

# Getting NJOY ready for ENDF/B-VIII.1

W. Haeck, N. Gibson, G. Siemers

ND2022, July 24-29, 2022

# Outline

- Getting NJOY ready for ENDF/B-VIII.1
  - Example: thermal scattering update
- NJOY modernisation work
  - Example: ACEtk - a toolkit for interacting with ACE files



# Making a new ENDF/B library ...

- 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



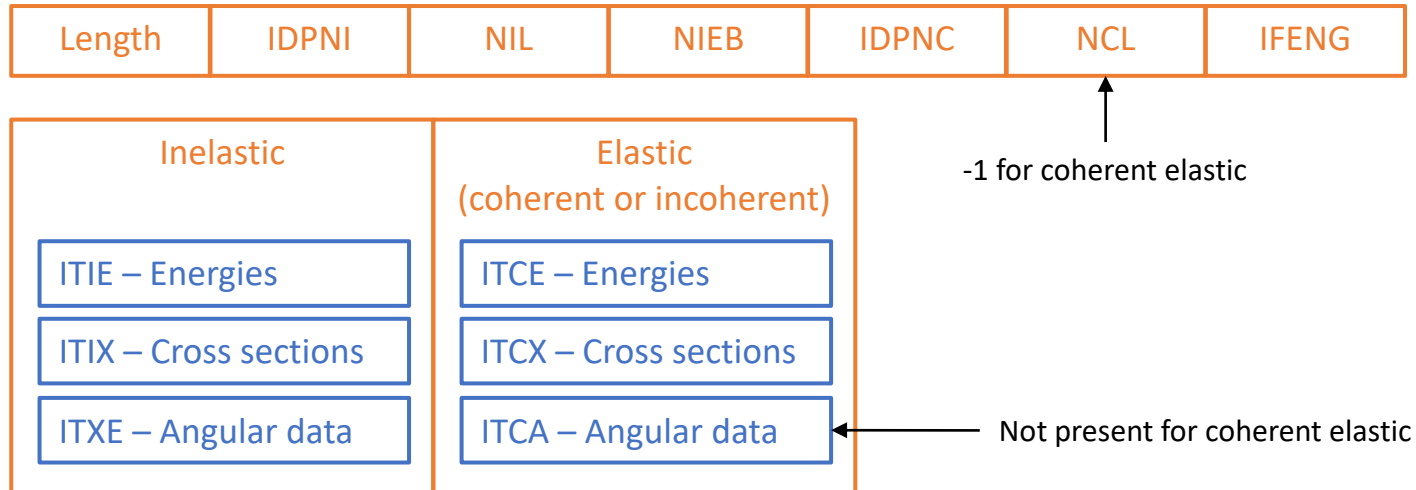
# Thermal scattering

- Nuclear data evaluations identify multiple categories of thermal scattering:
  - Coherent elastic: important in crystalline solids (graphite, metals, etc)
  - Incoherent elastic: important in solids with hydrogen (polyethylene, ZrH, etc.)
  - Coherent and incoherent inelastic: all solid and liquid materials (hydrogen in water)
- Prior to ENDF/B-VIII.1: either coherent or incoherent elastic scattering
  - Coherent and incoherent are not exclusive and neglecting one is an approximation
  - ENDF/B-VIII.1 will introduce mixed mode elastic scattering
- This feature is reflected in the ACE format itself
  - Only one elastic thermal scattering data block, which is either coherent or incoherent
  - We needed to add an optional second block when both are given



# The original thermal scattering format in ACE

- The thermal scattering format is relatively simple
  - Two main blocks: one for inelastic and one for elastic
  - The elastic block is either coherent (IDPNC=4) or incoherent (IDPNC=3)
  - Formatting parameters given in the NXS array



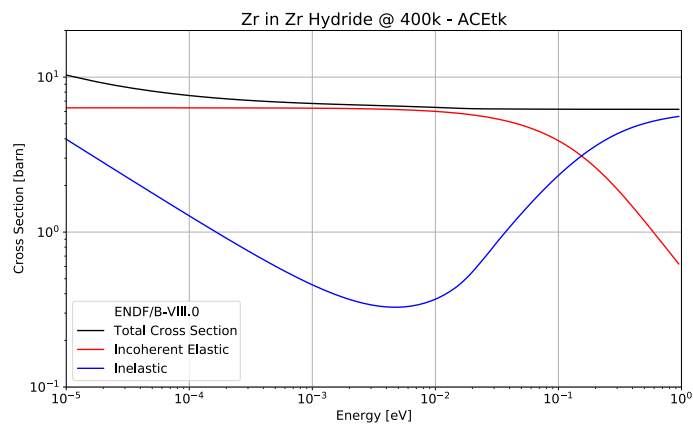
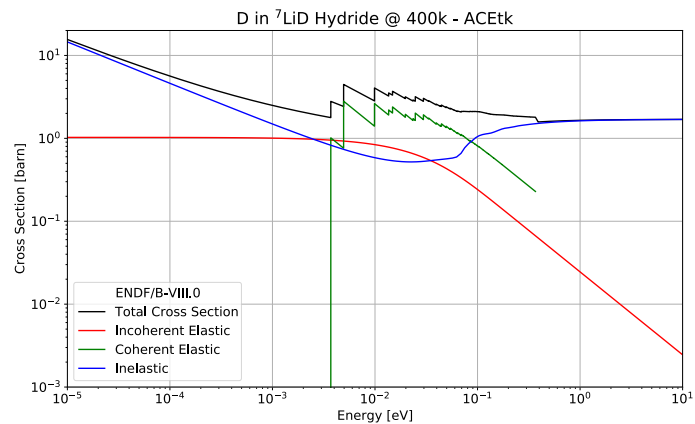
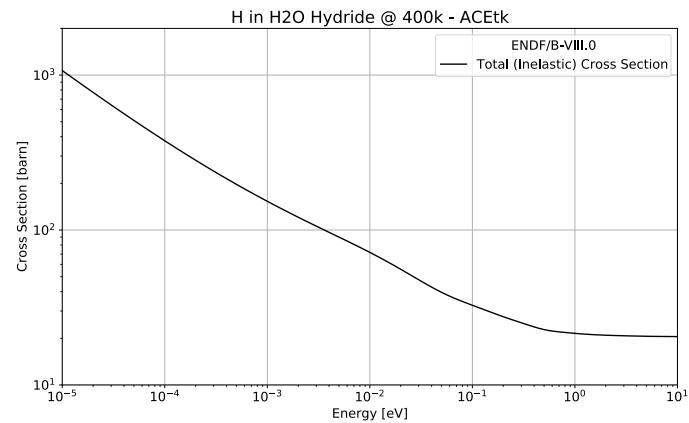
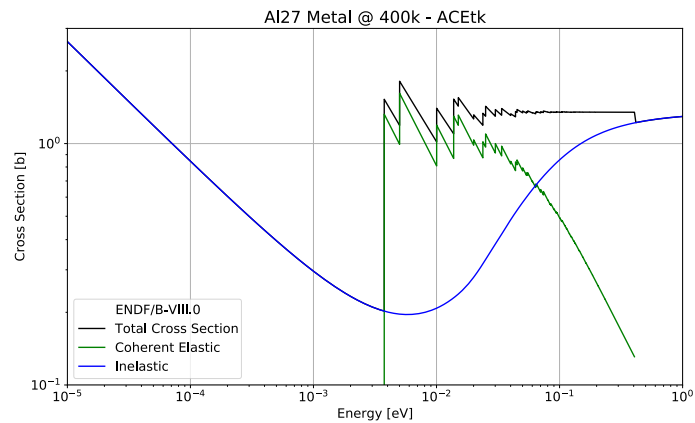
# The original thermal scattering format in ACE

- The old format is still VALID
  - When mixed mode is used, there will be an additional elastic block (IDPNC=5)
  - Coherent elastic is always given first, incoherent elastic is given after that
  - An additional formatting parameter: NCLI for the second elastic block only
    - NCL will always be -1 for IDPNC=5

Length	IDPNI	NIL	NIEB	IDPNC	NCL = -1	IFENG	NCLI
Inelastic			Coherent elastic		Incoherent elastic		
ITIE – Energies			ITCE – Energies		ITCEI – Energies		
ITIX – Cross sections			ITCX – Cross sections		ITCXI – Cross sections		
ITXE – Angular data			ITCA – Angular data		ITCAI – Angular data		

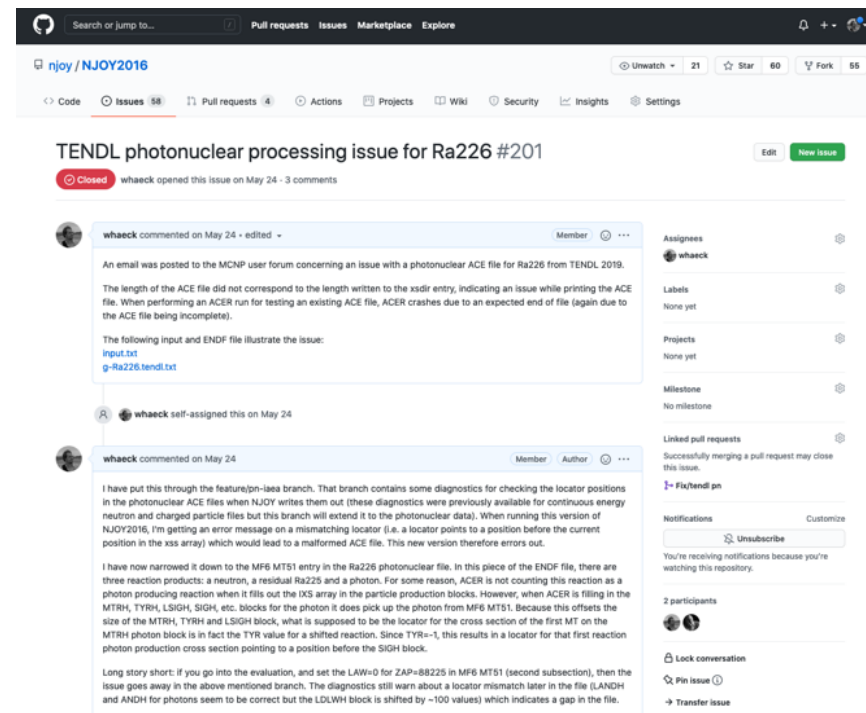


# Examples



# 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
  - TENDL, JENDL5, JEFF4, etc.
- An NJOY2016 release every 3 months



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'. The second comment, by 'whaeck', states they self-assigned the issue on May 24. The third comment, also by 'whaeck', provides a detailed explanation of the issue, mentioning the 'feature/pn-laea' branch and the 'M66 MT51' entry in the Ra226 photonuclear file. It explains that the issue is caused by a photon producing a reaction when it fills out the 'XS' array in the particle production blocks, but ACER is filling in the 'MTRH', 'TYRH', 'LSIGH', 'SIGH', etc. blocks for the photon it does pick up from 'M66 MT51', which offsets the size of the 'MTRH', 'TYRH' and 'LSIGH' block. The comment concludes with a 'Long story short' summary of the problem and the diagnostic results.



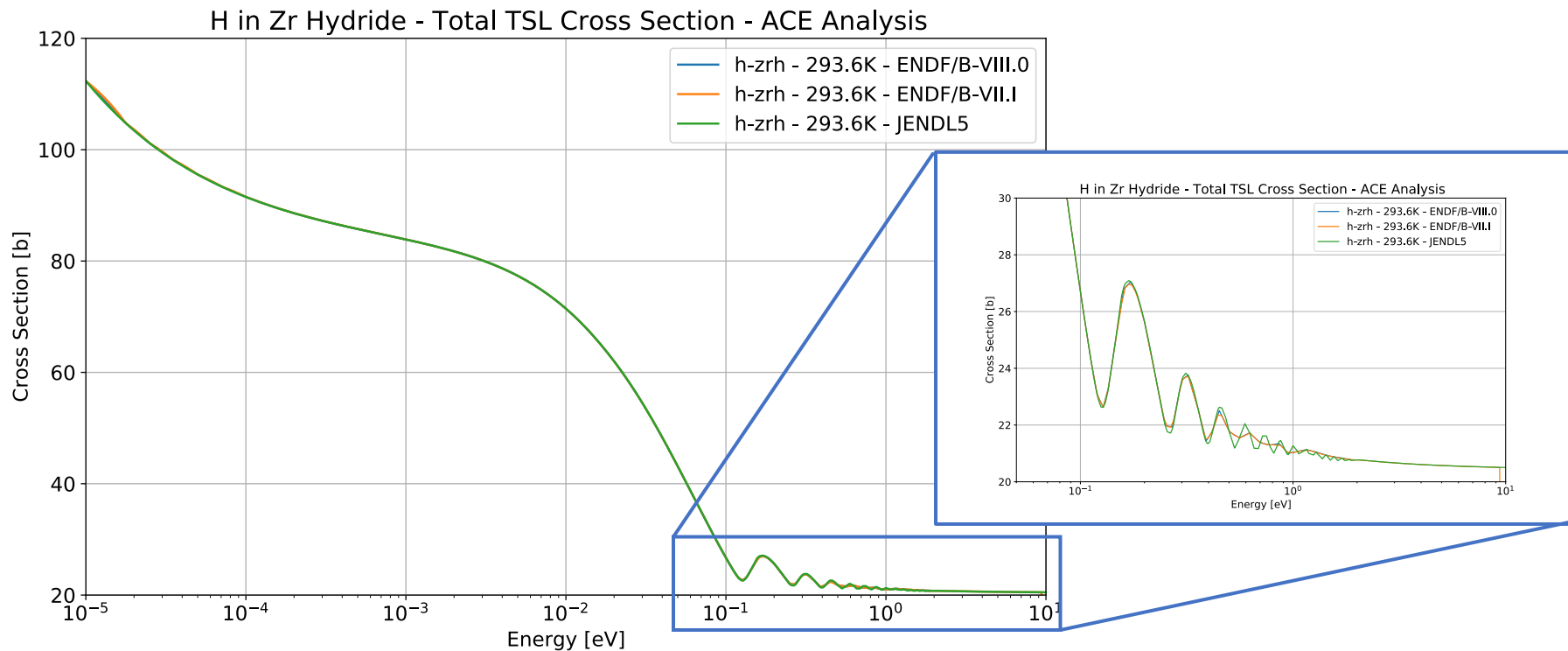


# ACEtk

- A toolkit to read, write, modify and create ACE tables
  - We want to be able to extract pieces from the ACE table and insert it elsewhere
  - Locators get handled under the hood without user intervention
- Simple interface that does not require (too much) knowledge of the ACE format
  - For now we implement a block-by-block interface
  - A convenience interface will be implemented once an entire table type is implemented
- Whenever possible, mimic the interface of existing components (e.g. ENDFtk)



# ACEtk – looking at more thermal scattering files



# One more thing ...

The screenshot shows the website [nucleardata.lanl.gov](https://nucleardata.lanl.gov) with the following content:

- Navigation bar: News & Media, Careers, Quick Links
- Los Alamos National Laboratory logo and menu: MISSION, SCIENCE & INNOVATION, COLLABORATION, COMMUNITY, ENVIRONMENT
- Search bar: Search
- Left sidebar: NUCLEAR DATA HOME, DATA LIBRARIES, ACE LIBRARIES (CP2020, ENDF80SaB2, Lib80x, EPRData14, ENDF71SaB, EPRData12, MCPLIB84)
- Breadcrumbs: NUCLEAR DATA / ACE / LIB80X
- Section: **Lib80x—Library based on ENDF/B-VIII.0**
- Released: 2018-06-29
- Description: This library is based on ENDF/B-VIII.0. It contains ACE files for continuous energy neutrons. These have been processed at the following temperatures (with their uncertainties):
  - .00c — 293.6 Kelvin (room temperature)
  - .01c — 600 Kelvin
  - .02c — 900 Kelvin
  - .03c — 1200 Kelvin
  - .04c — 2500 Kelvin
  - .05c — 0.1 Kelvin
  - .06c — 250 kelvin
- Text: The full documentation for the Lib80x library can be found in the docs directory after decompressing the download.

nucleardata.lanl.gov  
now has errata files!

The screenshot shows the **DOWNLOADS** and **ERRATA** sections of the website:

- DOWNLOADS**: Lib80x can be downloaded either as a zip file or as a compressed tarball.
  - Lib80x.zip (sha512: 801b9e3389ad75915c4f135d365668498...)
  - Lib80x.tgz (sha512: afa143e834ef02d8f5353570...)
- ERRATA**:
  - Date: 2022-07-06
  - Name: B-10 Lib80x
  - Description: After the release of ENDF/B-VIII.0 in February 2018, errors were discovered in the neutron B-10 evaluation. A fix was provided for the errata; this update uses the fixed B-10 evaluation. For more information on the updated/fixed evaluation, please see: <https://www.nndc.bnl.gov/endl/b8.0/errata.html>.
  - Download links for B-10 Lib80x.zip and B-10 Lib80x.tgz.
  - Note: If further information is required contact a member of the Data Team by e-mail at [nucldata@lanl.gov](mailto:nucldata@lanl.gov)



# Conclusions

- We continue to maintain and improve NJOY2016 for ENDF/B-VIII.1
  - Implement new ENDF features (e.g. thermal scattering files)
  - Processing new libraries as they come out (TENDL, JEFF, JENDL, etc.)
- We continue our work on NJOY modernisation
  - ACEtk and ENDFtk are production ready
  - GNDStk is still under development but we're almost there
  - Next year will be for processing components!

