

## Overview of NJOY work for NCSP FY22

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# Outline

1. Our main objective: ENDF/B-VIII.1 (and ENDF/B-IX)
2. NJOY2016
  1. What has changed since last year for NJOY2016?
  2. Priorities for this year
3. NJOY modernisation
  1. Overview of modern components available to users
  2. Priorities for this year



# 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



# 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
  - Use our issue tracker on GitHub!
- Test NJOY2016 processing of new libraries as they come out
  - Quite a few new libraries in 2022
  - TENDL, JENDL5, JEFF4

The screenshot shows a GitHub issue page for the repository 'njoy / NJOY2016'. The issue title is 'TENDL photonuclear processing issue for Ra226 #201', which is marked as 'Closed'. The issue was opened by user 'whaeck' on May 24 and has 3 comments. The first comment, also by 'whaeck', describes an email received from the MCNP user forum about a photonuclear ACE file for Ra226 from TENDL 2019. It notes that the length of the ACE file did not correspond to the length written to the xsdir entry, causing ACER to crash. The comment includes links to 'input.txt' and 'g-Ra226.tendl.txt'. A second comment by 'whaeck' indicates they self-assigned the issue on May 24. The third comment, also by 'whaeck', details the investigation: they narrowed it down to the MF6 MT51 entry in the Ra226 photonuclear file. It explains that three reaction products (neutron, residual Ra226, and photon) were present, but ACER was not counting the photon reaction as a photon-producing reaction, leading to a mismatch in the 'XS' array. The comment further explains that the mismatch was due to the photon block being shifted by the size of the MTRH, TYRH, and LSIGH blocks, which offsets the photon production cross section. A long story short, the issue was resolved by setting the LAW=0 for ZAP=89225 in the MF6 MT51 section, which corrected the photon production cross section.



# Overview of NJOY2016 updates in FY22

- 4 NJOY2016 updates were released (updates 2016.65 to 2016.68)
- 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 NJOY2016 updates in FY22

- 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
  - 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
- Due to an internal compiler error, gcc-11 will not be supported for NJOY2016
  - This internal compiler error occurs in ERRORR
  - Users should consider moving to gcc-12 or any version from gcc-7 to gcc-10.



# NJOY2016 priorities for FY23

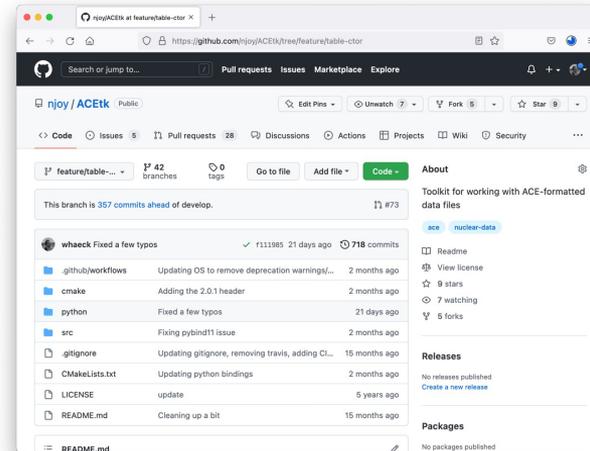
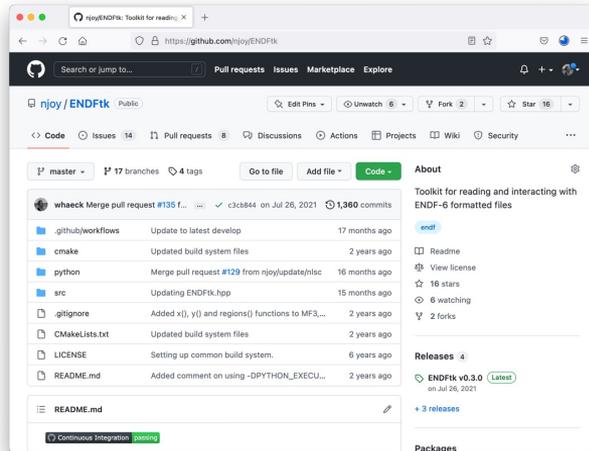
- More support for photonuclear data in ENDF/B-VIII.1
  - IAEA/PD-2019 evaluations may be pulled into ENDF/B-VIII.1
  - Some of these evaluations have features incompatible with NJOY2016.69
    - Photon data in MF12 and MF14 instead of MF6
    - Delayed neutron data for photo-fission 
  - Photonuclear data validation and verification work
- Thermal scattering data
  - New option(s) for the incident energy grid (currently a hardcoded grid)
- Heating calculation corrections
  - Looking into inconsistencies between HEATR and GROUPT

This may require changes in MCNP so it may be tricky



# 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

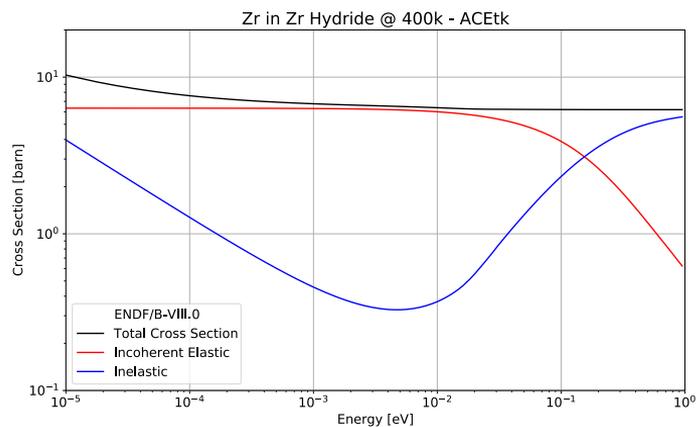
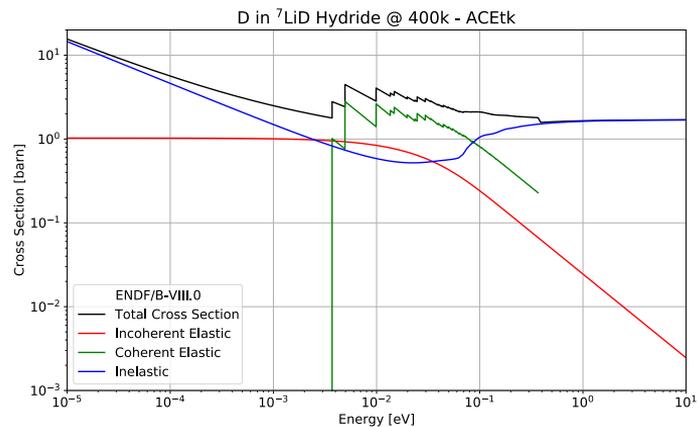
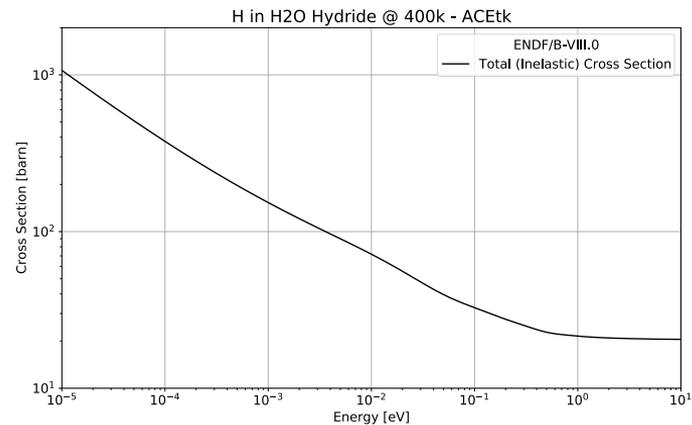
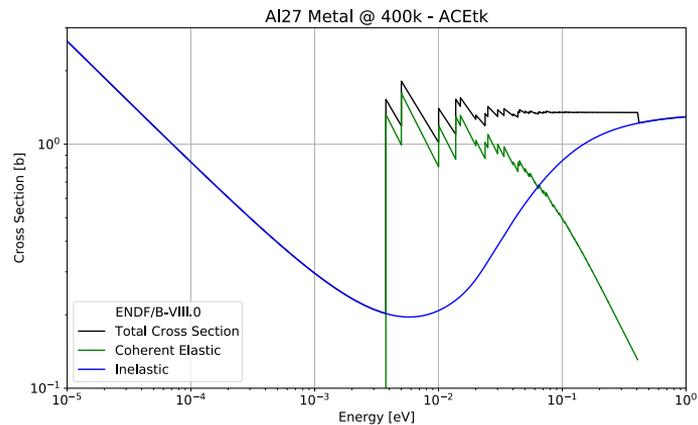


# ENDFtk and ACEtk development in FY22

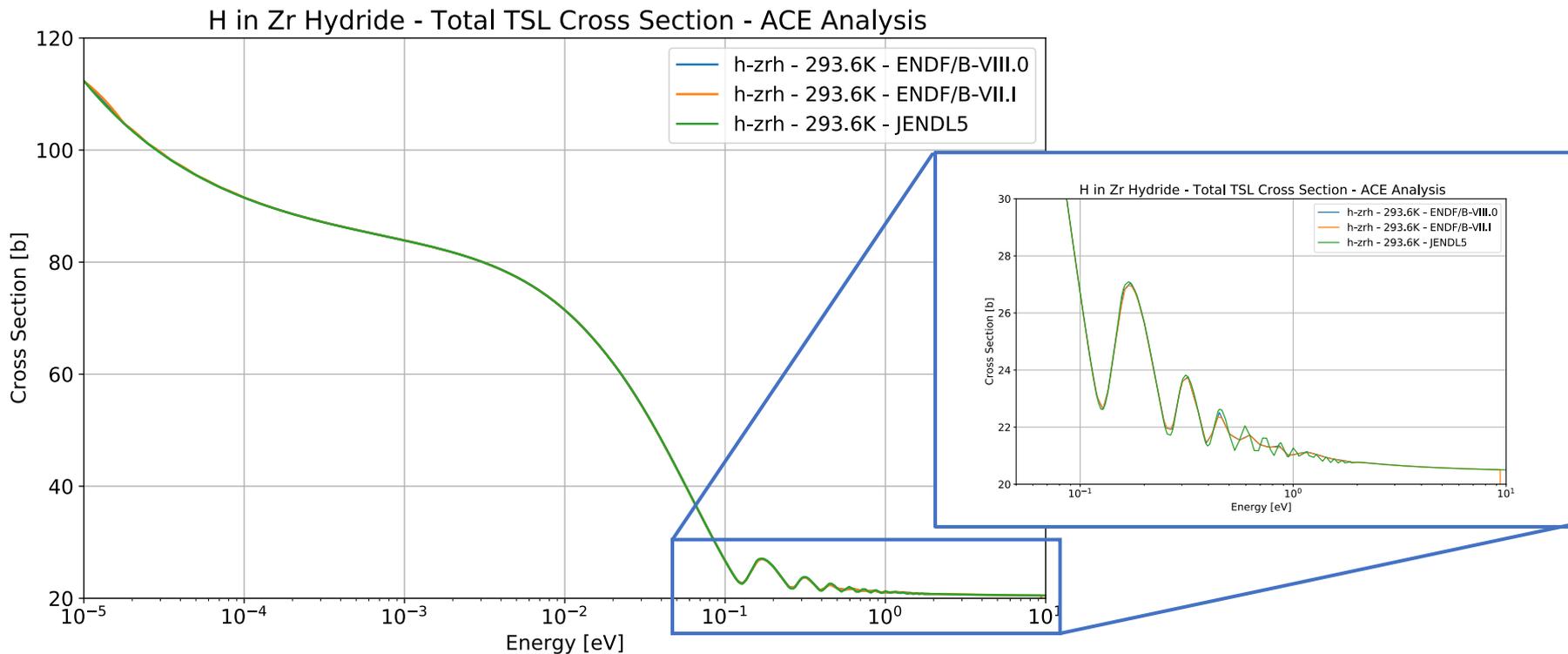
- ENDFtk: <https://github.com/njoy/ENDFtk>
  - Mainly work on covariance data: MF32, MF33, MF34 and MF35
  - Adding functionality for manipulating ENDF files
    - Inserting, replacing and removing materials, files and sections
    - Updating the directory of the ENDF file
  - Look out for a v1.0 release soon ...
  
- ACEtk: <https://github.com/njoy/ACEtk>
  - This was the main focus for us in FY22
  - 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
    - Dosimetry ACE files



# Plotting ACE data: thermal scattering data

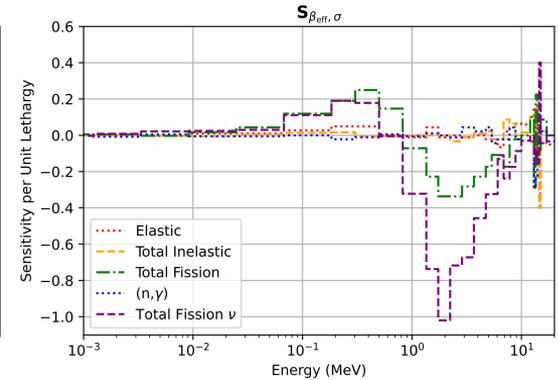
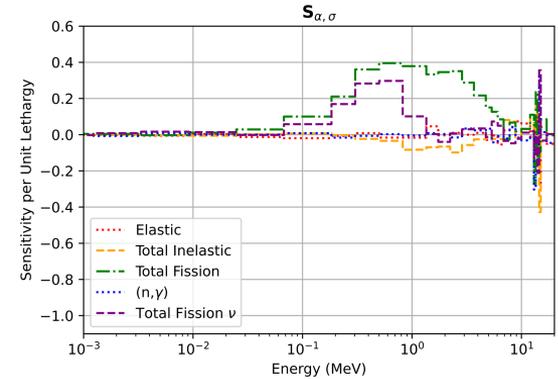
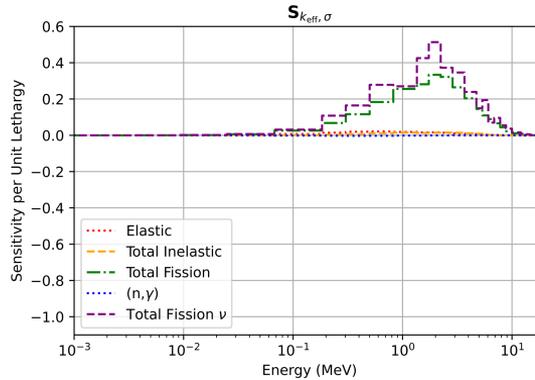
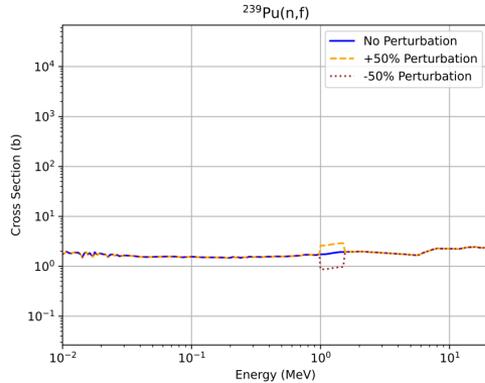


# Plotting ACE data: thermal scattering data



# 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



# NJOY modernisation priorities for FY23

- ENDFtk
  - Release ENDFtk v1.0 with full ENDF support
  - Maybe add some more convenience and abstracted interfaces
- ACEtk
  - Finalise ACE format specifications and maybe release a new document
    - Add the photonuclear, dosimetry and electron-photon (eprdata) ACE formats
  - Implement the electron-photon ACE format
- Resonance reconstruction
  - Add general R-matrix and relativistic kinematics
  - Python interface
  - Testing and debugging!



# Questions?

