

NJOY for ENDF/B-VIII.1

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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



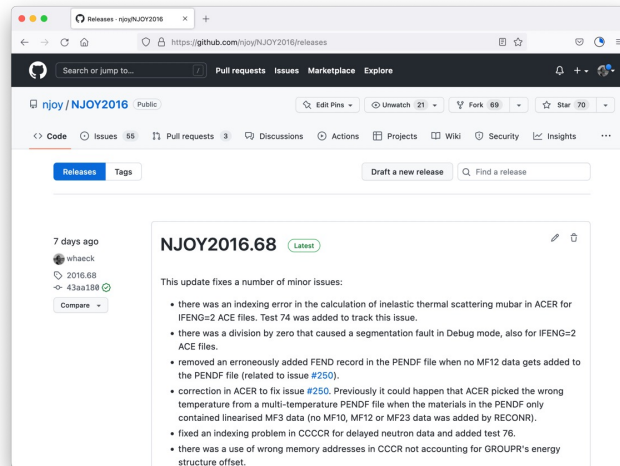
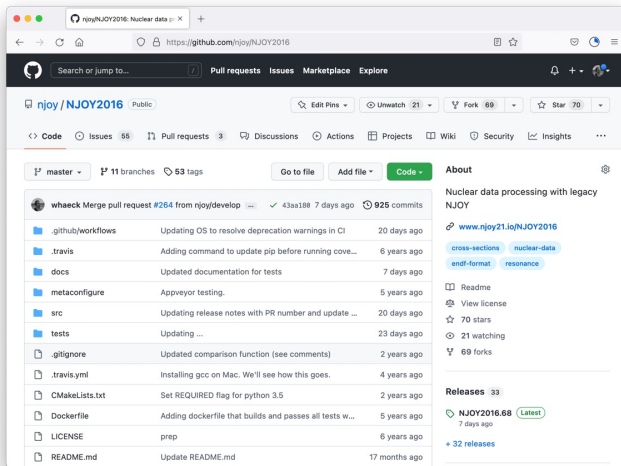
Which version of NJOY should you use?

- 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

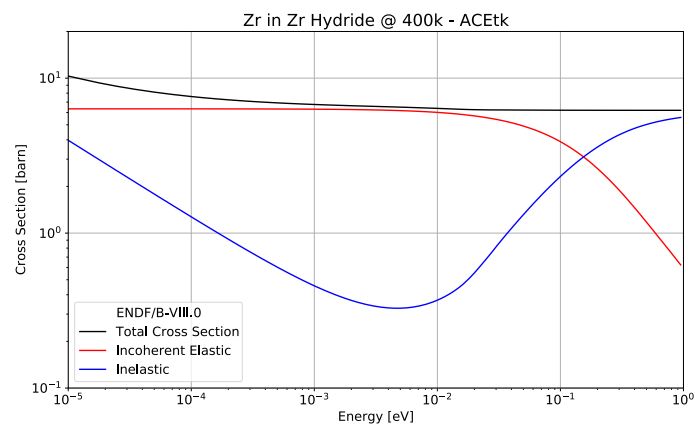
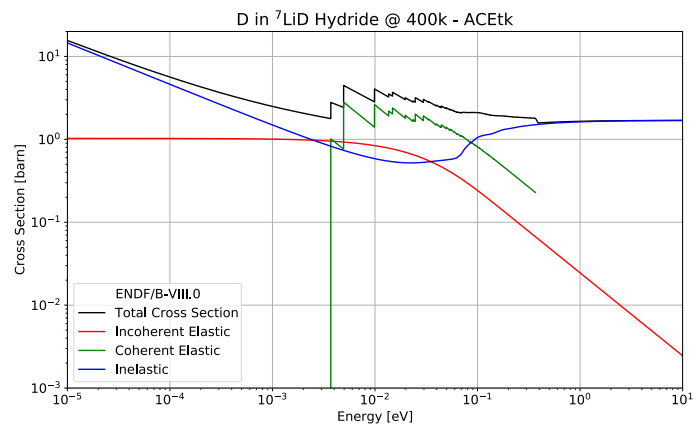
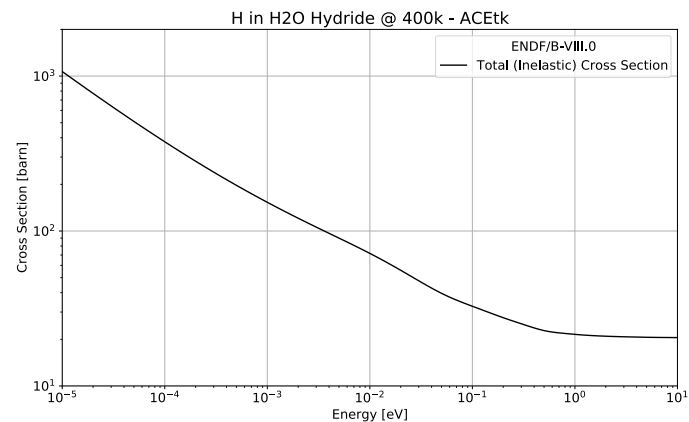
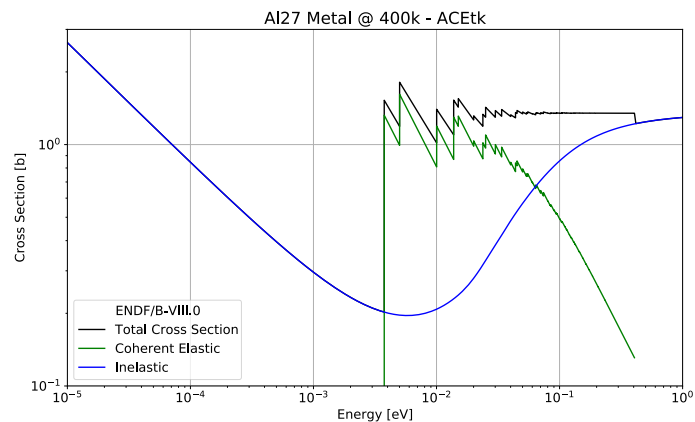


Our main objective: smooth processing of ENDF/B-VIII.1

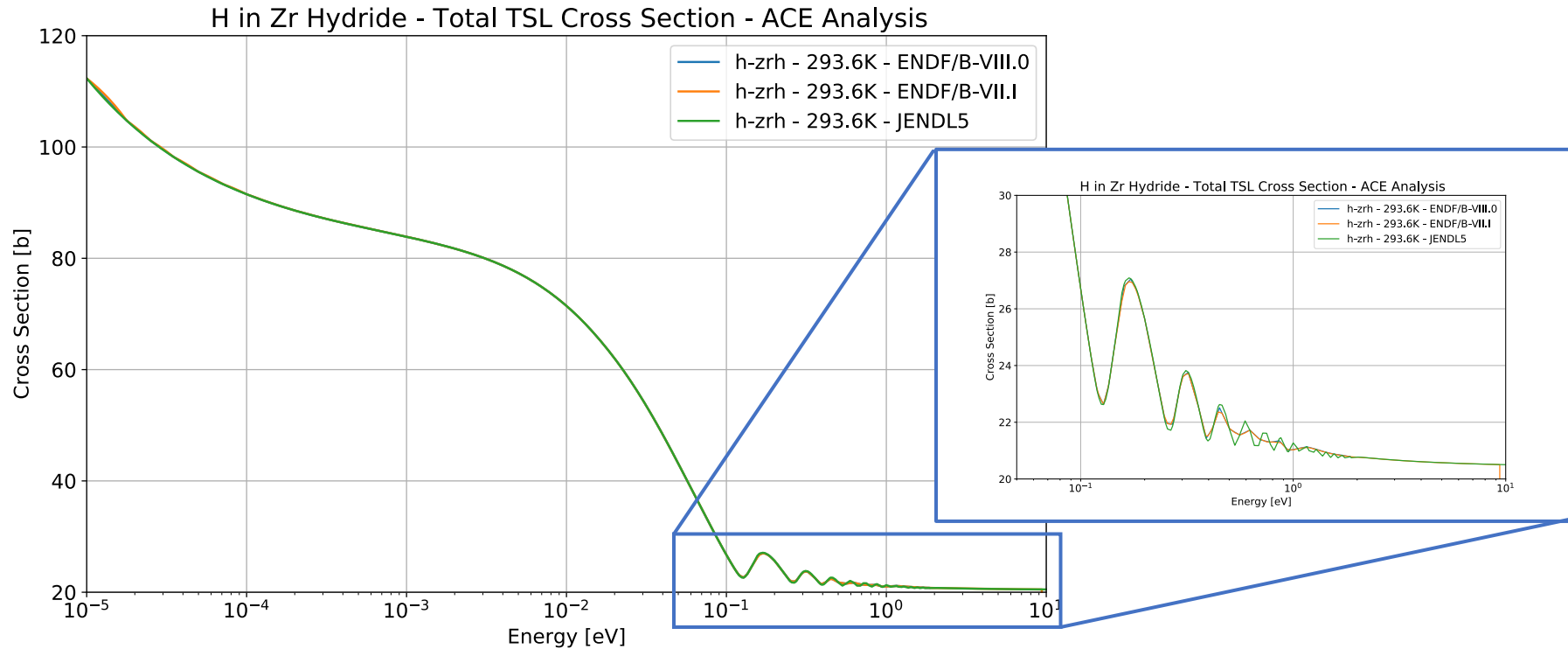
- Every new ENDF/B generation changes formats and adds new data
- The future library: ENDF/B-VIII.1
 - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
 - Improved photonuclear data
 - Background R-matrix elements for resonance parameters in MF2 MT151
 - General R-matrix formalism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

Search or jump to...

njoy / NJOY2016

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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



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



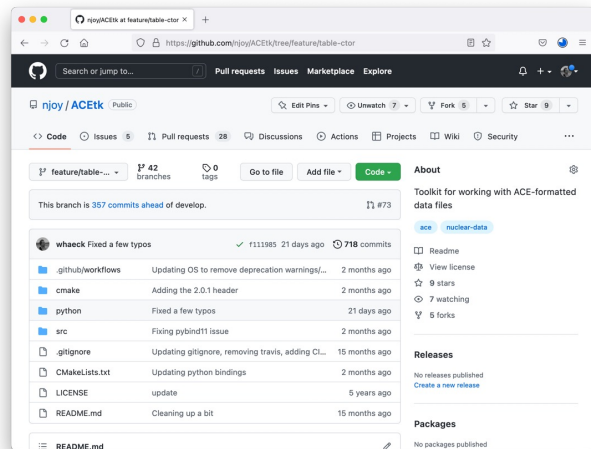
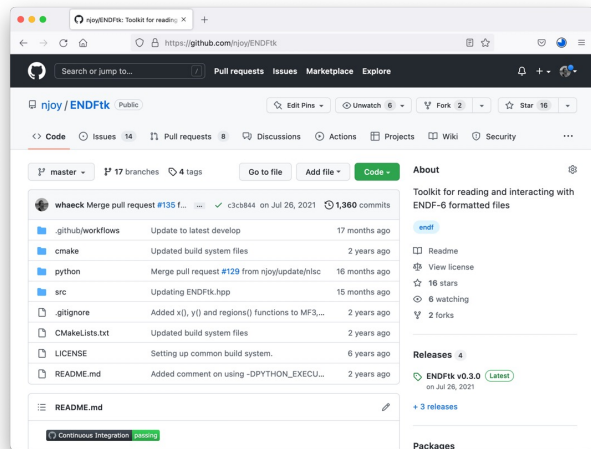
Overview of some of the NJOY2016 changes

- 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



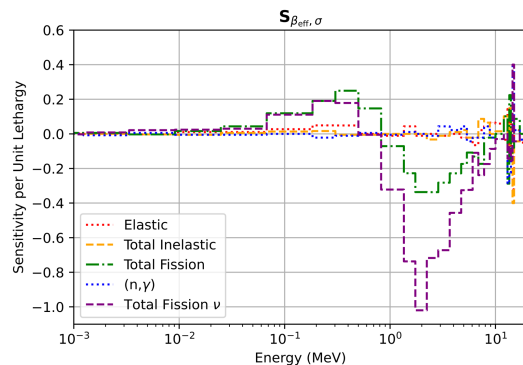
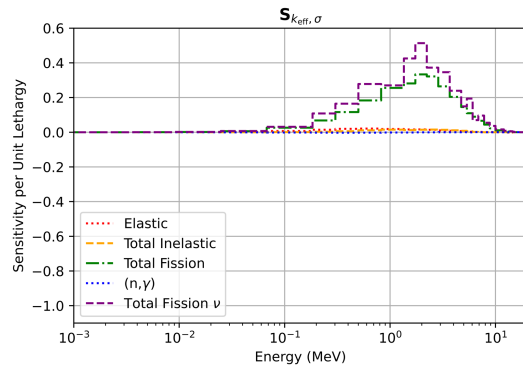
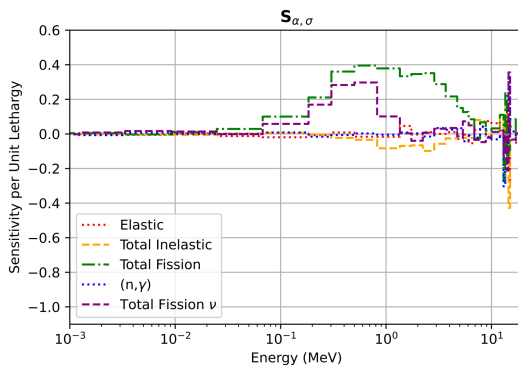
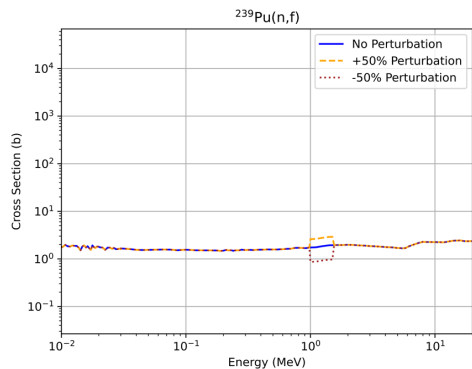
ENDFtk and ACEtk development

- 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

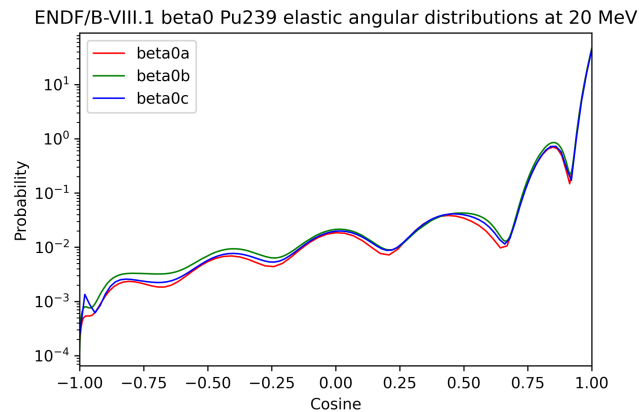
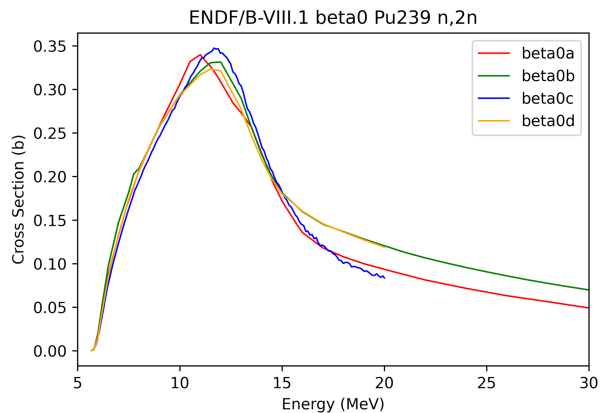
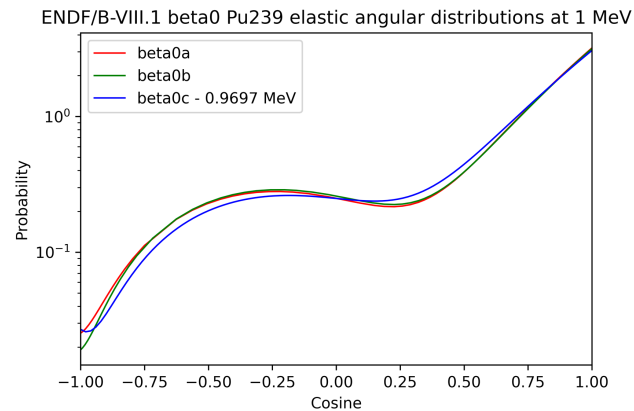
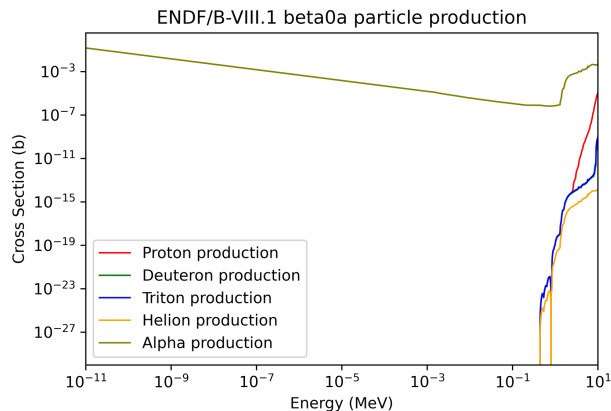


Perturbing existing ACE files for sensitivity calculation

- 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

