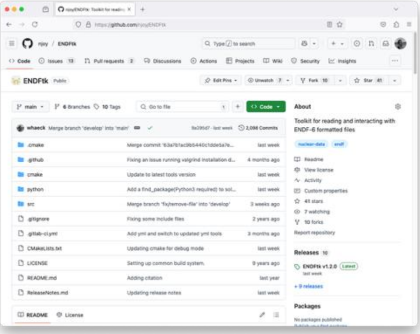
1. Change the ENDF/B format to match JENDL?
   - JENDL has many more evaluations with primary gammas in File 6, going back several releases
2. Formalize the divergence between ENDF/B and JENDL?
   - Just needs to be documented so the processing codes can handle it
3. Disallow primary gammas in File 6 in ENDF/B, only allow them in File 12?

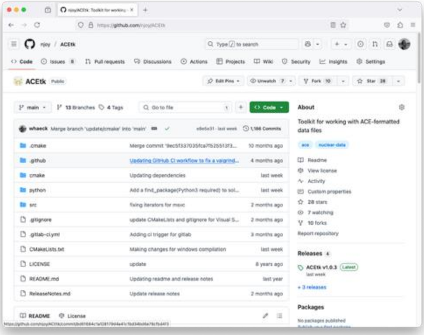
Why do we need to modernise our processing code?

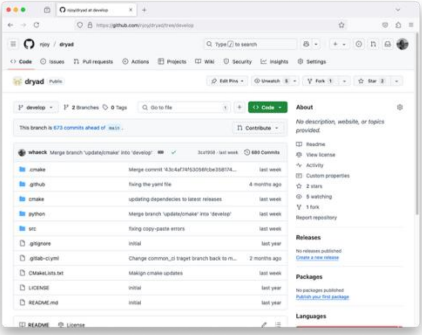
- New nuclear data features are hard to introduce in NJOY2016
  - Energy dependent fission yield data
  - Incident charged particle resonance parameters
- Better knowledge of implemented methods
  - Modernisation allows us to explore different methods and identify shortcomings
- NJOY2016 is too closely linked to the ENDF-6 format
  - Introducing new evaluation formats like GNDS is “impossible” in NJOY2016
- Our users have needs that NJOY2016 does not provide
  - NJOY2016 does not linearise MF9 data
  - NJOY2016 cannot produce the photoatomic and electroatomic ACE files (eprdata)

A component-based modernisation strategy

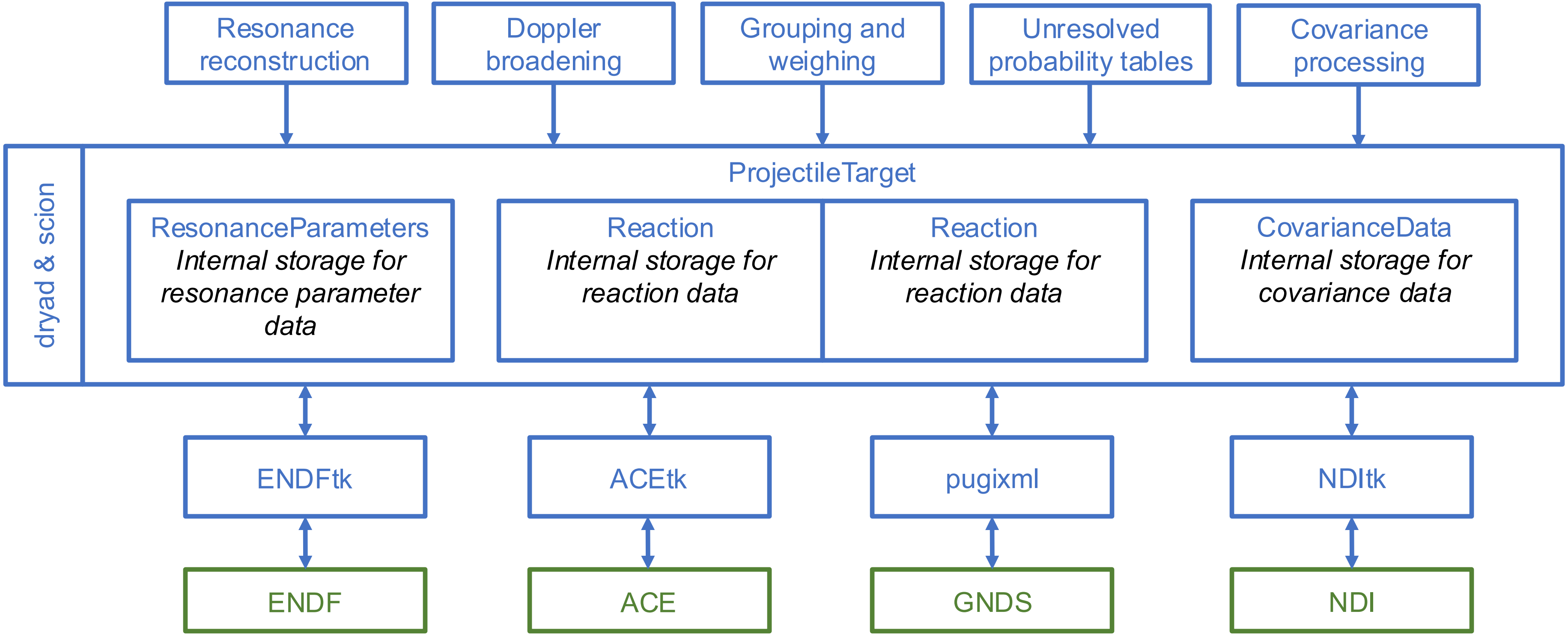
- Modernised modules are built from components
  - Format components: `ENDFtk`, `ACEtk`, `NDItk`
  - Mathematical operations and generic data representation: `scion`
  - Format agnostic nuclear and atomic data access and interpretation: `dryad`
  - Modernised modules like `reconr`, `broadr`, etc. will interact with the `dryad` interface
- Components can be developed and deployed faster than modules
  - Entirely developed in C++ and with Python bindings



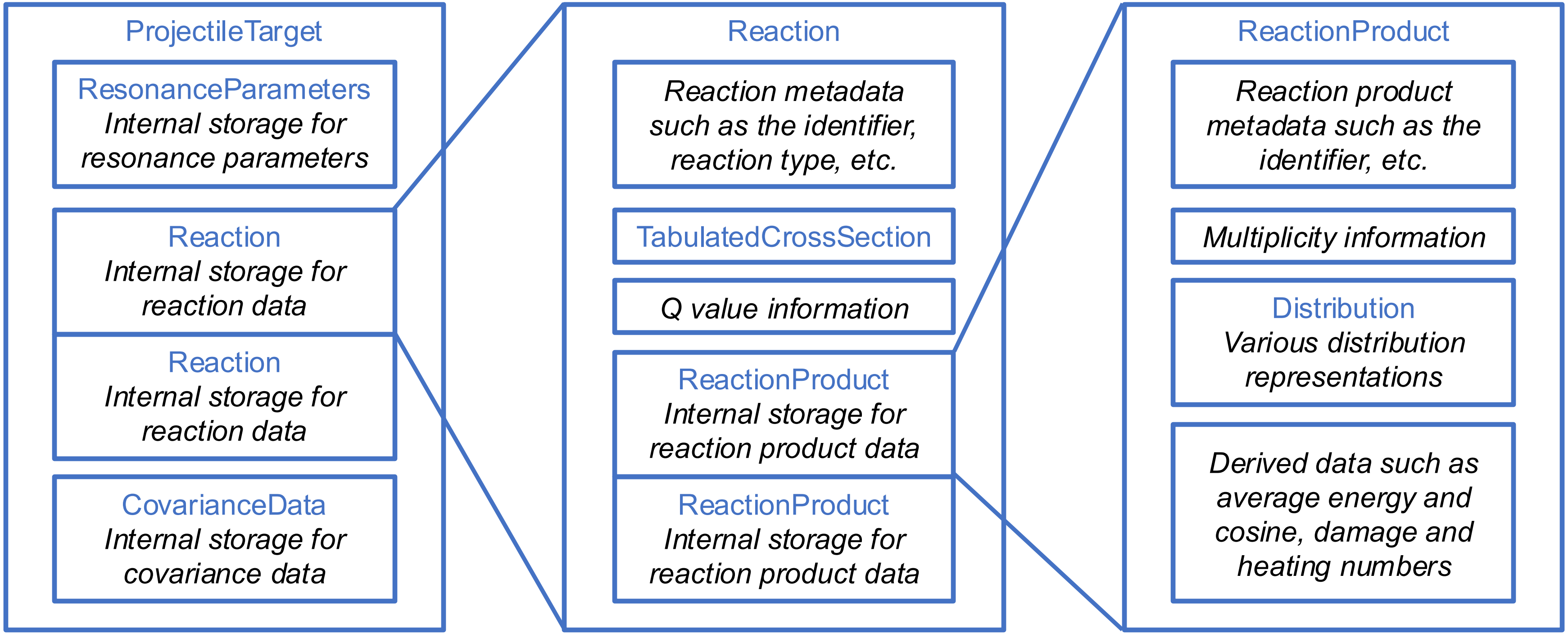




A component-based modernisation strategy



Format agnostic data interface and structures



Data format support in modern NJOY

Photoatomic and electroatomic data	ENDF	GNDS	ACE
Atomic relaxation data			N/A
Cross section data			
Products, energy and angular distribution data			
Incident neutron, charged particle and photonuclear data	**ENDF**	**GNDS**	**ACE**
Resonance parameters			N/A
Cross section data			
Products, energy and angular distribution data			
Covariance data			N/A (?)
Other data types	**ENDF**	**GNDS**	**ACE**
Radioactive decay data and fission yield data			N/A
Thermal scattering data			

Reaction and other identifiers

- We aim for a format agnostic data interface so no ENDF-6/GNDS speak
  - That includes identifiers, so no MT numbers – ever!
  - Identifiers can be made using standardised strings that actually mean something

- `ParticleID` for particle identifiers (these follow the GNDS standard)
  - `n`, `p`, `d`, `t`, `h`, `a` for fundamental particles
  - `U` or `Uranium` for an element
  - `U{1s1/2,2s1/2}` for an atom with electron shell vacancies
  - `H1` or `H1_e0` for a ground state nuclide
  - `H1_e1` for a nuclide in an excited state (we do not support metastable aliases yet)
  - And yes, you can ask for `Aluminium` and `Aluminum`

Reaction and other identifiers

- `ReactionID` for nuclear and atomic reaction identifiers
  - Fully specified symbols:
    - `n,U235->n,U235` and `n,U235->2n,a,Th232[all]` for traditional reactions
    - `n,U235->total` and `n,U235->fission` for special reactions
  - Incomplete reaction symbols can be used when initialising a reaction identifier
    - `n,U235->n(0)` for `n,U235->n,U235` (elastic)
    - `n,U235->2n,a` and `n,U235->2n,a(t)` for `n,U235->2n,a,Th232[all]`

```
from njoy.dryad import ProjectileTarget
from njoy.dryad.id import ParticleID, ReactionID

# open the GNDS file for Be9
be9 = ProjectileTarget.from_gnds_file( 'be9.gnds' )

# create some identifiers
n = ParticleID.neutron()
elastic_id = ReactionID( 'n,Be9->n(0)' )

# get the elastic reaction and neutron reaction product
elastic = be9.reaction( elastic_id )
neutron = elastic.product( n )
```

Resonance reconstruction

- We are in the process of integrating resonance reconstruction in `njoy.dryad`
  - Based on the `resonanceReconstruction` library developed in 2019 – 2020
  - Complete redesign to allow for Python bindings and fix known issues

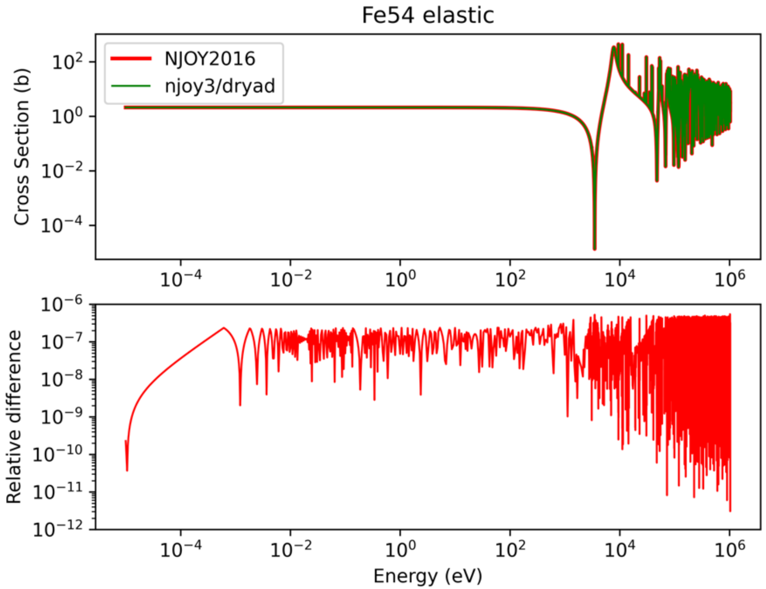
- Current status:
  - Supports ENDF-6 LRF=3 and LRF=7 resolved formats (GNDS partially implemented)
  - Supports general R-matrix and relativistic kinematics (untested)
- Cross sections are calculated by spin group
  - Intermediate matrices are available if the user so desires

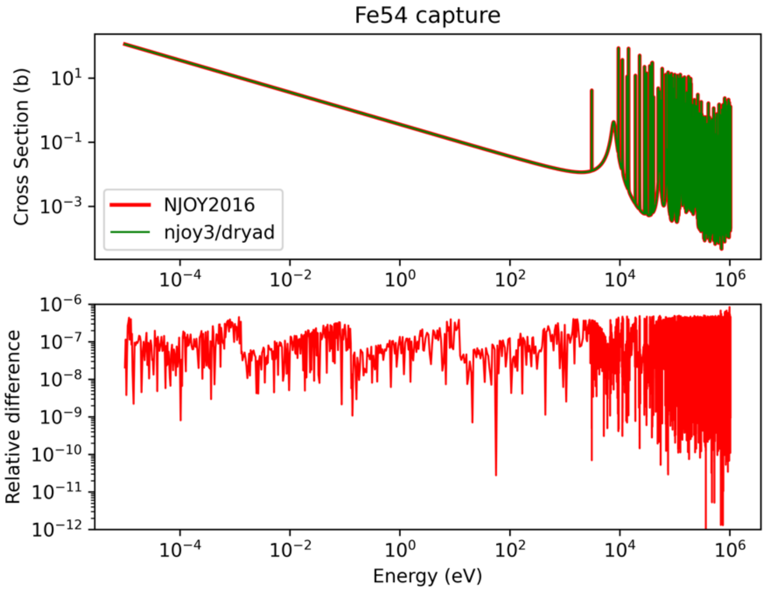
$$\sigma_{cc'} = \frac{\pi}{k^2} g_J \left| e^{iw_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'}$$

$$U = \Omega W \Omega = \Omega(I + 2iX)\Omega \qquad X = P^{1/2} R_L P^{1/2} = P^{1/2} \boxed{[(I - RL)^{-1} R]} P^{1/2}$$

Resonance reconstruction

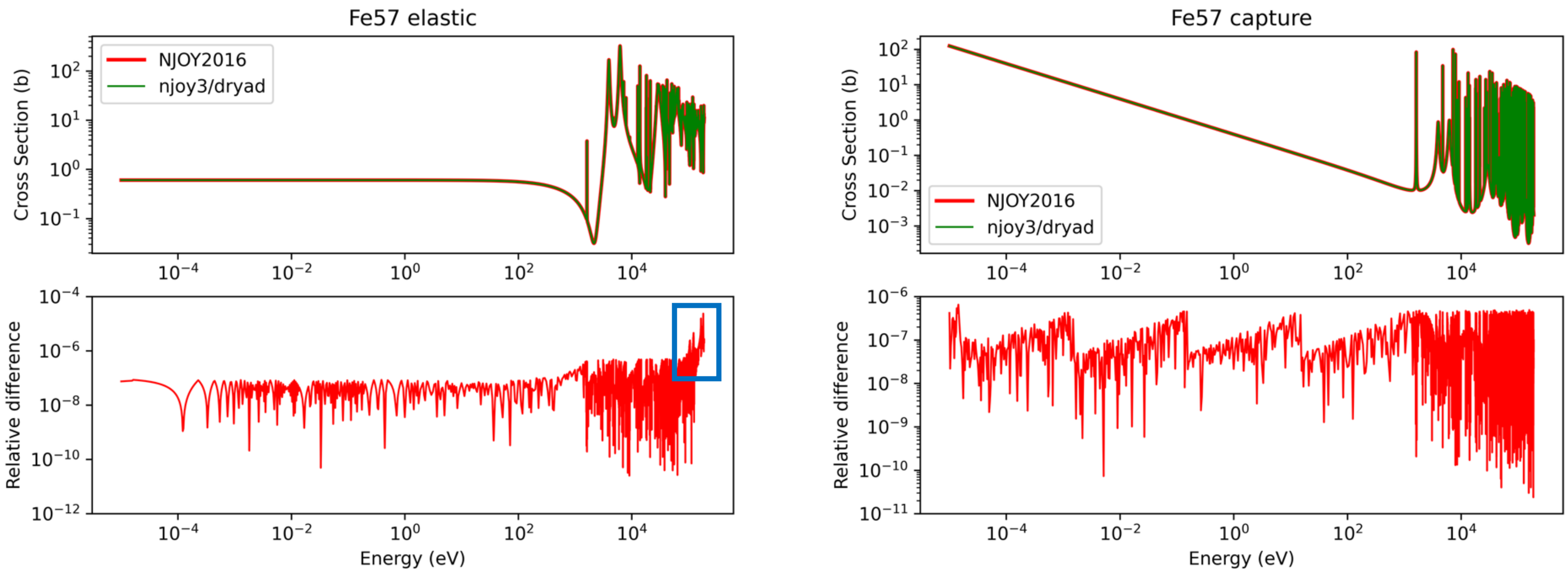
- Test case 1 : ENDF/B-VIII.1 Fe54 - elastic and capture
  - Evaluation uses LRF=7 with background cross sections (removed for test)





Resonance reconstruction

- Test case 2 : ENDF/B-VIII.1 Fe57 – elastic, inelastic (MT51) and capture
  - Evaluation uses LRF=7 without background cross sections



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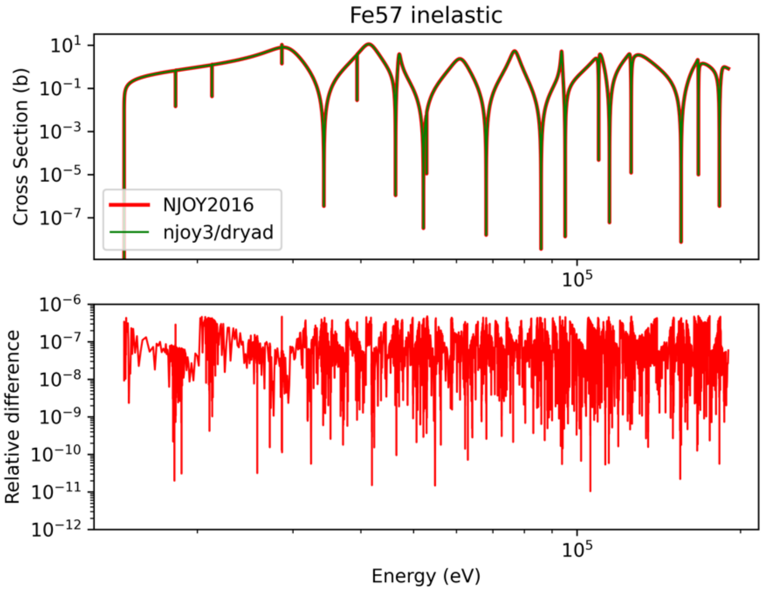
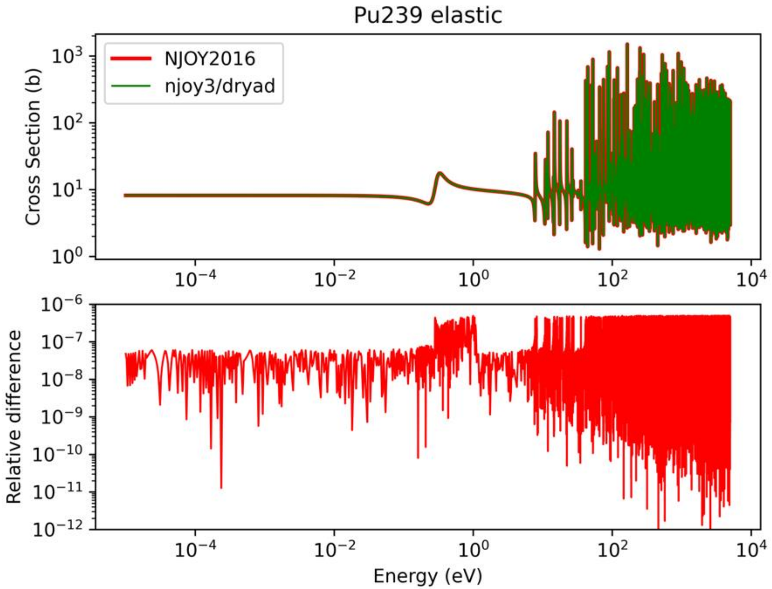
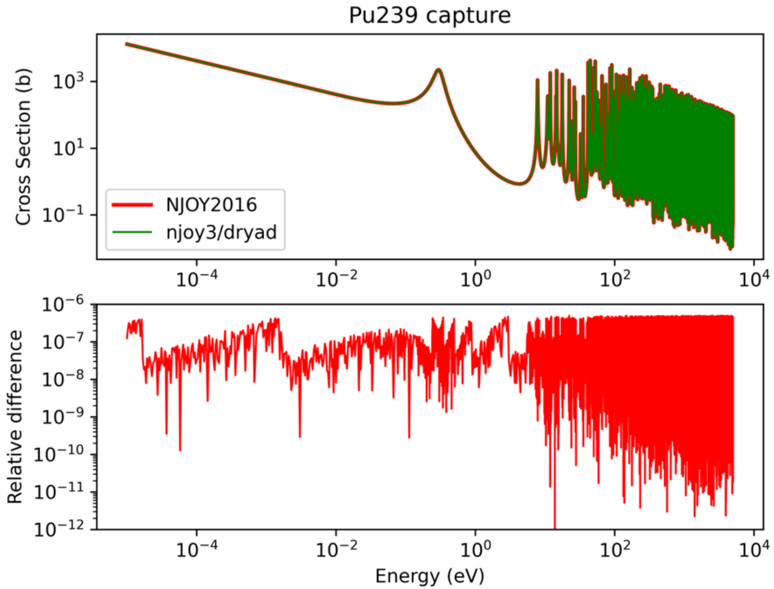


Resonance reconstruction

- Test case 3 : ENDF/B-VIII.1 Pu239 – elastic, fission and capture
  - Evaluation uses LRF=7 (duplicate energies were corrected for this test)





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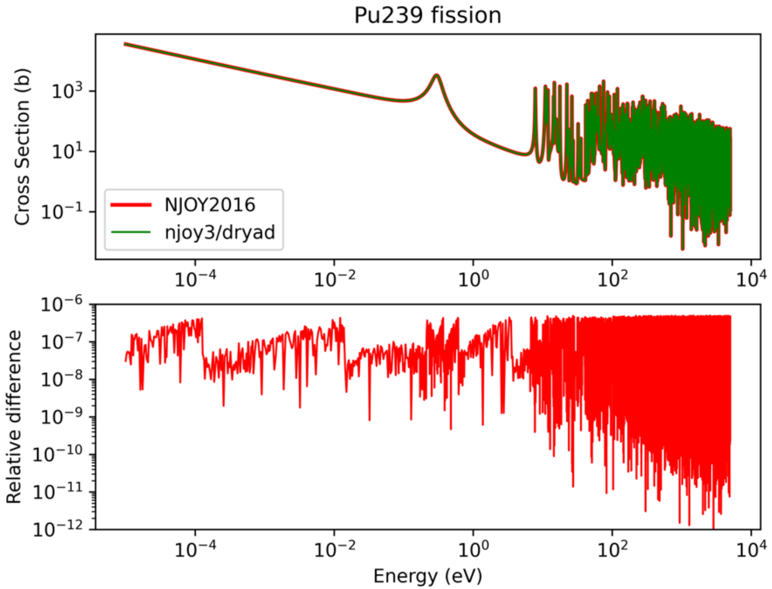
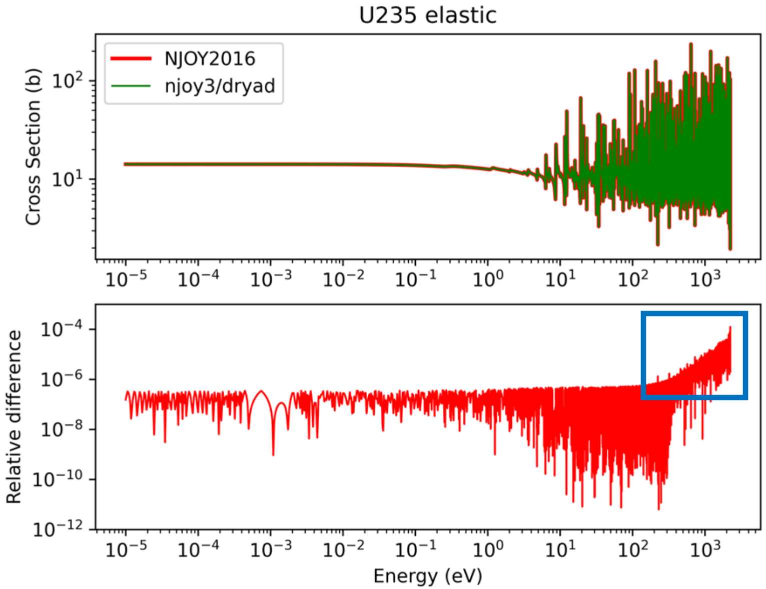
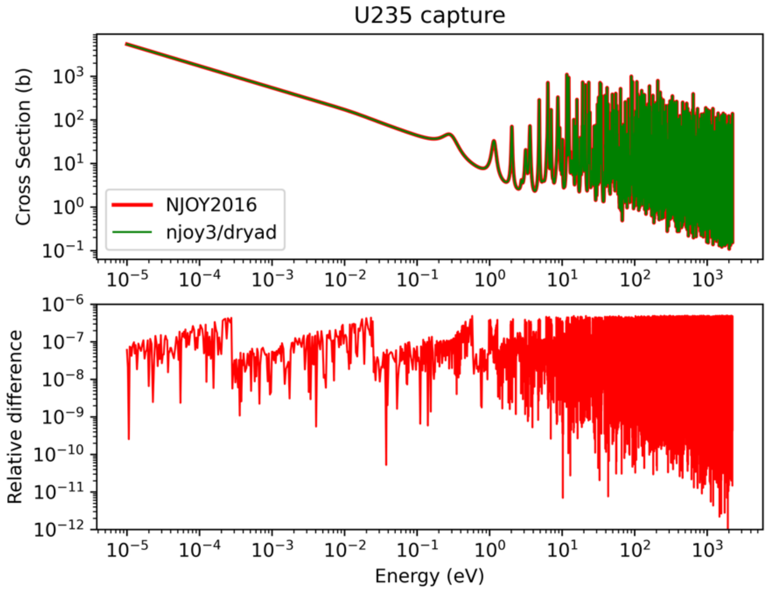


Resonance reconstruction

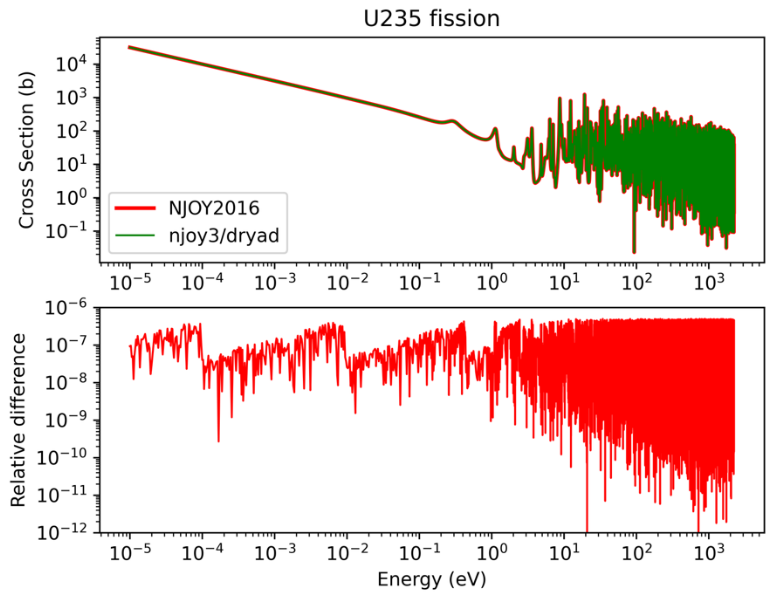
- Test case 4 : ENDF/B-VIII.1 U235 – elastic, fission and capture
  - Evaluation uses LRF=3 (translated to spin groups by modern NJOY)





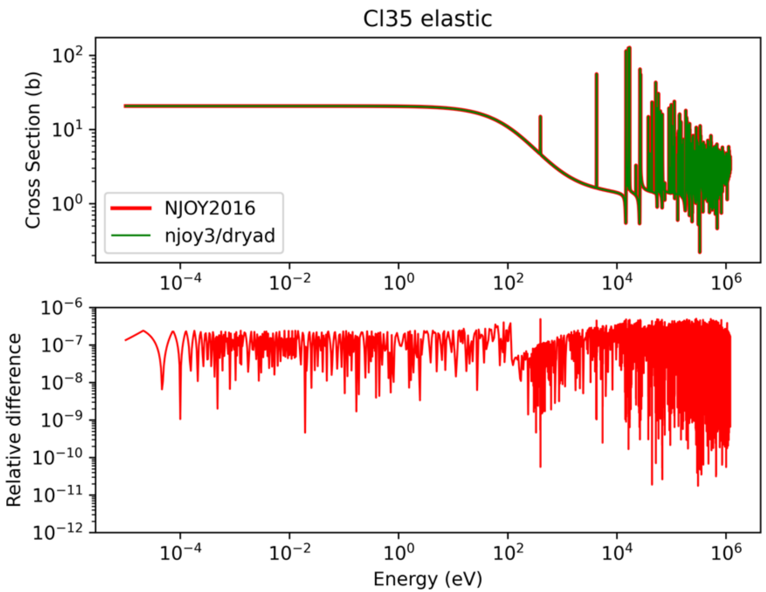
Resonance reconstruction

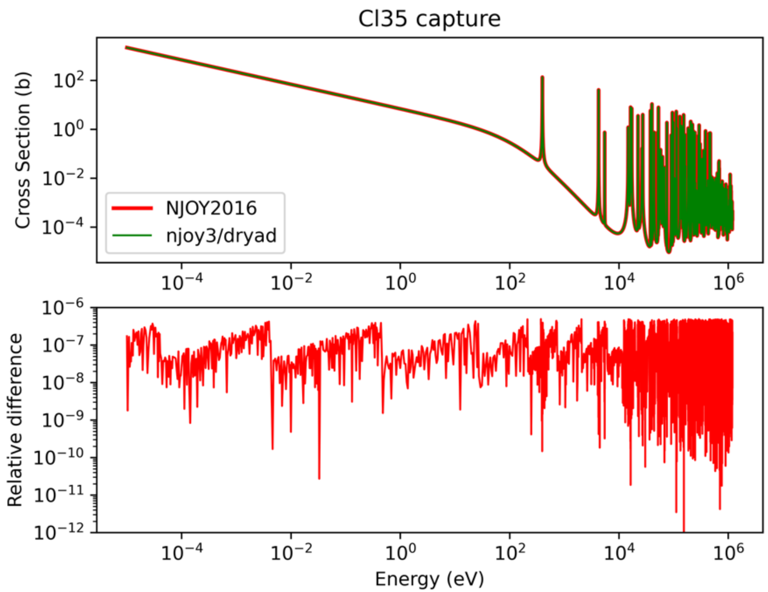
- Test case 4 : ENDF/B-VIII.1 U235 – elastic, fission and capture
  - Evaluation uses LRF=3 (translated to spin groups by modern NJOY)



Resonance reconstruction

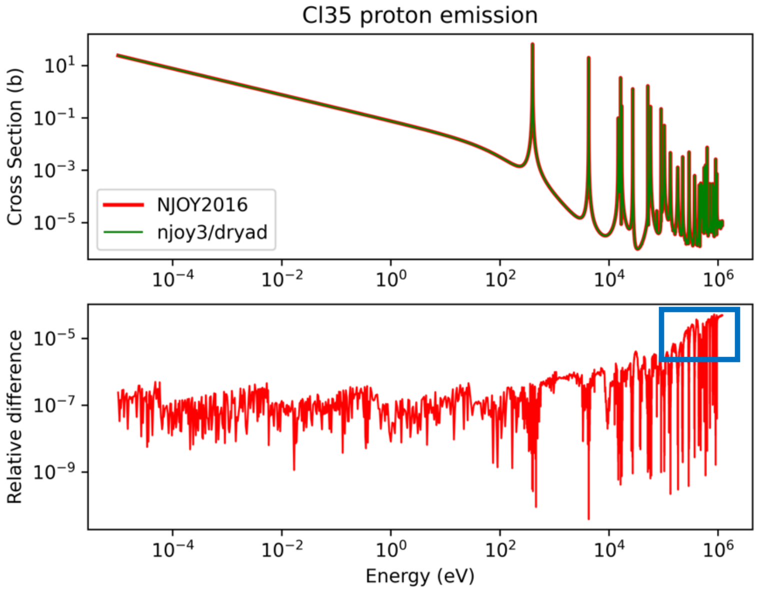
- Test case 5 : ENDF/B-VIII.1 Cl35 – elastic, p emission and capture
  - Evaluation uses LRF=7 and has one charged particle channels





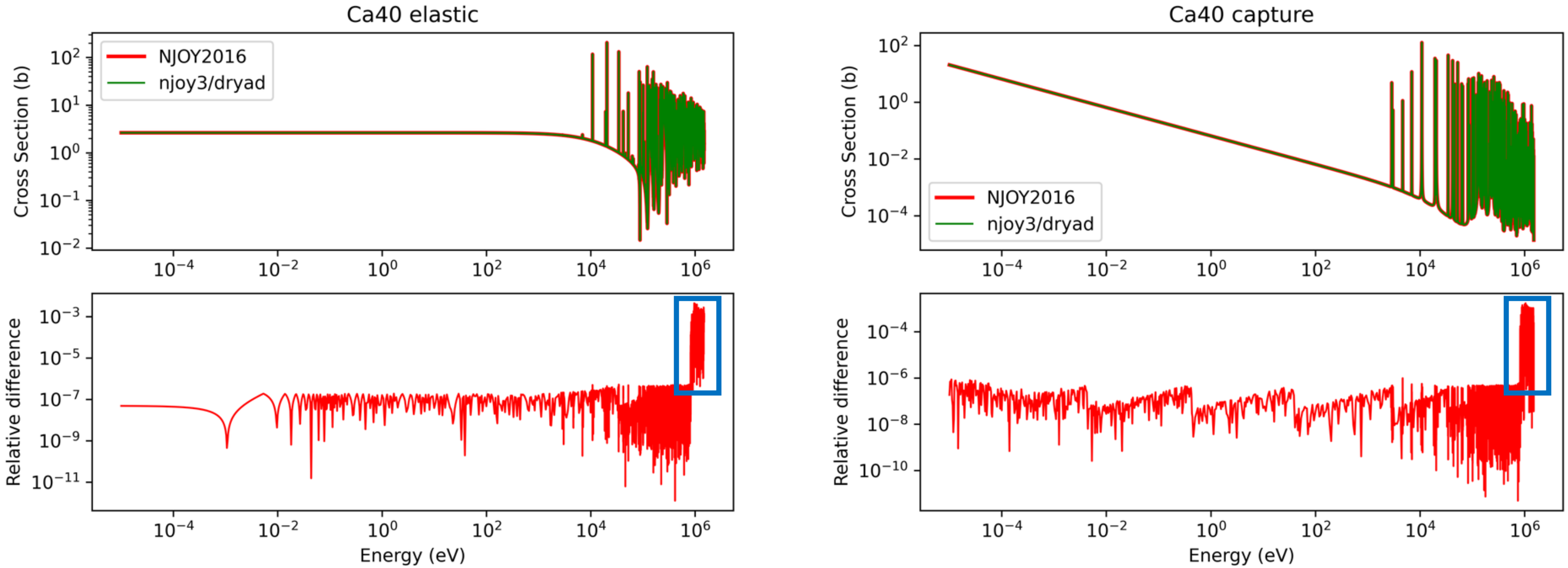
Resonance reconstruction

- Test case 5 : ENDF/B-VIII.1 Cl35 – elastic, p emission and capture
  - Evaluation uses LRF=7 and has one charged particle channels



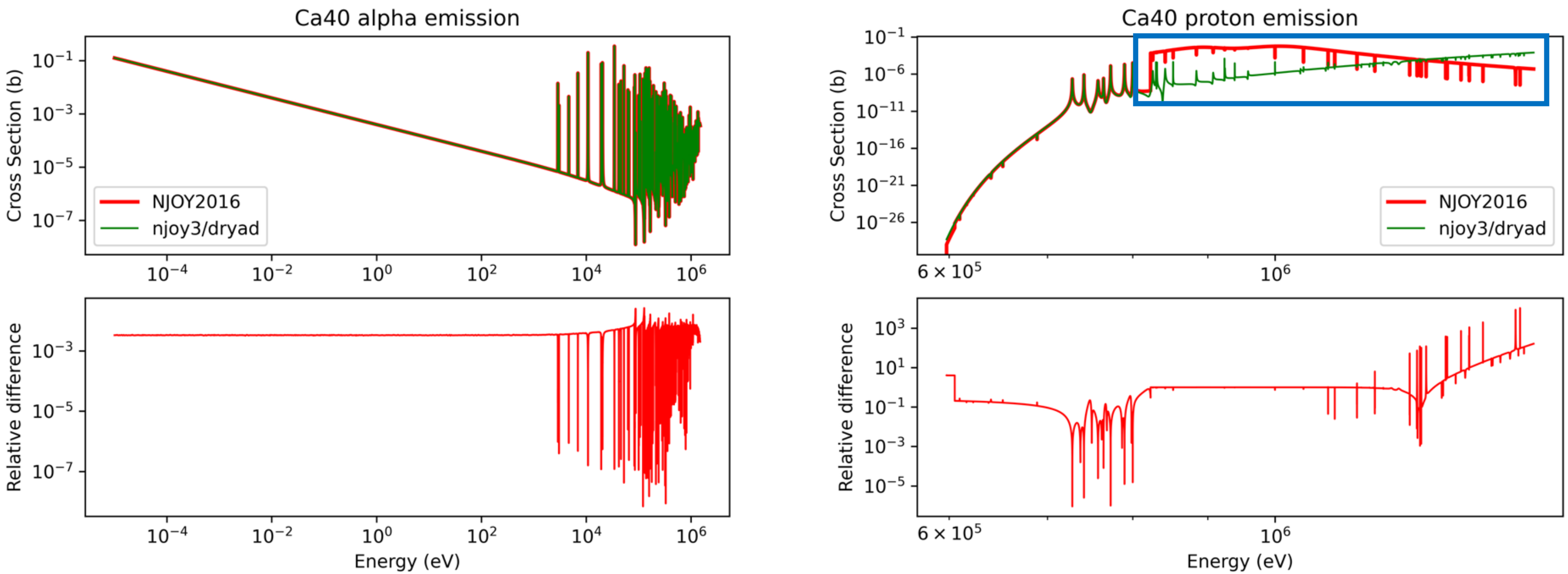
Resonance reconstruction

- Test case 6 : ENDF/B-VIII.1 Ca40 – elastic, p and α emission, and capture
  - Evaluation uses LRF=7 and has two charged particle channels



Resonance reconstruction

- Test case 6 : ENDF/B-VIII.1 Ca40 – elastic, p and α emission, and capture
  - Evaluation uses LRF=7 and has two charged particle channels



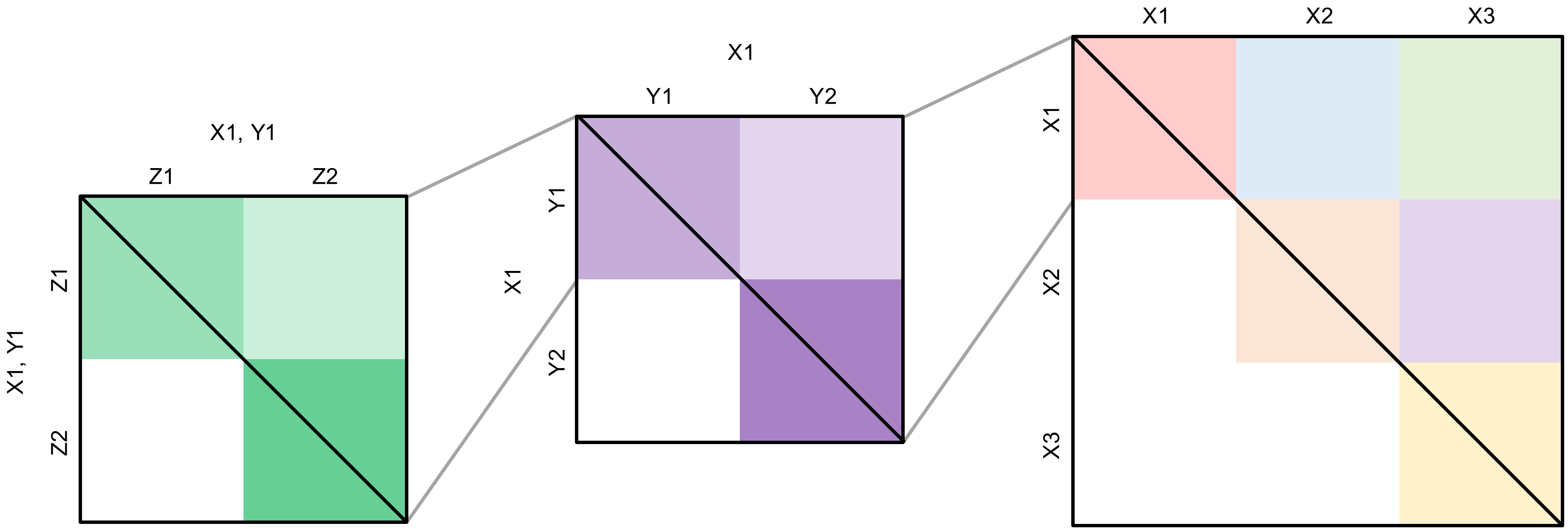
Resonance reconstruction

- Comparing run time with legacy NJOY2016 coding is difficult
  - RECONR does more than reconstructing resolved resonances
    - Both resolved and unresolved resonances
    - Linearisation and unionisation of cross sections on the same energy grid

Case	Number energies	njoy3/dryad [s]	NJOY2016/RECONR [s]
Fe54	47745	0.375	0.4
Fe57	17043	0.075	0.1
Pu239	237738	13.9	5.9
U235	232410	33.2	9.4
Cl35	25788	4.64	2.4
Ca40	29869	5.26	0.6

Covariance data structures

- A new covariance data structure that can hold covariance matrices of any dimensionality and supports on- and off-diagonal submatrices



Covariance data structures

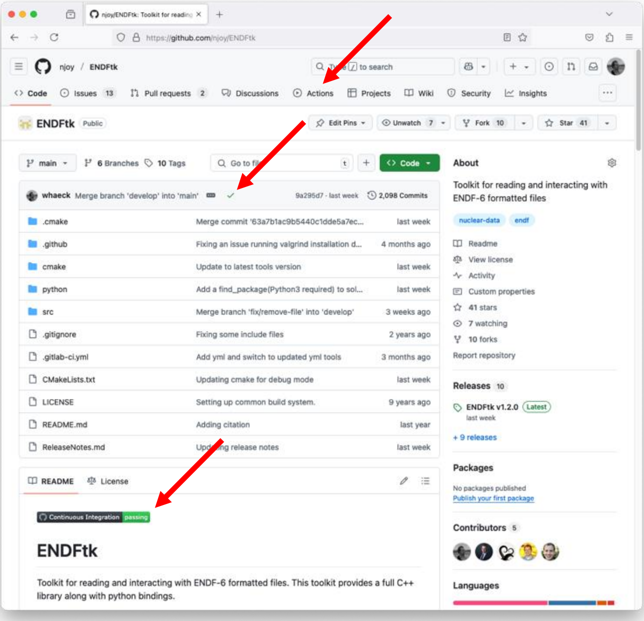
- Basic capabilities that are available in the covariance data structure:
  - Create data using covariance matrix or standard deviations and correlations
  - Derive data from the covariance matrix:
    - Covariance matrix
    - Standard deviations
    - Correlation matrix
    - Eigenvalues (eigenvectors are not stored for the moment)
  - Extraction of submatrices
- Current available for the following covariance types:
  - Cross section covariance data
  - Product multiplicity covariance data (fission yield covariances)
- Populating these from ENDF and GNDS is underway

Continuous integration

- We have traditionally used GitHub for our Continuous Integration efforts

- Great but there are limitations
  - Limited number of compilers
  - No access to the actual runners to reproduce failures
  - Runner configurations change often

Operating system	Architecture	Compilers
Ubuntu 22.02	x86_64	gcc-12, clang 14
MacOS 13	x86_64	gcc-12, clang 15
MacOS 14	Arm64 (M1)	gcc-12, clang 15



Continuous integration at LANL

- We now have Continuous Integration internally at LANL
  - More compilers, more operating systems and more architectures
  - Easier debugging since we have access to the runners used

- All development is now done on internal repositories at LANL
  - Merges into the `main` and `develop` branches are pushed to GitHub automatically
  - External contributions through GitHub are still possible

Operating system	Architecture	Compilers
Red Hat 8	x86_64	gcc-7 through gcc-15, intel-classic 2021.9.0, intel-llvm 2024.2.1
Windows	x86_64	msvc 19.42
MacOS 15	arm64 (M2)	Apple clang 17.0.0, clang-llvm 16.0.5, 17.0.6 and 18.1.8

Conclusions and future work

- The following ENDF/B-VIII.1 libraries for MCNP have been released
  - Incident neutron data: Lib81
  - Thermal scattering data: ENDF81SaB
- We are working on a few errata files:
  - Primary gamma data processing in ACER has issues
- NJOY modernization work foreseen in FY26:
  - Thermal scattering data structures in `njoy.dryad` (thank you ORNL)
  - More secondary particle distributions in `njoy.dryad`
  - Resolved resonance reconstruction
  - Covariance data from ENDF-6 and GNDS with some basic processing
  - Photoatomic and electroatomic ACE files