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Title:	Another NJOY update for MCNP users
Author(s):	Haeck, Wim Gibson, Nathan Andrew
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Los Alamos
NATIONAL LABORATORY

Another NJOY update for MCNP users

W. Haeck, N. Gibson

2022 MCNP User Symposium 2, October 17-21, 2022

Outline

- Introduction
- What has changed since last year for NJOY2016?
- NJOY modernisation work over the last year

We have a longer session this afternoon on all things nuclear data

Introduction

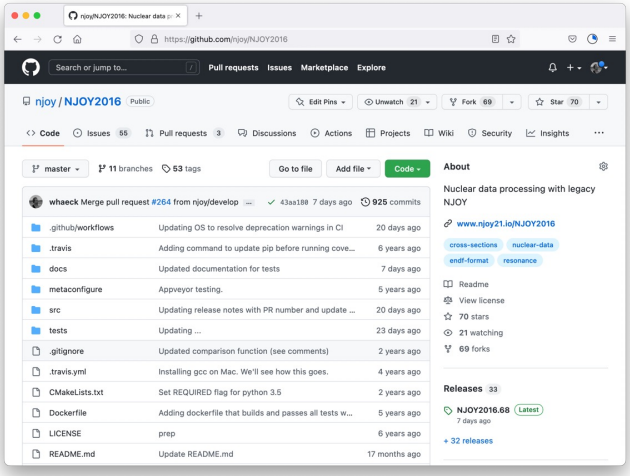
- Some of the main tasks of the XCP-5 Nuclear Data Team at LANL:
  - Maintain nuclear data libraries for LANL simulation codes (MCNP, PARTISN, etc.)
  - Verify and validate new data libraries when they become available

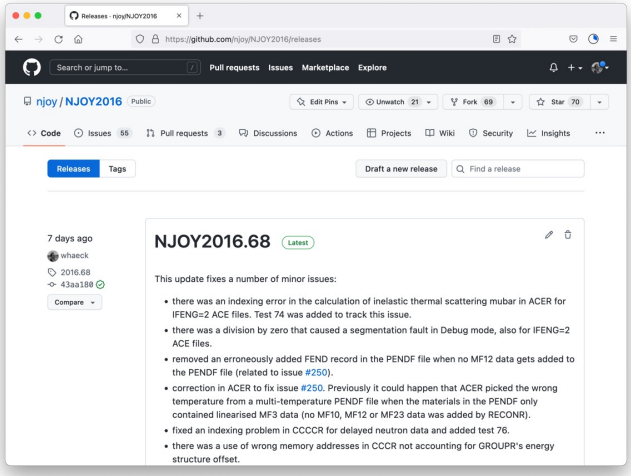
- NJOY is the nuclear data processing software develop at Los Alamos
  - Initially developed in the ‘70s as a single package to replace individual programs
  - Originally written in Fortran-77

- We are actively working on modernising NJOY
  - But we maintain our production version: NJOY2016 (Fortran)
  - While developing modernised NJOY components

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

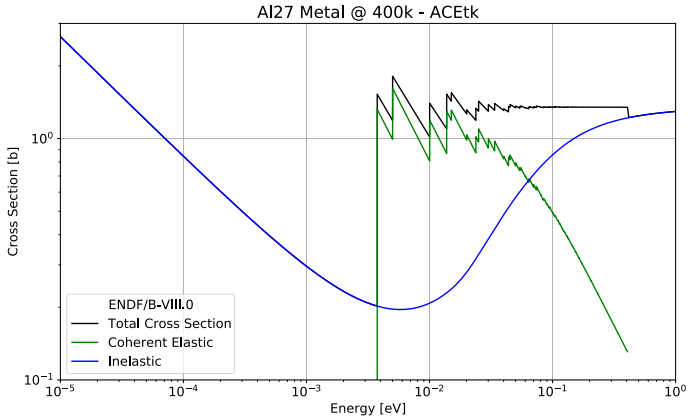
Our main objective: smooth processing of ENDF/B-VIII.1

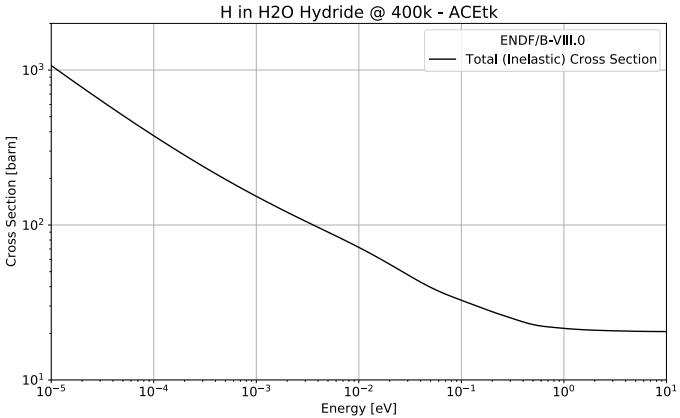
- Every new ENDF/B generation changes formats and adds new data

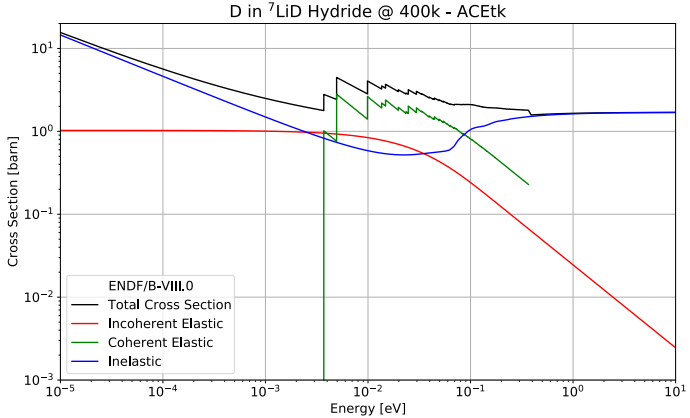
- The future library: ENDF/B-VIII.1
  - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
  - Improved photonuclear data
  - Background R-matrix elements for resonance parameters in MF2 MT151
  - General R-matrix formalism (KRM = 4) in MF2 MT151

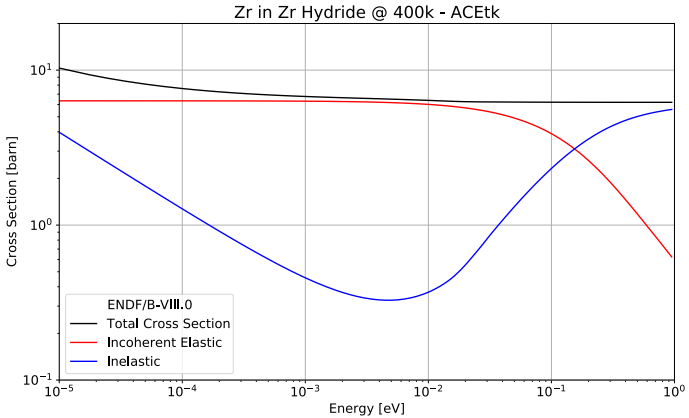
- Caveat: if these impact the ACE format, MCNP needs to be updated too
  - These changes are prioritised due to the involvement of MCNP
  - Changes are made in collaboration with the MCNP development team

Thermal scattering data

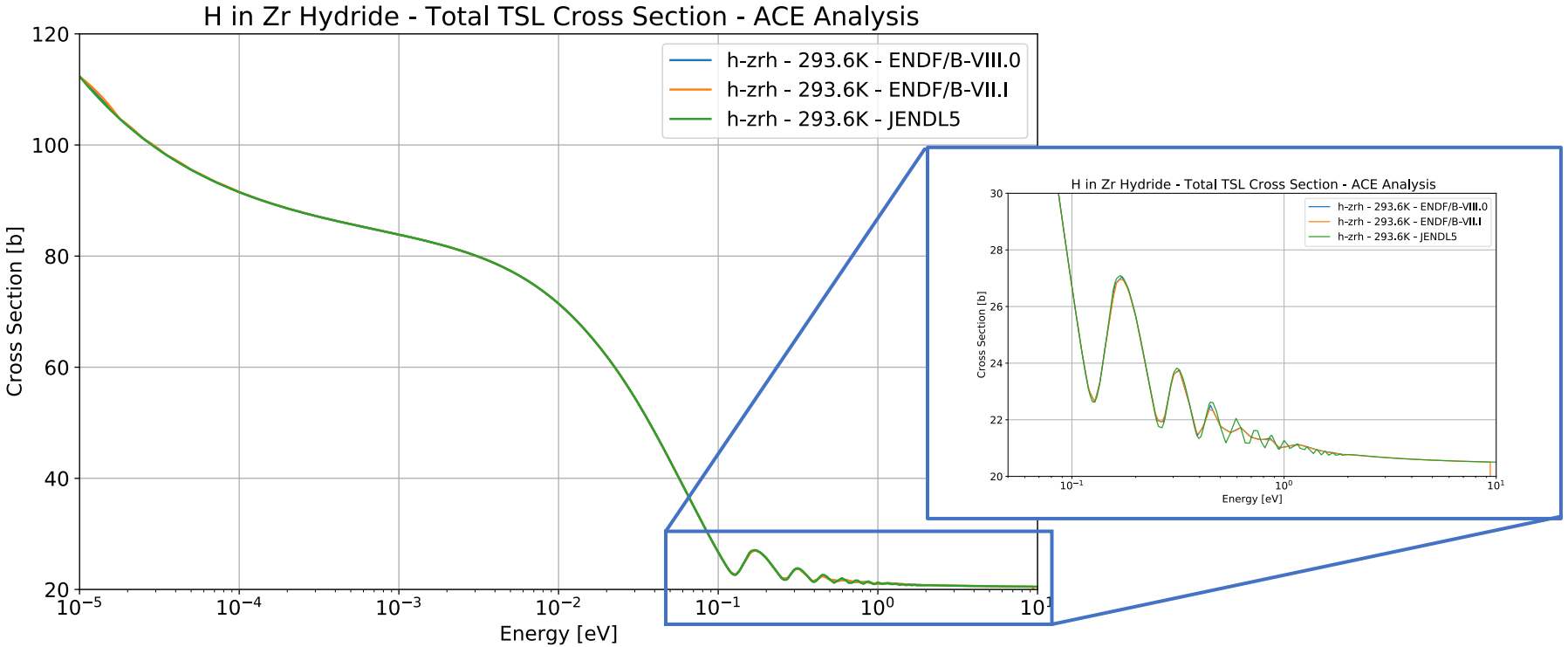






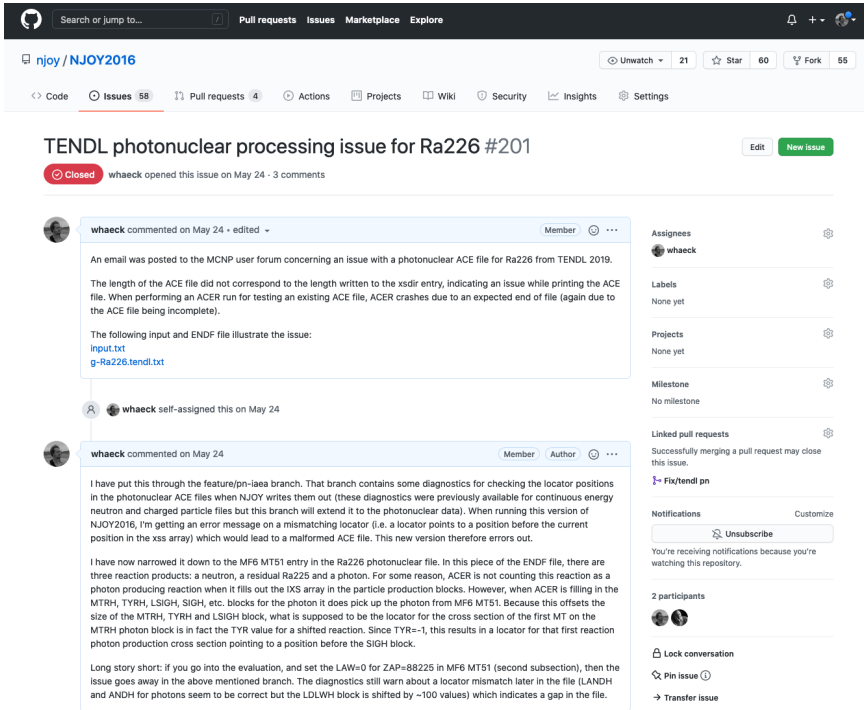


Thermal scattering data



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



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

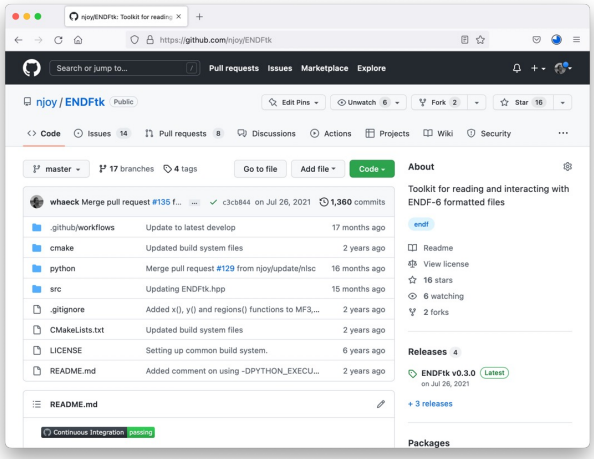
- Angular covariance data processing in ERRORR (NJOY2016.66)
  - ENDF MF34 format allows for multiple sub-subsection associated to pieces of the covariance matrix associated to MT1 L1, MT2 L2 pairs
  - Previous versions of NJOY2016 crashed on files that had multiple sub-subsections
    - For example: 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

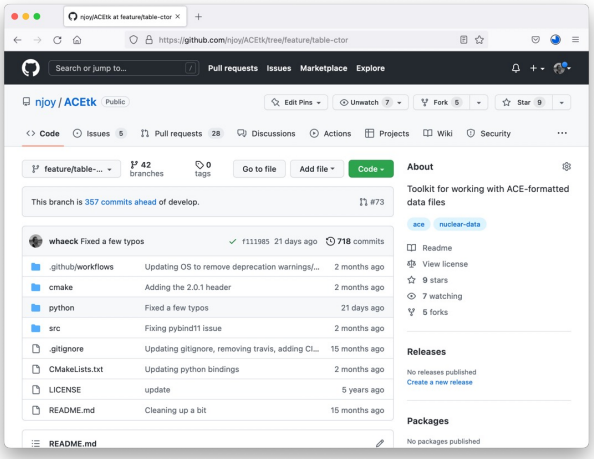
- Updated ACE locator consistency checks (NJOY2016.66)
  - Locator checking for photonuclear and thermal scattering files has been enabled
  - Previously only available for incident neutron and charged particle ACE files

- 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

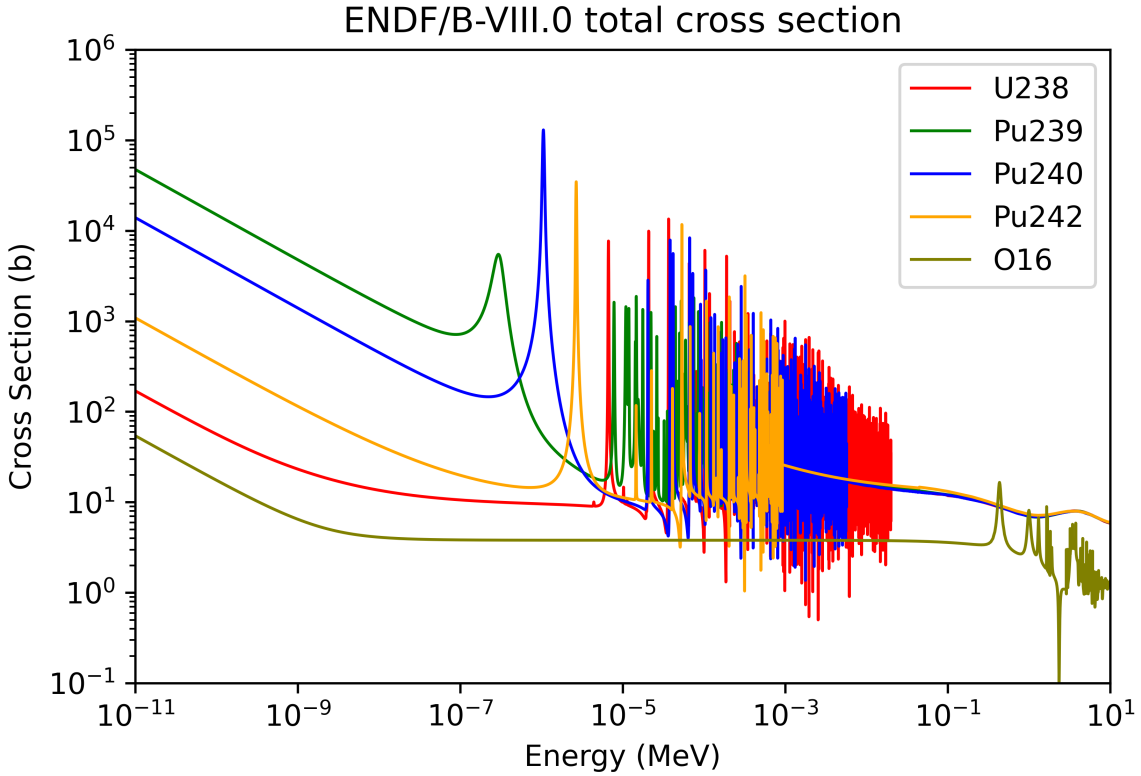
- ENDFtk: https://github.com/njoy/ENDFtk
  - Mainly work on covariance data: MF32, MF33, MF34 and MF35
  - Adding functionality for manipulating ENDF files
    - Inserting, replacing and removing materials, files and sections
    - Updating the directory of the ENDF file
  - Look out for a v1.0 release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

- ACEtk: https://github.com/njoy/ACEtk
  - This was the main focus for us in 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

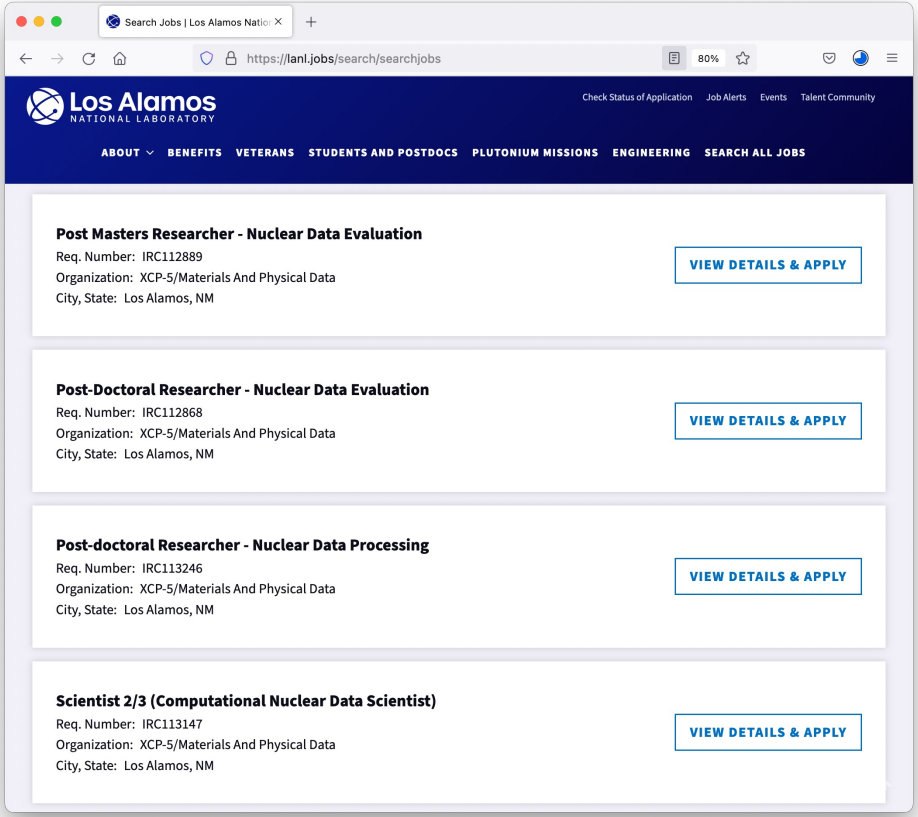
Behold the power of ACEtk …

```
import ACEtk
import matplotlib.pyplot as plot

U238 = ACEtk.ContinuousEnergyTable.from_file( '92238.800nc' )
Pu239 = ACEtk.ContinuousEnergyTable.from_file( '94239.800nc' )
Pu240 = ACEtk.ContinuousEnergyTable.from_file( '94240.800nc' )
Pu242 = ACEtk.ContinuousEnergyTable.from_file( '94242.800nc' )
O16 = ACEtk.ContinuousEnergyTable.from_file( '8016.800nc’ )

plot.plot( U238.ESZ.energies, U238.ESZ.total, label = 'U238', color = 'red', linewidth = 1.0 )
plot.plot( Pu239.ESZ.energies, Pu239.ESZ.total, label = 'Pu239', color = 'green', linewidth = 1.0 )
plot.plot( Pu240.ESZ.energies, Pu240.ESZ.total, label = 'Pu240', color = 'blue', linewidth = 1.0 )
plot.plot( Pu242.ESZ.energies, Pu242.ESZ.total, label = 'Pu242', color = 'orange', linewidth = 1.0 )
plot.plot( O16.ESZ.energies, O16.ESZ.total, label = 'O16', color = 'olive', linewidth = 1.0 )
plot.xlabel( 'Energy (MeV)' )
plot.ylabel( 'Cross Section (b)' )
plot.title( 'ENDF/B-VIII.0 total cross section' )
plot.xlim( 1e-11, 10 )
plot.ylim( 1e-1, 1e+6 )
plot.xscale( 'log' )
plot.yscale( 'log' )
plot.legend()
plot.show()
```

Behold the power of ACEtk …



One last thing …



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.)

- We continue our work on NJOY modernisation
  - ACEtk and ENDFtk are production ready
  - This fiscal year will be for processing components!

- See you this afternoon for an introduction to ENDF, NJOY and ACE