Los Alamos
NATIONAL LABORATORY

NJOY for ENDF/B-VIII.1

W. Haeck, N. Gibson, N. Kleedtke

CSEWG, October 31 – November 4, 2022

Outline

- Which version of NJOY should you use?
- What has changed since last year for NJOY2016?
- NJOY modernisation work over the last year

Which version of NJOY should you use?

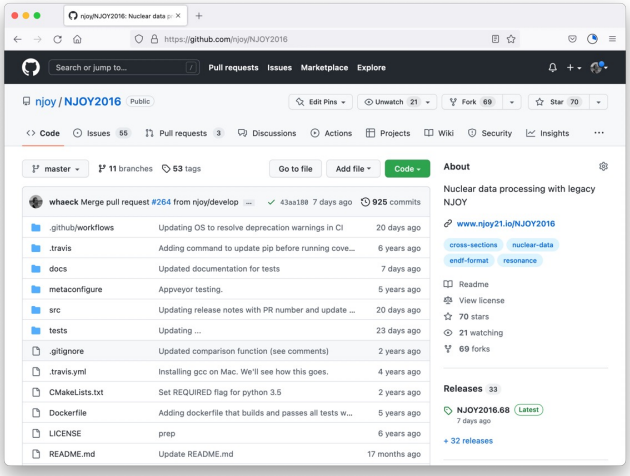
- NJOY has been around for over 40 years now
  - Major versions: NJOY99, NJOY2012, NJOY2016, NJOY21

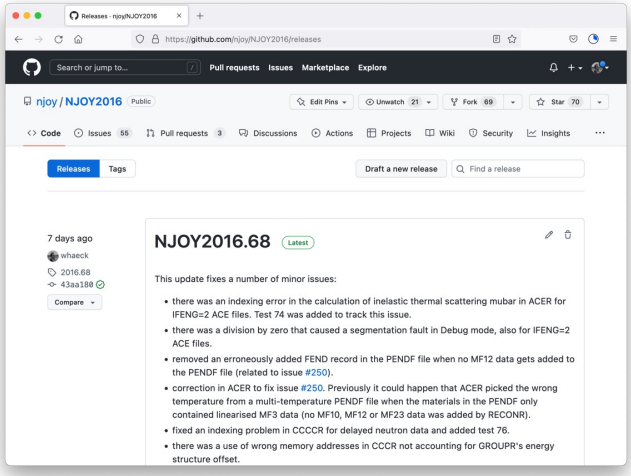
- NJOY2016 is the production version in use at LANL
  - The MCNP ENDF/B-VIII.0 library was produced using NJOY2016
  - The MCNP ENDF/B-VIII.1 library be produced using NJOY2016
  - Latest version is NJOY2016.68 (September 2022)

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

Maintaining our production version

- 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

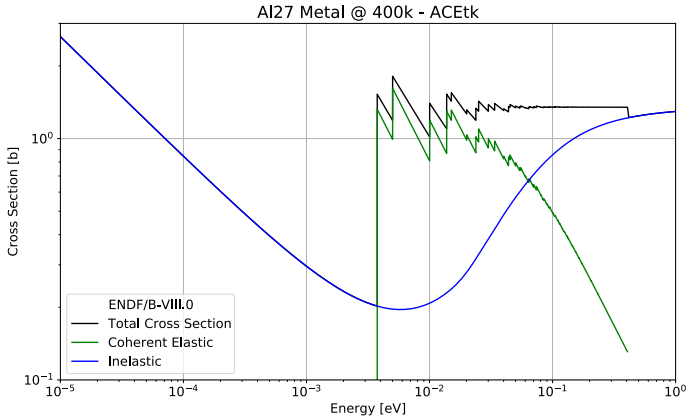
Our main objective: smooth processing of ENDF/B-VIII.1

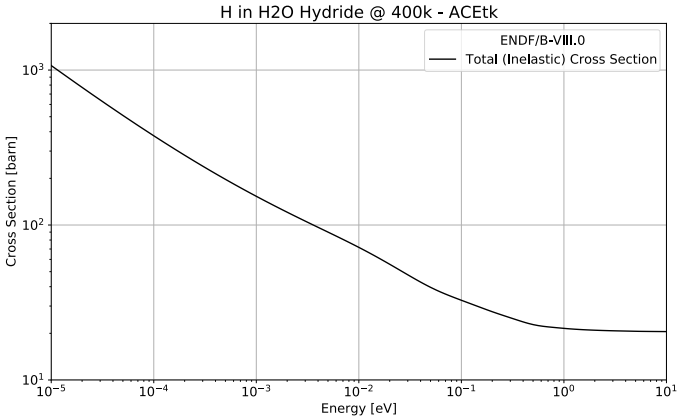
- Every new ENDF/B generation changes formats and adds new data

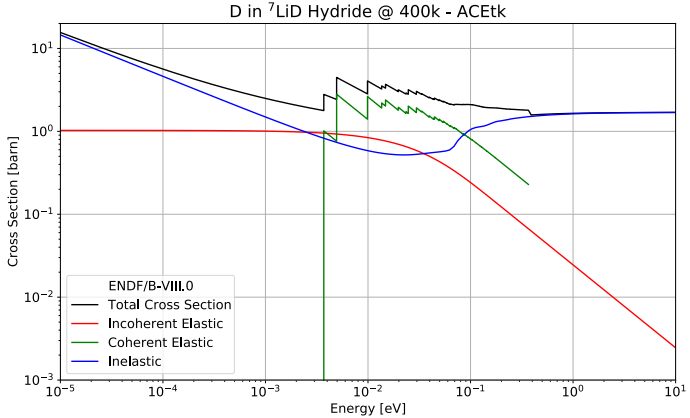
- The future library: ENDF/B-VIII.1
  - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
  - Improved photonuclear data
  - Background R-matrix elements for resonance parameters in MF2 MT151
  - General R-matrix formalism (KRM = 4) in MF2 MT151

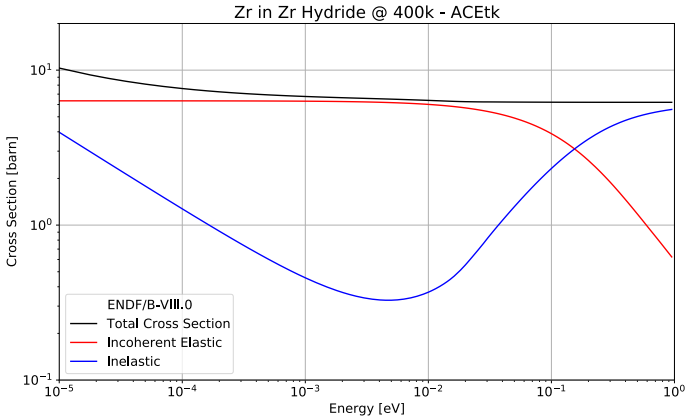
- Caveat: if these impact the ACE format, MCNP needs to be updated too
  - These changes are prioritised due to the involvement of MCNP
  - Changes are made in collaboration with the MCNP development team

Thermal scattering data

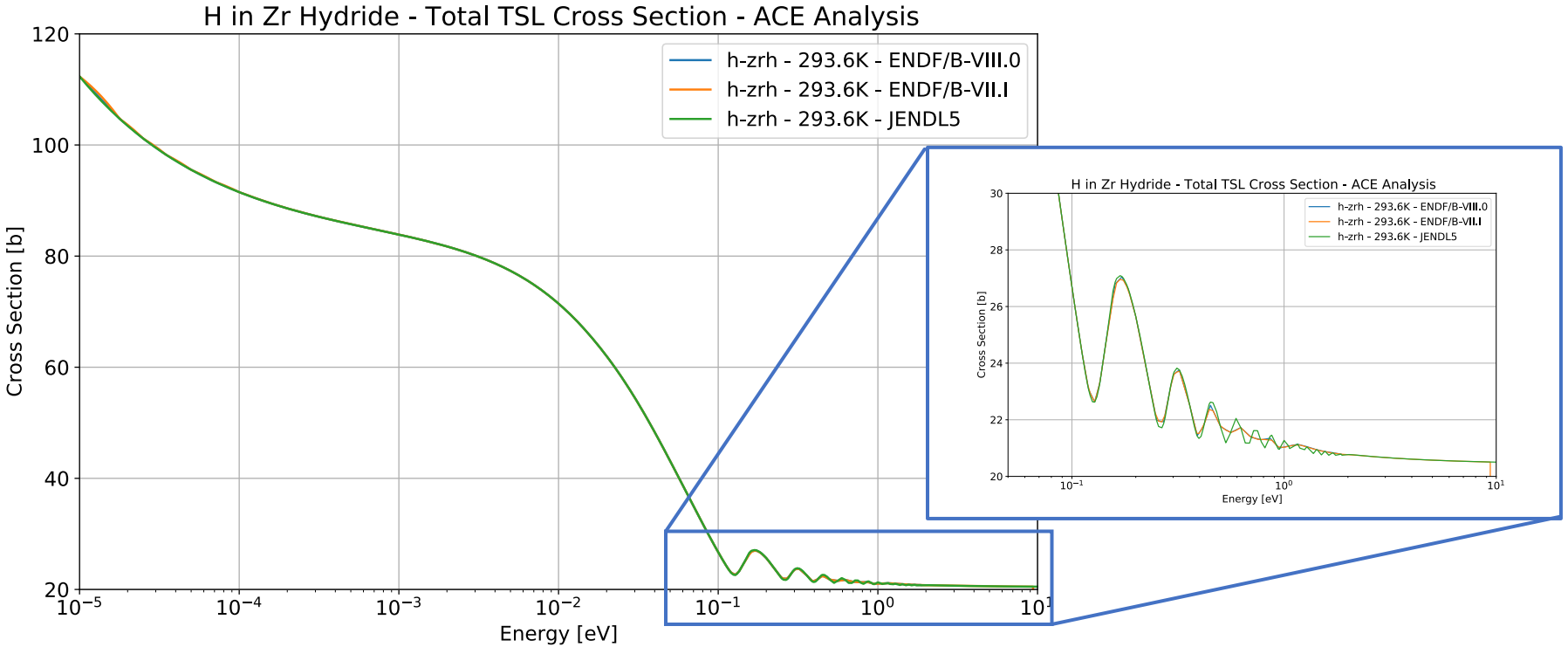






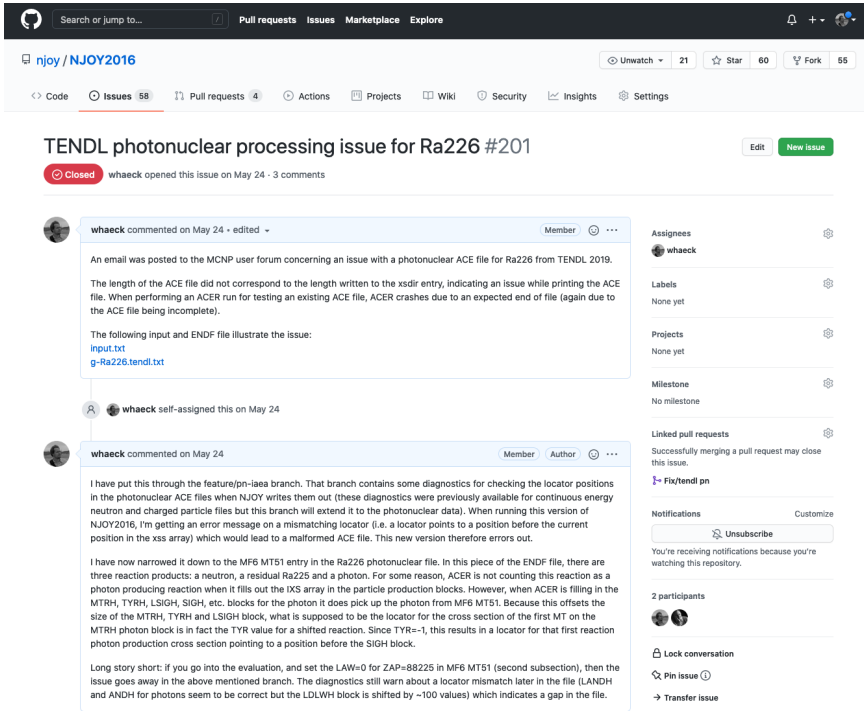


Thermal scattering data



What else are we doing to prepare for ENDF/B-VIII.1?

- Fix issues in NJOY2016 as soon as they become apparent
  - When you see something, say something
- Test NJOY2016 processing of new libraries as they come out
  - Quite a few new libraries in 2022
  - TENDL, JENDL5, JEFF4



Processing the ENDF/B-VIII.1 beta0 libraries

- The first beta version has been processed into MCNP data libraries
  - A single temperature (293.6 K) instead of our multi-temperature libraries
  - Validation work is ongoing (see the validation session)

- No major processing issues have been detected so far, but …
  - This is only the incident neutron library and does not include all ENDF/B-VIII.1 candidate evaluations (e.g. Ta, O16, etc.)
  - No thermal scattering evaluations were included in the beta0 release

- We are going to process more ENDF/B-VIII.1 sub-libraries
  - Incident charged particle data
  - Photonuclear and/or photoatomic data

Overview of some of the NJOY2016 changes

- Mixed mode elastic thermal scattering (NJOY2016.66)

- Photonuclear ACE files in ACER (NJOY2016.66)
  - Secondary photon distributions traditionally given using the LAW=1 LANG=1 format using a single Legendre coefficient (i.e., an isotropic distribution)
    - This assumption was hardcoded in NJOY2016's ACER module
    - This changed with the new IAEA photonuclear data library
  - Secondary photon distributions in the ACE file can now be tabulated (ACELAW = 61)

- Caveat: MCNP6.3 is required for photonuclear and thermal scattering ACE files produced by NJOY2016.66 and above

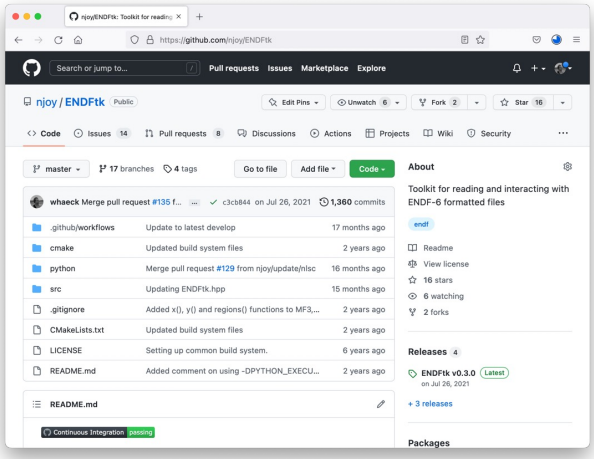
Overview of some of the NJOY2016 changes

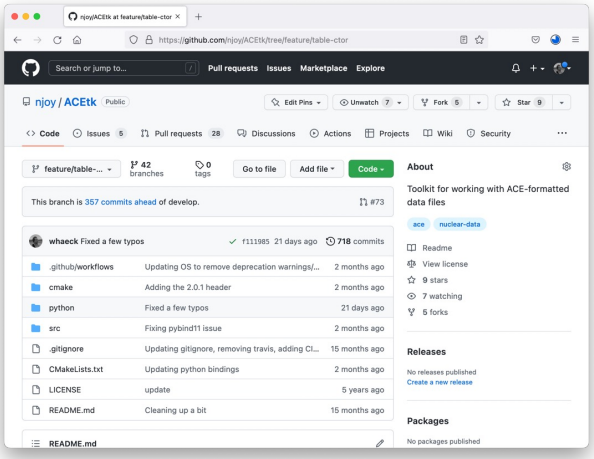
- Angular covariance data processing in ERRORR (NJOY2016.66)
  - ENDF MF34 format allows for multiple sub-subsection associated to pieces of the covariance matrix associated to MTA LA, MTB LB pairs
  - Previous versions of NJOY2016 crashed on files that had multiple sub-subsections
    - For example: U235 from ENDF/B-VIII.0
  - This crash has been fixed but we need an updated GENDF format for the results
    - Only the first sub-subsection is printed out
  - Note: there still is an issue when running multiple MF34 calculations in a single run

- Updated ACE locator consistency checks (NJOY2016.66)
  - Locator checking for photonuclear and thermal scattering files has been enabled
  - Previously only available for incident neutron and charged particle ACE files
- NJOY2016.67 and NJOY2016.68 provide minor fixes

What does the future bring?

- NJOY21: shift from a module based to a component-based modernisation
  - Modernised modules are built from components
    - Components provide formats (ENDF, ACE) or processing operations (resonance reconstruction)
    - 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





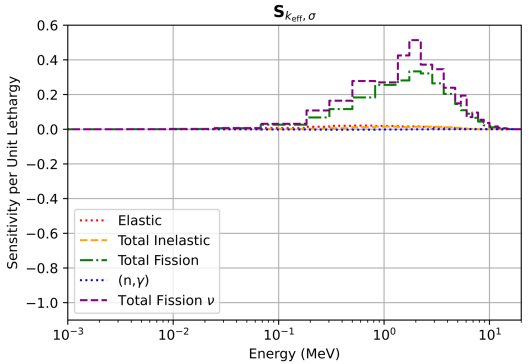
ENDFtk and ACEtk development

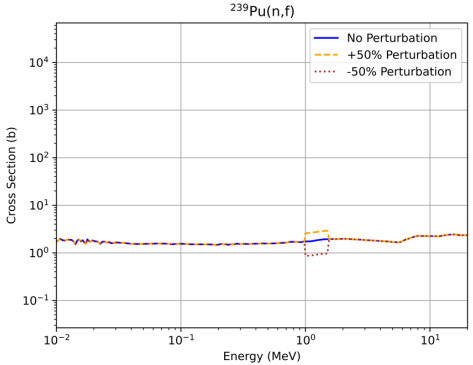
- ENDFtk: https://github.com/njoy/ENDFtk
  - Mainly work on covariance data: MF31, MF32, MF33, MF34, MF35 and MF40
  - Adding functionality for manipulating ENDF files
    - Inserting, replacing and removing materials, files and sections
    - Updating the directory of the ENDF file
  - Look out for a v1.0 release soon …

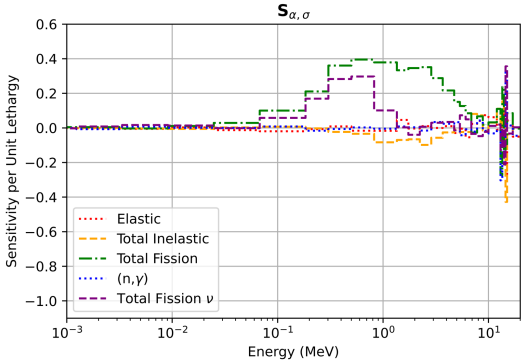
- ACEtk: https://github.com/njoy/ACEtk
  - This was the main focus for us in FY21
  - We now have full support for the following ACE file types:
    - Incident neutron and charged particle ACE files
    - Photoatomic and photonuclear ACE files
    - Thermal scattering ACE files

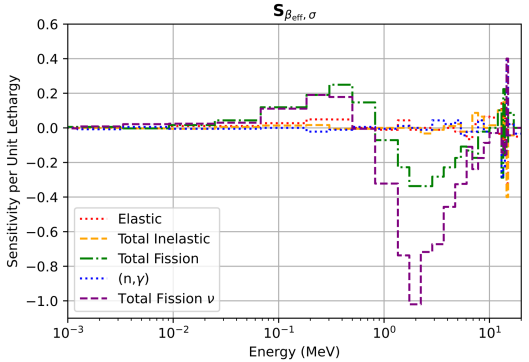
Perturbing existing ACE files for sensitivity calculation

- Perturbing individual reactions in an ACE file
  - Change the cross section in the requested energy region
  - Rebalance total and disappearance
  - Adjust internal ACE locators
- Useful for the calculation of sensitivity profiles

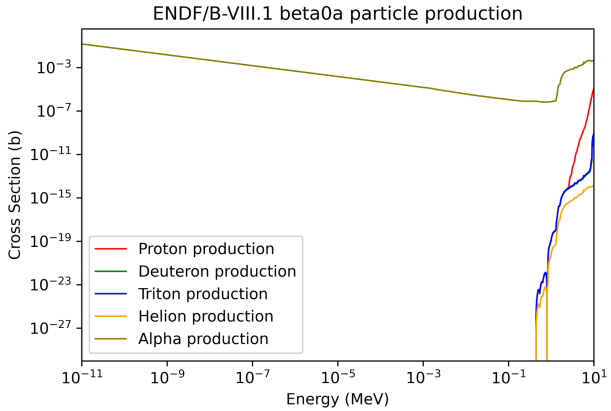


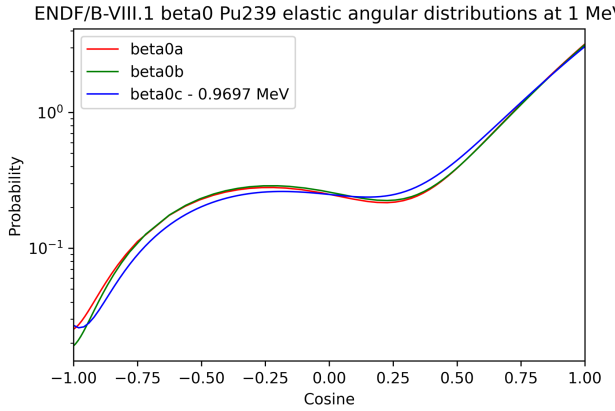


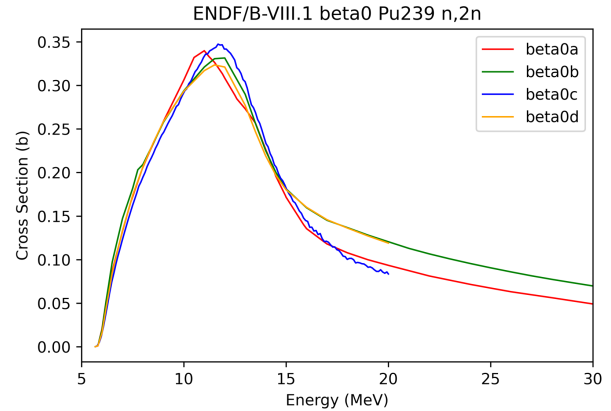


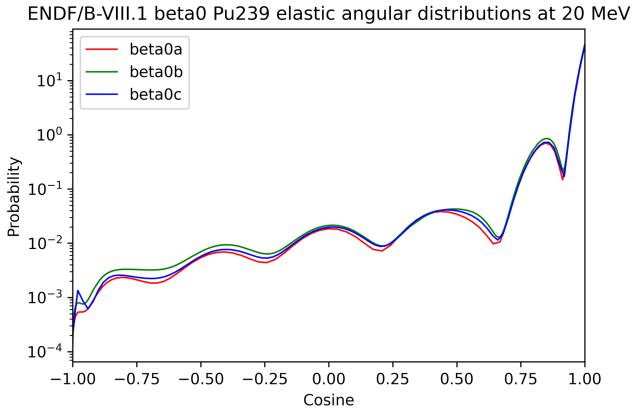


Plotting data out of ACE files









Conclusions

- We continue to maintain and improve NJOY2016 for ENDF/B-VIII.1
  - Implement new ENDF features (e.g. thermal scattering files)
  - Fix issues in NJOY2016 as soon as they become apparent
  - Processing new libraries as they come out (TENDL, JEFF, JENDL, etc.)
  - Processing all ENDF/B-VIII.1 beta libraries as they will come out

- We continue our work on NJOY modernisation
  - ACEtk and ENDFtk are production ready
  - This fiscal year will be for processing components!
    - Interpretation, linearisation, etc.
    - General R-matrix in resonance reconstruction