

LA-UR-22-30849

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Title: Another NJOY update for MCNP users

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Intended for: 2022 MCNP User Symposium, 2022-10-17/2022-10-21 (Los Alamos, New Mexico, United States)

Issued: 2022-10-14



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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



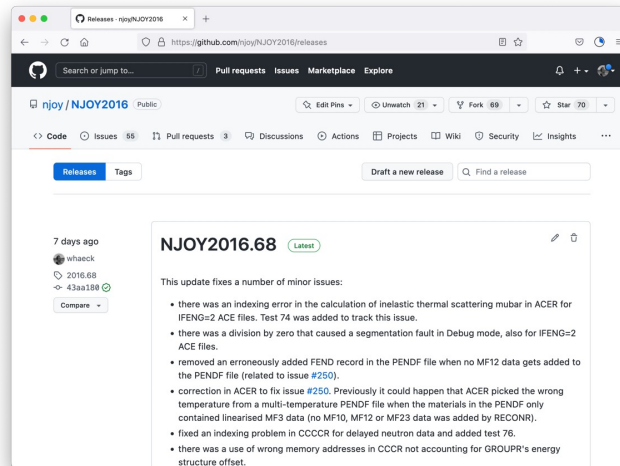
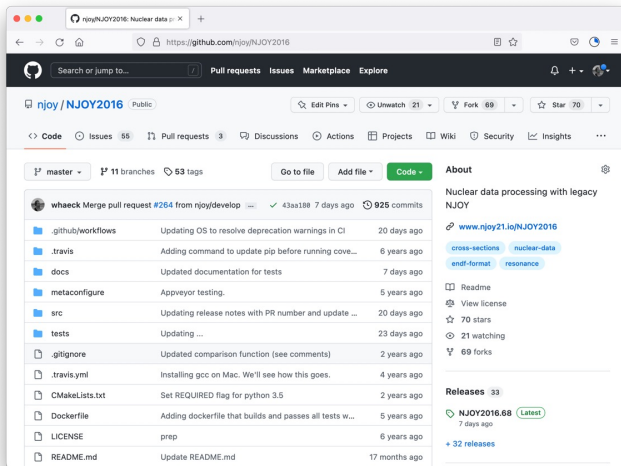
Introduction

- 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 developed 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

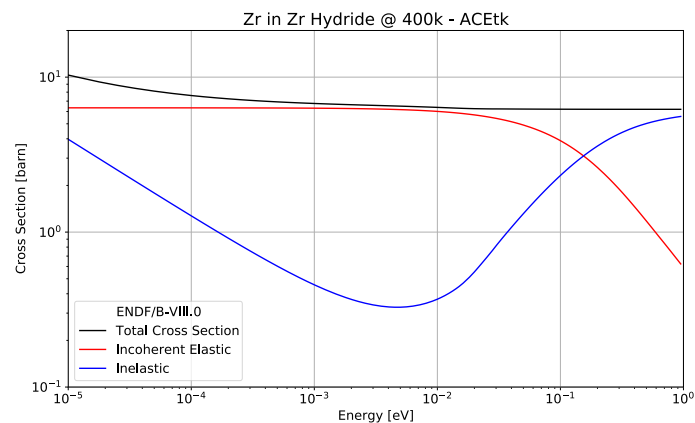
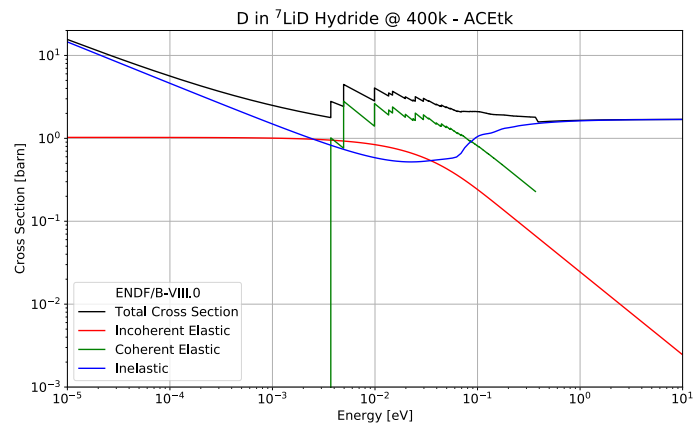
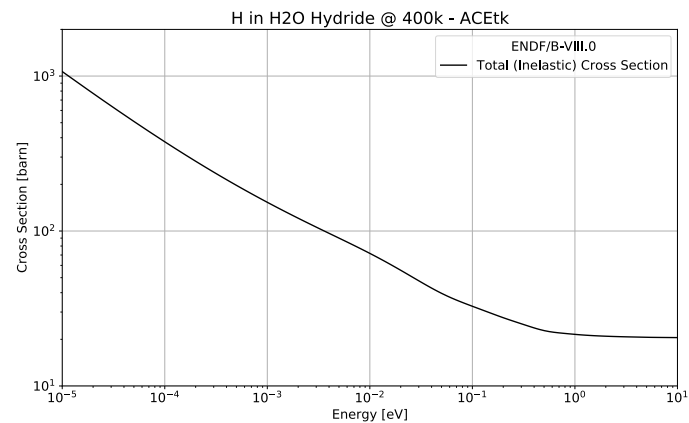
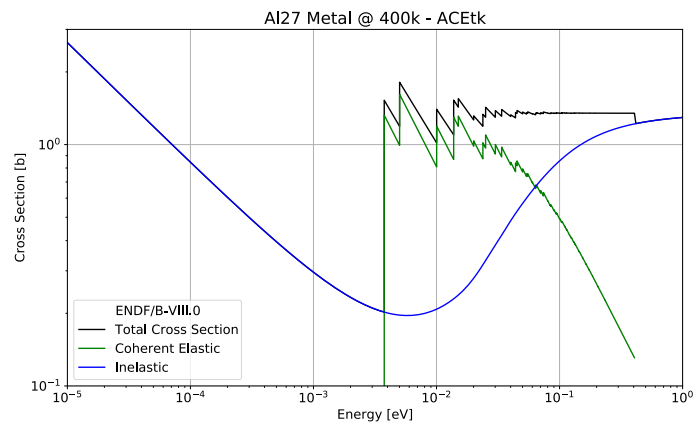


Our main objective: smooth processing of ENDF/B-VIII.1

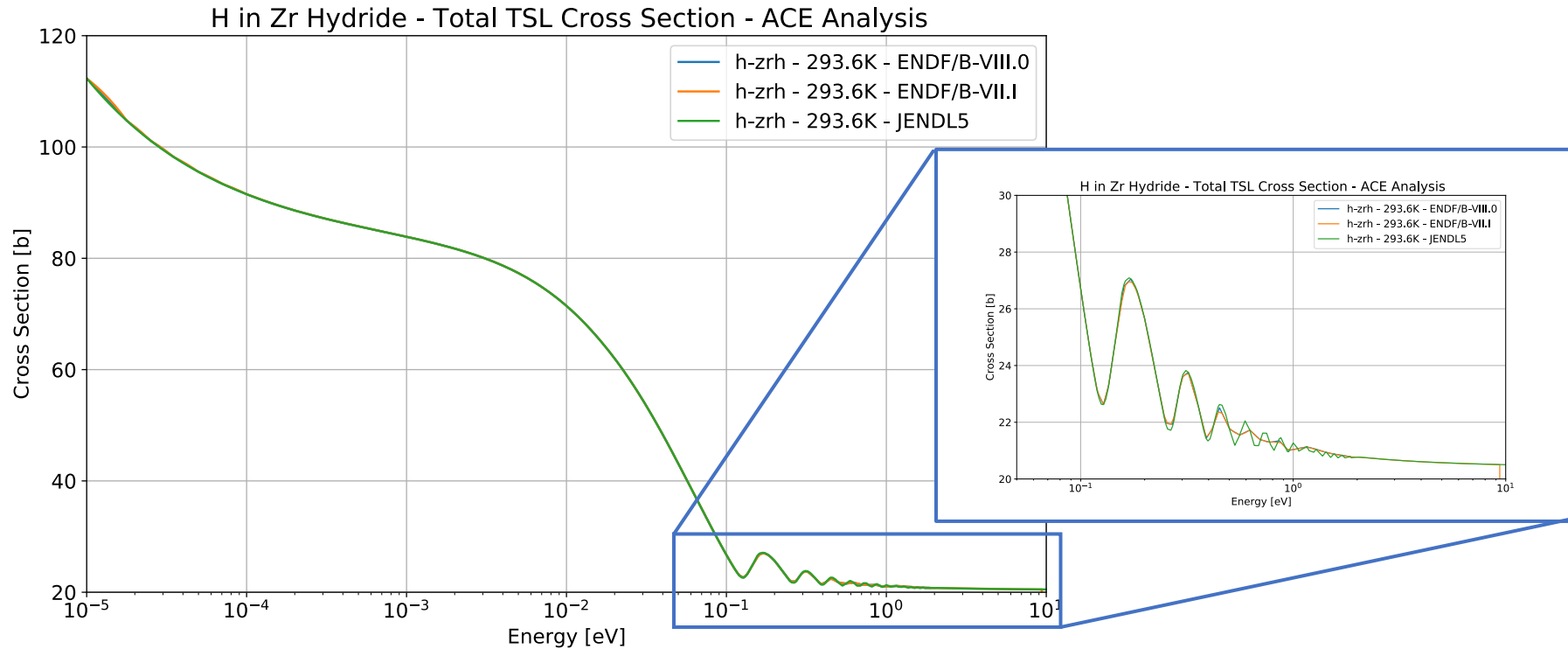
- Every new ENDF/B generation changes formats and adds new data
- The future library: ENDF/B-VIII.1
 - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
 - Improved photonuclear data
 - Background R-matrix elements for resonance parameters in MF2 MT151
 - General R-matrix formalism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

Search or jump to...

njoy / NJOY2016

Unwatch 21 Star 60 Fork 55

Code Issues 58 Pull requests 4 Actions Projects Wiki Security Insights Settings

TENDL photonuclear processing issue for Ra226 #201

Closed whaeck opened this issue on May 24 · 3 comments

whaeck commented on May 24 · edited

Member

An email was posted to the MCNP user forum concerning an issue with a photonuclear ACE file for Ra226 from TENDL 2019.

The length of the ACE file did not correspond to the length written to the xsdir entry, indicating an issue while printing the ACE file. When performing an ACER run for testing an existing ACE file, ACER crashes due to an expected end of file (again due to the ACE file being incomplete).

The following input and ENDF file illustrate the issue:

[Input.txt](#)
[g-Ra226.tendl.txt](#)

whaeck self-assigned this on May 24

whaeck commented on May 24

Member Author

I have put this through the feature/pn-iaea branch. That branch contains some diagnostics for checking the locator positions in the photonuclear ACE files when NJOY writes them out (these diagnostics were previously available for continuous energy neutron and charged particle files but this branch will extend it to the photonuclear data). When running this version of NJOY2016, I'm getting an error message on a mismatching locator (i.e. a locator points to a position before the current position in the xss array) which would lead to a malformed ACE file. This new version therefore errors out.

I have now narrowed it down to the MF6 MT51 entry in the Ra226 photonuclear file. In this piece of the ENDF file, there are three reaction products: a neutron, a residual Ra225 and a photon. For some reason, ACER is not counting this reaction as a photon producing reaction when it fills out the XS array in the particle production blocks. However, when ACER is filling in the MTRH, TYRH, LSIGH, SIGH, etc. blocks for the photon it does pick up the photon from MF6 MT51. Because this offsets the size of the MTRH, TYRH and LSIGH block, what is supposed to be the locator for the cross section of the first MT on the MTRH photon block is in fact the TYR value for a shifted reaction. Since TYR=-1, this results in a locator for that first reaction photon production cross section pointing to a position before the SIGH block.

Long story short: if you go into the evaluation, and set the LAW=0 for ZAP=88225 in MF6 MT51 (second subsection), then the issue goes away in the above mentioned branch. The diagnostics still warn about a locator mismatch later in the file (LANDH and ANDH for photons seem to be correct but the LDLWH block is shifted by ~100 values) which indicates a gap in the file.

Assignees: whaeck

Labels: None yet

Projects: None yet

Milestone: No milestone

Linked pull requests: Successfully merging a pull request may close this issue.

Fix/tendl/pn

Notifications: Unsubscribe

You're receiving notifications because you're watching this repository.

2 participants

Lock conversation

Pin issue

Transfer issue



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



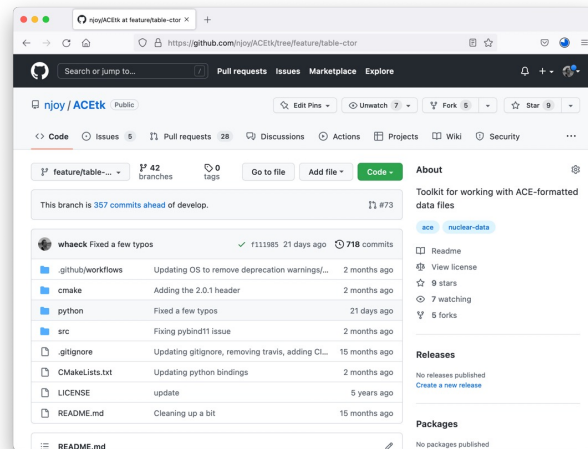
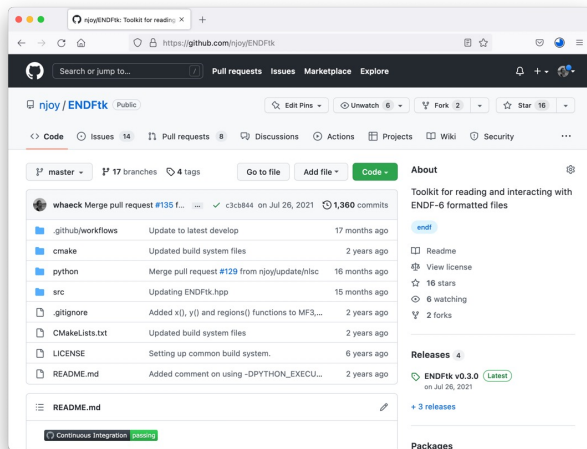
Overview of some of the NJOY2016 changes

- 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 ...

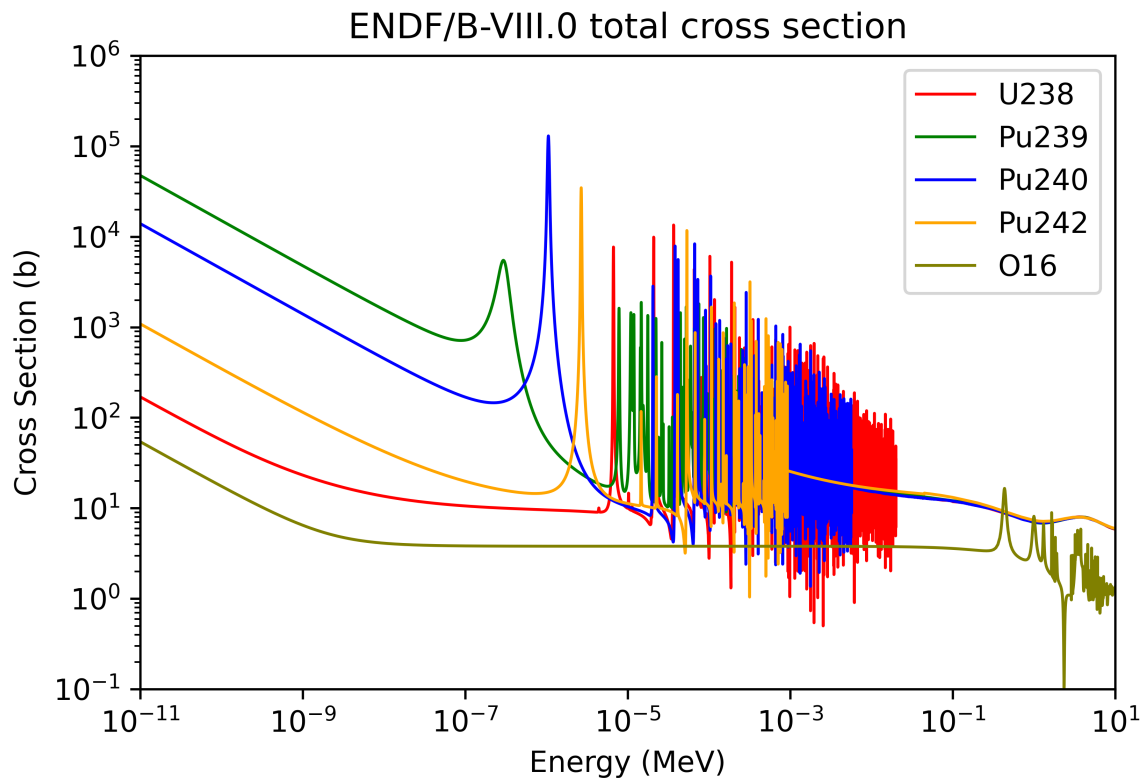
```
import ACETk
import matplotlib.pyplot as plot

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' )

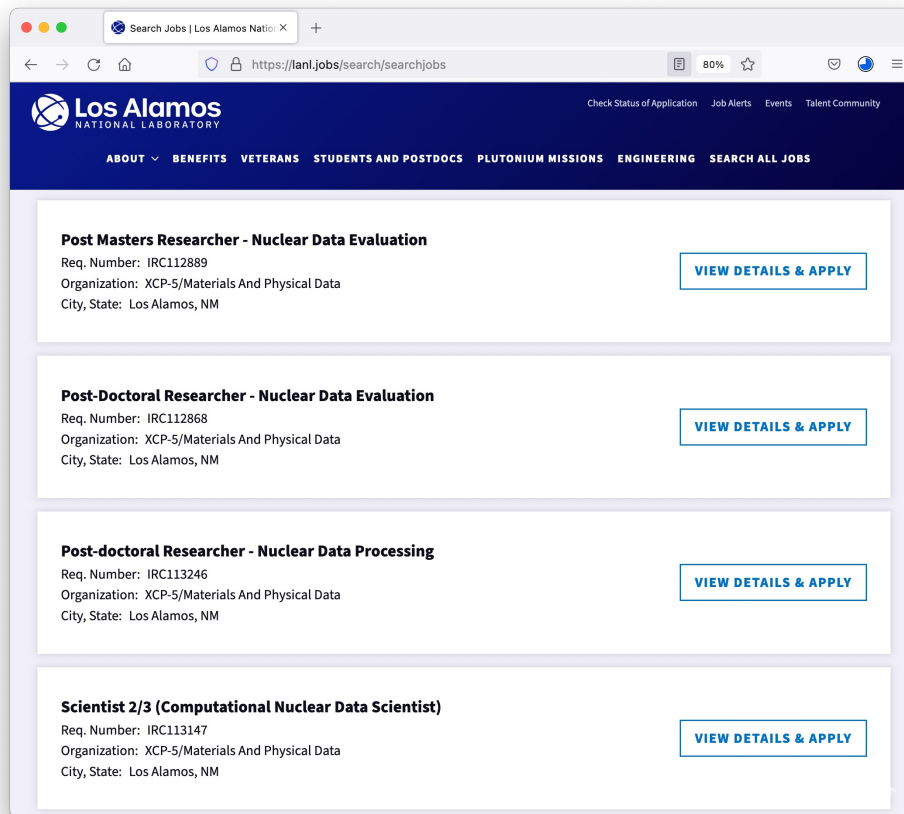
plot.plot( U238.ESZ.energies, U238.ESZ.total, label = 'U238', color = 'red', linewidth = 1.0 )
plot.plot( Pu239.ESZ.energies, Pu239.ESZ.total, label = 'Pu239', color = 'green', linewidth = 1.0 )
plot.plot( Pu240.ESZ.energies, Pu240.ESZ.total, label = 'Pu240', color = 'blue', linewidth = 1.0 )
plot.plot( 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

