Los Alamos NATIONAL LABORATORY

Overview of NJOY work for NCSP FY23

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Outline

- Updates to NJOY2016 related to ENDF/B-VIII.1
  - MF7 MT451
  - Background R-matrix elements
  - Other notable changes
- Update on the NJOY modernisation
  - ENDFtk, ACEtk
  - scion

Our main objective: smooth processing of ENDF/B-VIII.1

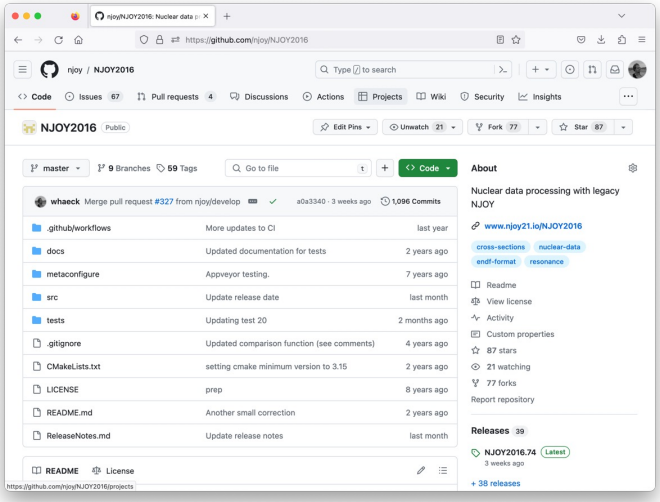
- Every new ENDF/B generation changes formats and adds new data

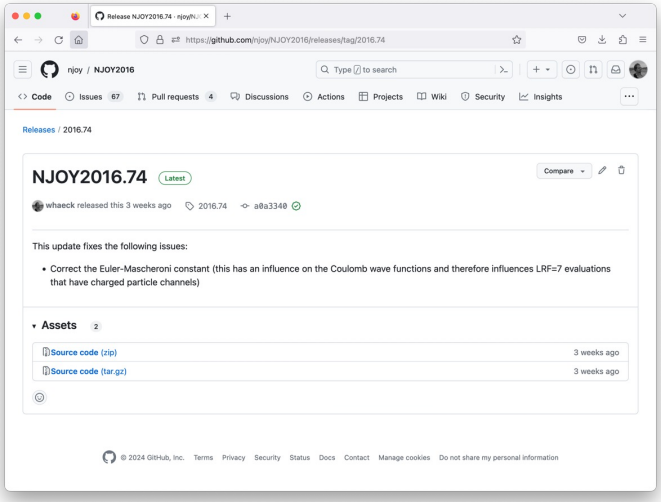
- The future library: ENDF/B-VIII.1 (somewhere in 2024)
  - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
  - Improved photonuclear data
  - Thermal scattering information in MF7 MT451
  - Background R-matrix elements for resonance parameters in MF2 MT151

- NJOY2016 should be able to handle or at the very least be able to read these
  - New features that require changes in MCNP have been prioritised
  - As a result, MCNP6.3 already supports these new ENDF/B-VIII.1 features

Maintaining our production version

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





- Latest version is NJOY2016.74 (January 2024)
  - 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

Thermal scattering information in MF7 MT451

- MF7 MT451 was approved as a format option this year
  - It provides composition and other relevant data on the molecule or crystal unit cell
  - A number of LIST elements per element
  - Each list gives isotopes, isomeric state, abundance, AWR and cross section values

- NJOY2016 does not use this data but can handle its presence in an ENDF file
  - Modifications were made to MODER only
  - We will make use of this in a modernised version of NJOY

- NJOY2016.71 (July 2023) is required when MF7 MT451 is present

Background R-matrix elements in MF2 MT151

- MF2 MT151 changes were approved in 2021
  - Background R-matrix elements have been in the ENDF manual for a long time
  - The format description had errors in it that were fixed

- Multiple options are available:
  - No background
  - Arbitrarily tabulated complex function
  - SAMMY parametrisation
  - Frohner parametrisation

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_\lambda - E - i\,\Gamma_{\lambda\gamma}/2} + R_c^{\mathrm{bkg}}\, \delta_{cc'} \right] \delta_{JJ'}. \qquad \text{(D.76)}$$

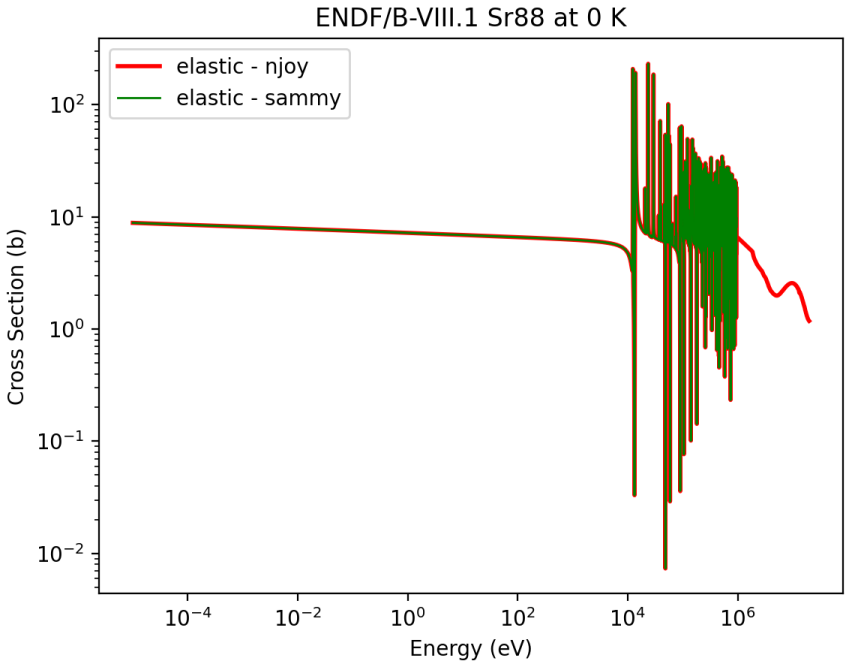
- An ORNL Sr88 evaluation now uses the SAMMY parametrisation option

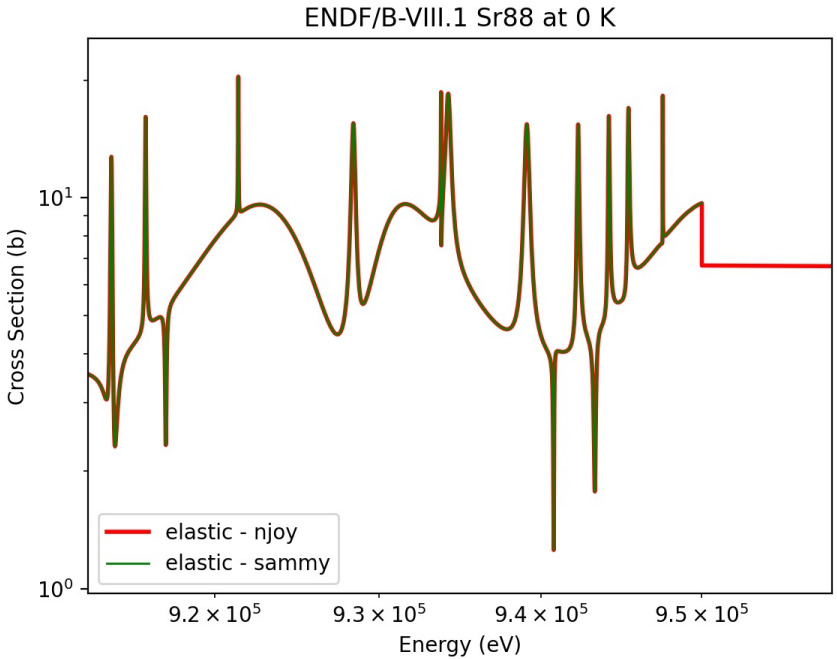
- NJOY2016.73 (November 2023) is required for background R-matrix elements

Background R-matrix elements in MF2 MT151

- Changes were required in the following NJOY2016 modules:
  - MODER:
    - read over the background R-matrix element information
  - RECONR:
    - Add a few requirement tests to protect against NJOY2016 limitations
      - Background R-matrix elements are only allowed in LRF=7, KRM=3 (Reich-Moore)
      - NJOY2016 does not handle reduced resonance widths (IFG=1)
    - Add the background R-matrix element to the R-matrix
    - All options are supported although we only validated the SAMMY parametrisation
      - This new capability was tested in collaboration with ORNL
  - ERRORR:
    - Add derivatives to the background R-matrix elements
    - This currently only supports the SAMMY parametrisation and has not been validated

Background R-matrix elements in MF2 MT151



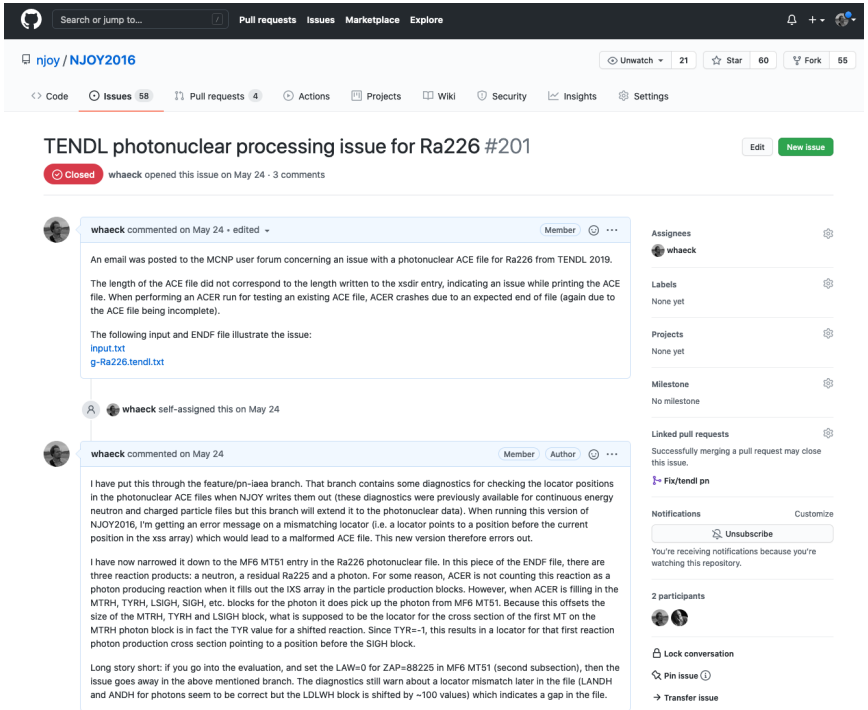


Other noteworthy updates to NJOY2016

- NJOY2016.70:
  - Primarily fixes in HEATR that may lead to differences with previous versions
- NJOY2016.72:
  - ERRORR now allows for the selection of the MF34 sub-subsection to be calculated
  - By default, the L=1,L1=1 sub-subsection will be calculated which in almost all cases will correspond to the first sub-subsection in the MF34 data
- NJOY2016.73:
  - Fixes in LEAPR to properly run some of the input files used for the ENDF/B-VIII thermal scattering files

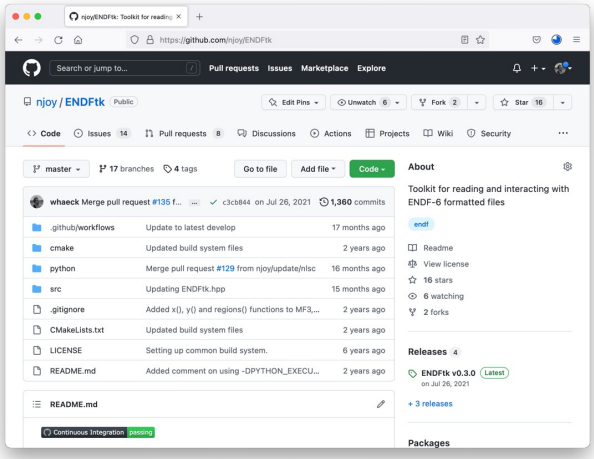
When you see something, say something

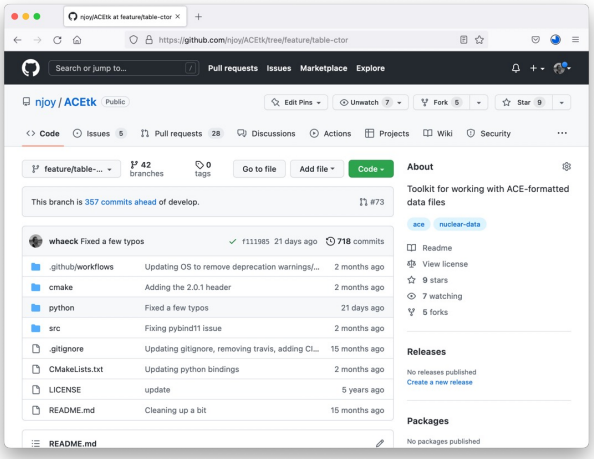
- We try to fix issues in NJOY2016 as soon as they become apparent
  - Sr88 R-matrix background elements
  - LEAPR input files segfaulting
  - IAEA updates



So what about the NJOY modernisation?

- NJOY21: shift from a module based to a component based modernisation
  - Modernised modules are built from components
    - Components provide formats (e.g. ENDF, ACE, GNDS) or processing operations (e.g. scion)
    - Components can be developed and deployed faster than modules
  - Using a C++ and Python API at the same time
  - Regular releases with testing and validation





ENDFtk and ACEtk development is almost completed

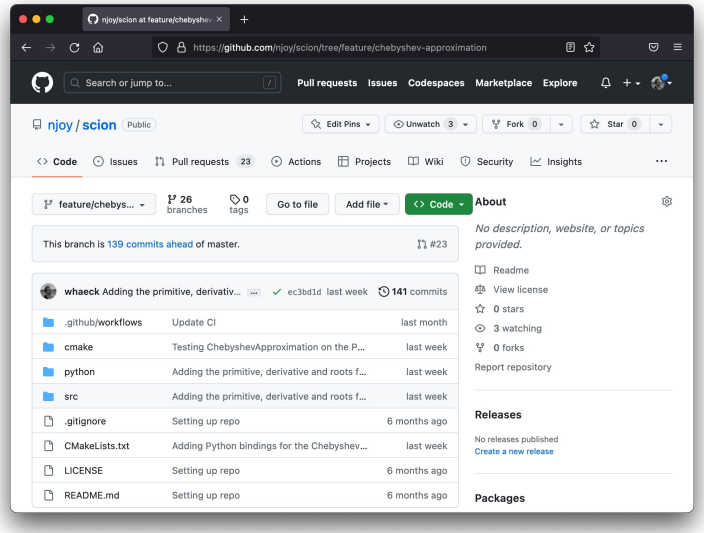
- ENDFtk: https://github.com/njoy/ENDFtk
  - ENDFtk v1.0.0 (February 5, 2024): now with full ENDF compatibility
- ACEtk: https://github.com/njoy/ACEtk
  - ACEtk v0.1.0:
    - Incident neutron and charged particle ACE files
    - Photoatomic (including eprdata files) and photonuclear ACE files
    - Thermal scattering ACE files
    - Dosimetry ACE files

- Look out for v1.0 releases of both toolkits soon!
  - Updating cmake build systems and unit test framework update
  - Add an installation option
  - Updating dependencies

So we can read and write data, now what?

- Most NJOY modules need to perform a common set of operations:
  - Interpretation of various data representations (tables, analytical functions, etc.)
  - Linearisation of various data representations
  - Unionisation of data on a common energy grid, etc.
  - Differentiation and integration of the data

- This will be the job of SCION
  - SCientific interpretatION, linearisatION, differentiatION, integratION and more IONs
  - It will provide a format agnostic data interface

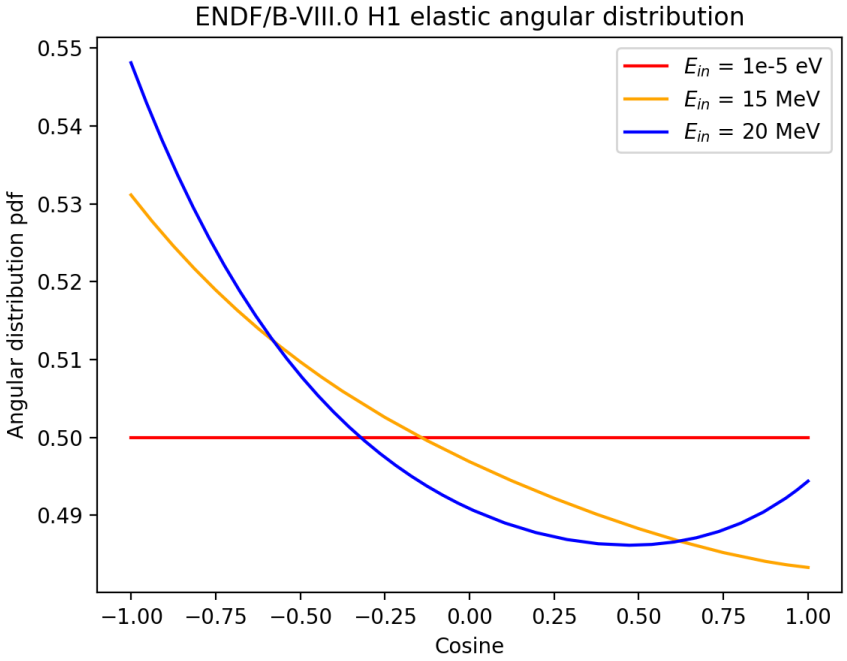


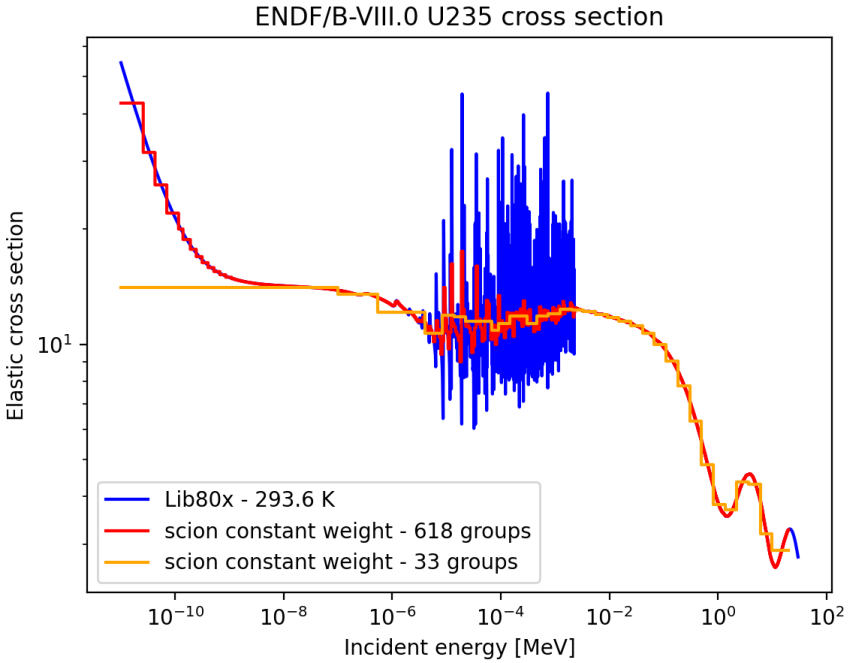
Current capabilities in SCION

- Functional interpretation of tabulated data using various interpolation schemes
- Functional interpretation of polynomial based expansions
  - Normal power series, Legendre series and Chebyshev series
  - Root finding for the general case f(x) = a using the companion matrix
  - Integration and differentiation can be performed using a functional interface

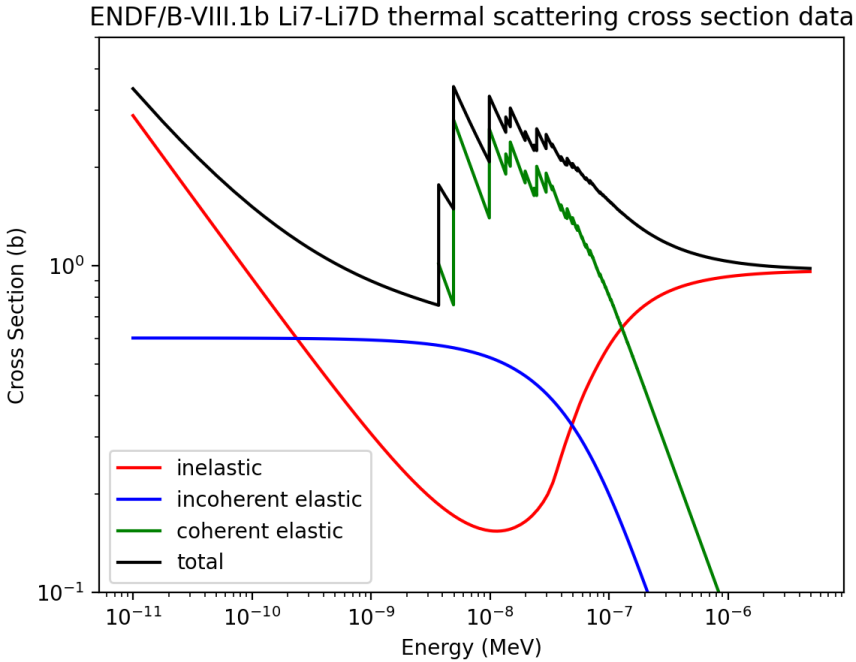
- Generic linearisation of functions
  - Extensible interface for convergence and panel splitting
- Common mathematical capabilities
  - Horner and Clenshaw recursion for polynomial evaluation
  - Newton-Raphson for root finding
  - Special mathematical functions

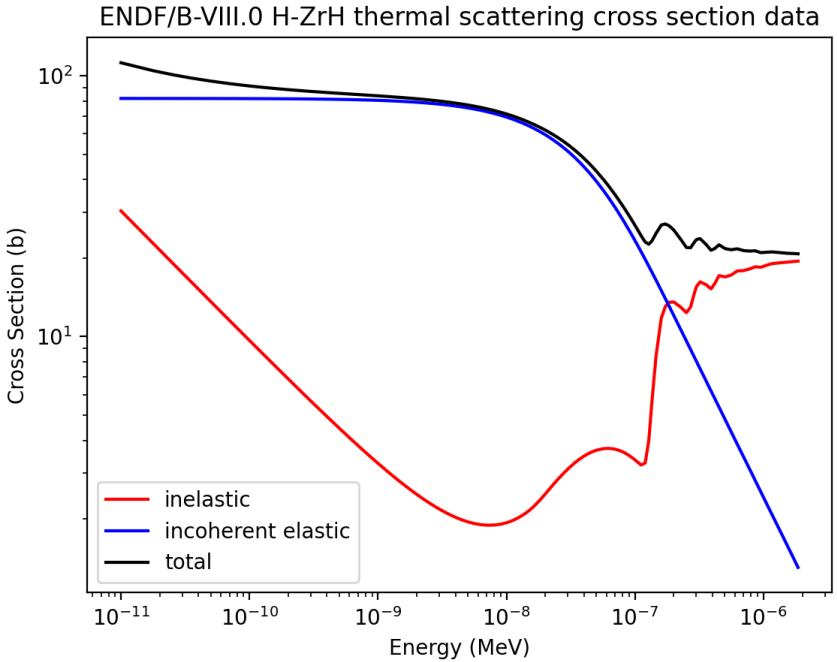
Current capabilities in SCION





Current capabilities in SCION





Our focus for next year

- Continue maintenance of NJOY2016 with respect to ENDF/B-VIII.1
  - This includes updating the NJOY2016 dependency in NJOY21 for those who use it

- NJOY modernisation:
  - Covariance related work (codex)
  - Resonance reconstruction overhaul
  - Processing the latest photoatomic and electron (EPICS) data into ACE files for MCNP