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Los Alamos NATIONAL LABORATORY

The road to a modernized NJOY

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MCNP User Symposium, August 19 – February 22, 2024

Outline

- An NJOY2016 update
  - New MCNP libraries for ENDF/B-VIII.1
  - Background R-matrix elements
  - Other notable changes
- Progress on the NJOY modernisation
  - Modern NJOY component overview
  - A first application: photo-atomic and electro-atomic ACE files

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

- The release of ENDF/B-VIII.1 is almost upon us
  - Release currently foreseen on August 30

- We will provide MCNP ACE formatted data libraries for this new library
  - A multi-temperature incident neutron and thermal scattering data library
  - A new photo-atomic and electro-atomic (eprdata) library
  - We might also release a photonuclear and incident charged particle data library

Introduction

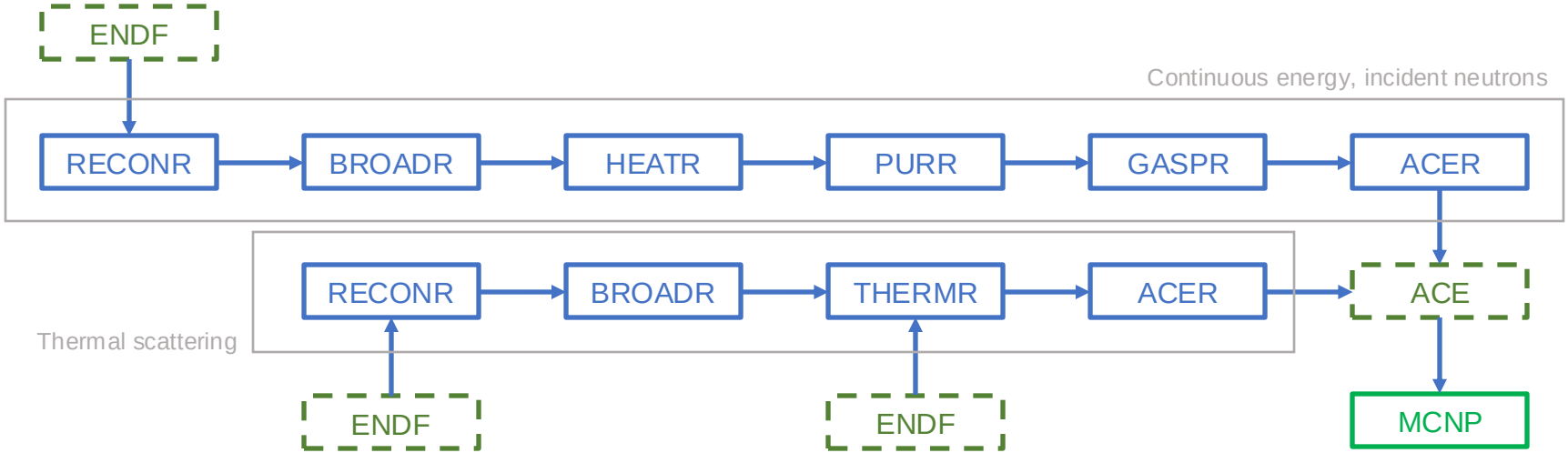
- NJOY is the nuclear data processing software developed at Los Alamos
  - Initially developed in the ‘70s as a single package to replace individual programs
  - Originally written in Fortran-77
  - Known as MINX-II prior to a printer malfunction

```
M + 1 = N
I + 1 = J
N + 1 = O
X + 1 = Y
```

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

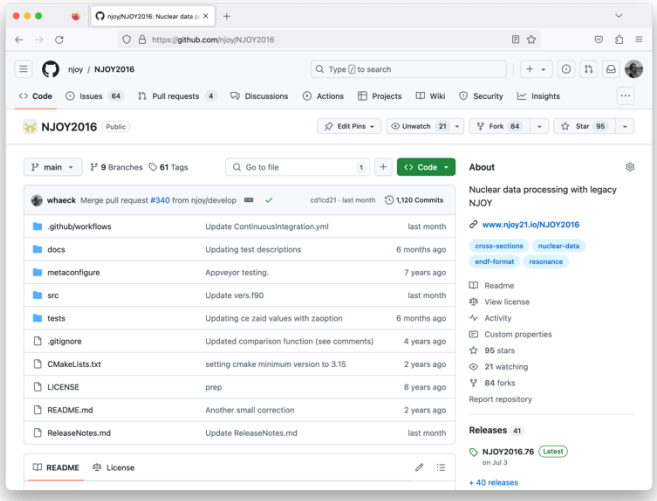
Introduction

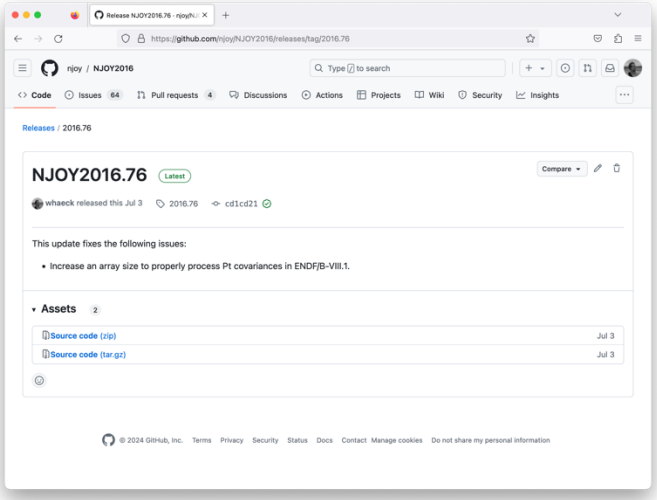
- NJOY provides a set of data processing modules that are called sequentially
  - Different processing paths for different library types and applications
  - Incident neutron, incident charged particles, thermal scattering, photonuclear, etc.



Maintaining our production version

- Get it at https://github.com/njoy/NJOY2016





- Latest version is NJOY2016.76 (July 2024)
  - 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

Background R-matrix elements in MF2 MT151

- MF2 MT151 changes were approved in 2021
  - Background R-matrix elements have been in the ENDF manual for a long time
  - The format description had errors in it that were fixed

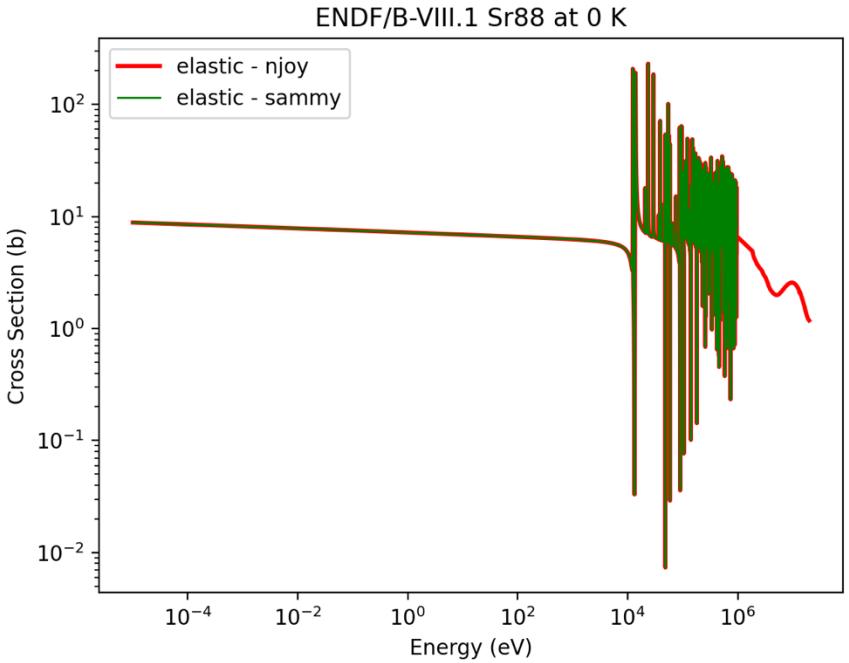
- Multiple options are available:
  - No background
  - Arbitrarily tabulated complex function
  - SAMMY parametrisation
  - Frohner parametrisation

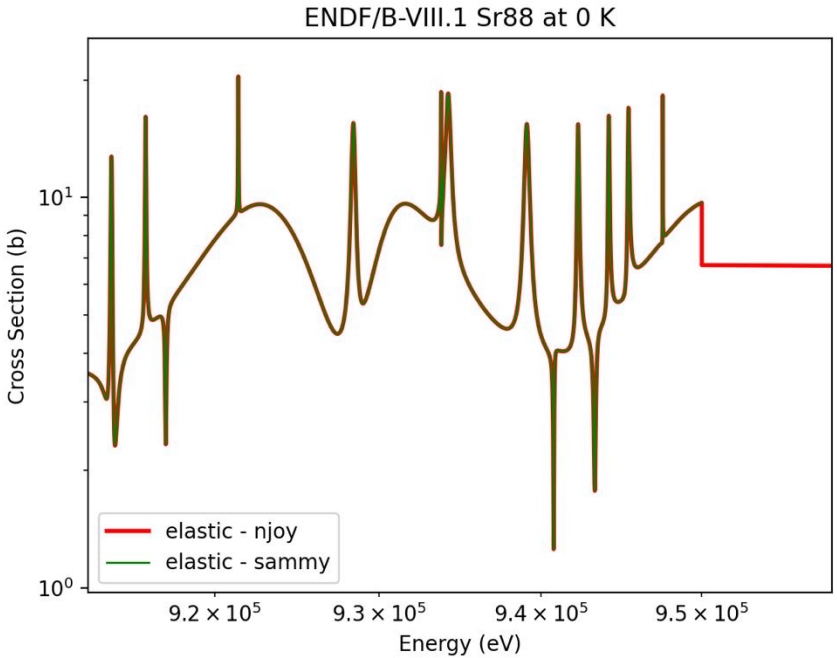
$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_\lambda - E - i\,\Gamma_{\lambda\gamma}/2} + R_c^{\mathrm{bkg}}\, \delta_{cc'} \right] \delta_{JJ'}. \qquad \text{(D.76)}$$

- An ORNL Sr88 evaluation now uses the SAMMY parametrisation option

- NJOY2016.73 (November 2023) is required for background R-matrix elements

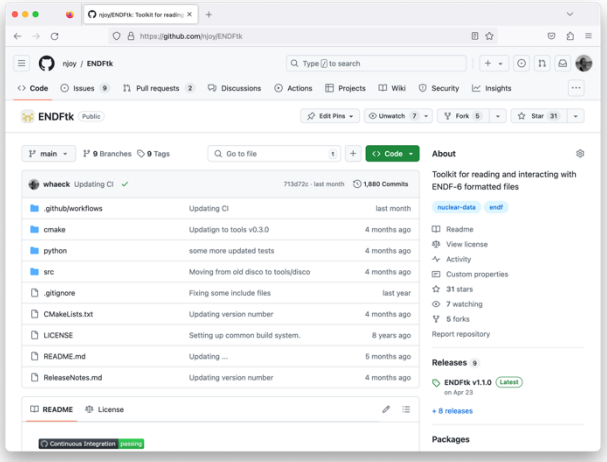
Background R-matrix elements in MF2 MT151

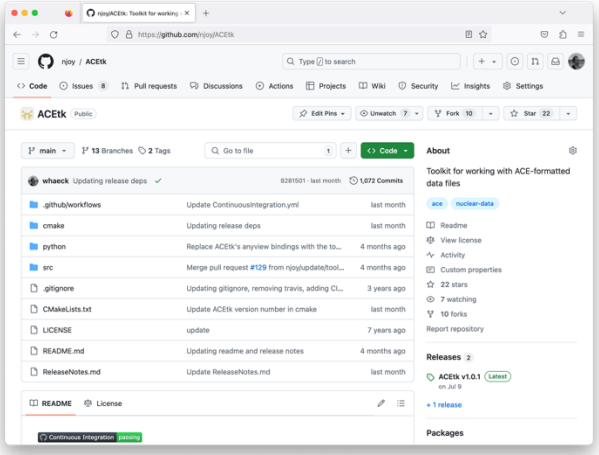




So what about the NJOY modernisation?

- We have shifted from a module based to a component based modernisation
  - Modernised modules are built from components
    - Components provide formats (e.g. ENDF, ACE, GNDS) or processing operations
    - 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





Formatting components

- ENDFtk v1.1.0 has been released (April 23, 2024)
  - Adding some missing interface functions related to TAB1 and TAB2 records
  - Fixing a parser issue where numbers are sometimes off by a very small value
  - Parsing ENDF files is now 10-20% faster as well
  - Get it on GitHub: https://github.com/njoy/ENDFtk

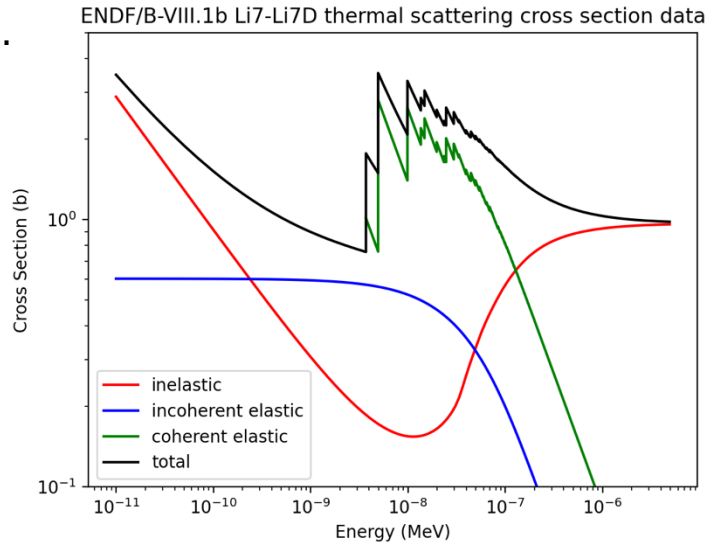
- ACEtk v1.0.0 has been released (April 24, 2024)
  - Changes to python bindings to allow ACEtk and ENDFtk to interface properly
  - Fixing the same parser issue as in ENDFtk resulting in faster parsing as well
  - Get it on GitHub: https://github.com/njoy/ACEtk

- Other format components we are working on: NDItk and GNDStk

The core math component: SCION

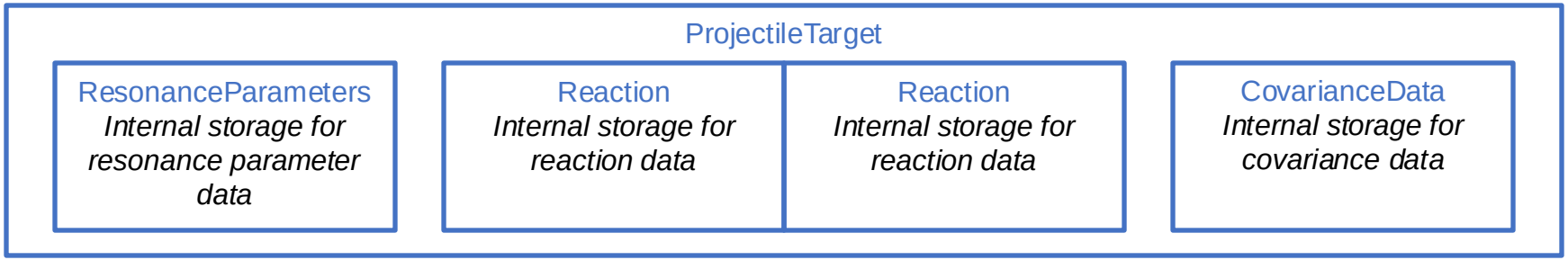
- Most NJOY modules need to perform a common set of operations:
  - Interpretation of various data representations (tables, analytical functions, etc.)
  - Linearisation of various data representations
  - Unionisation of data on a common energy grid, etc.
  - Addition, subtraction, multiplication, etc.
  - Differentiation and integration of data

- SCION provides these capabilities
  - SCientific interpretatION, linearisatION, differentiatION, integratION and more IONs
  - The basis of a format agnostic data interface

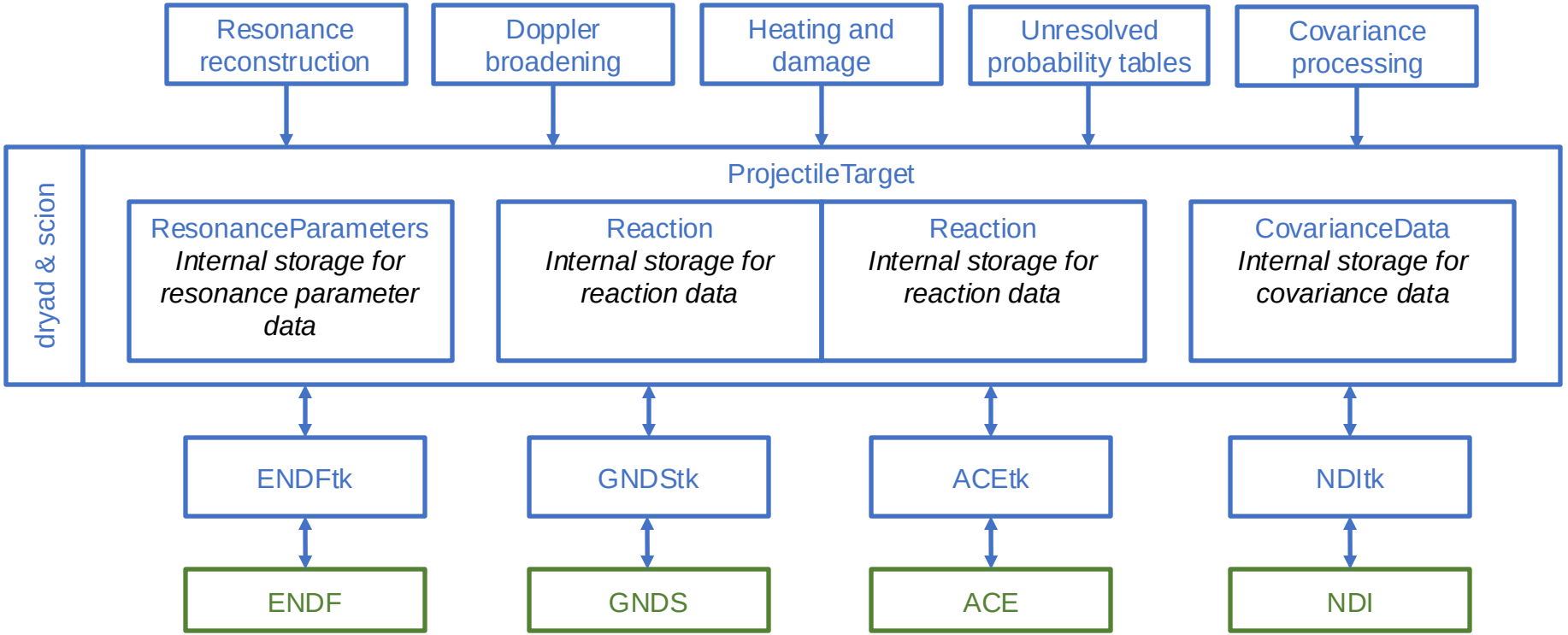


A format agnostic data interface: DRYAD

- A nuclear data user should not have to worry about format details
- For example:
  - ENDF MF4 Legendre data does not include the order 0 coefficient (equal to 1/2)
  - ENDF MF6 LAW1 Legendre data includes the order 0 coefficient but is not normalised
- Data is represented in its most generic form and can be translated to/from different formats

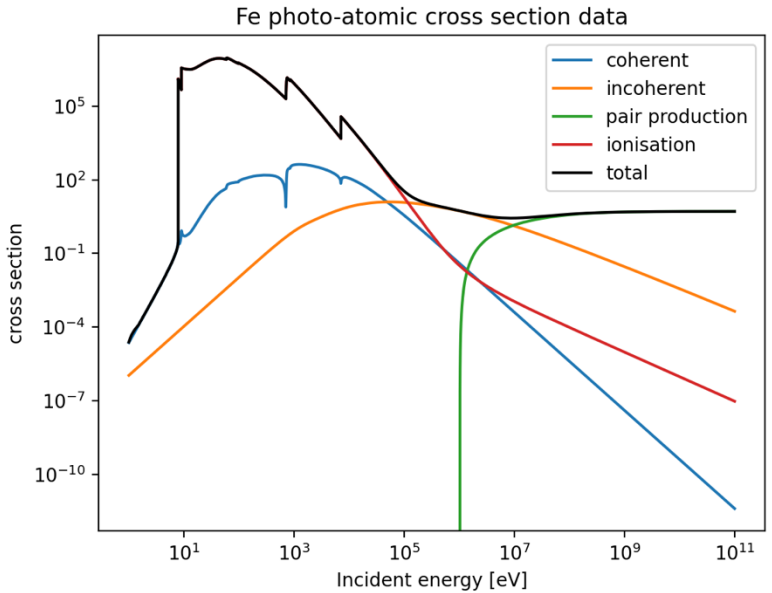


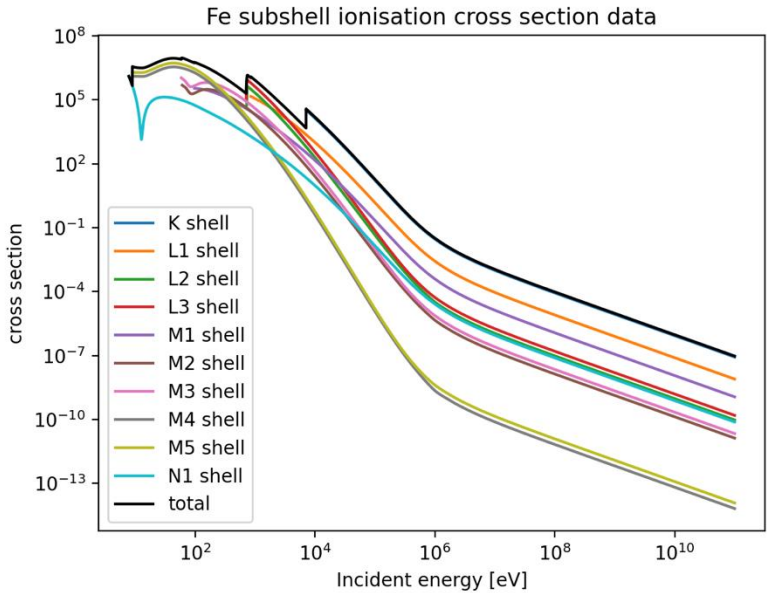
Putting it all together



A first application: photo- and electro-atomic ACE files

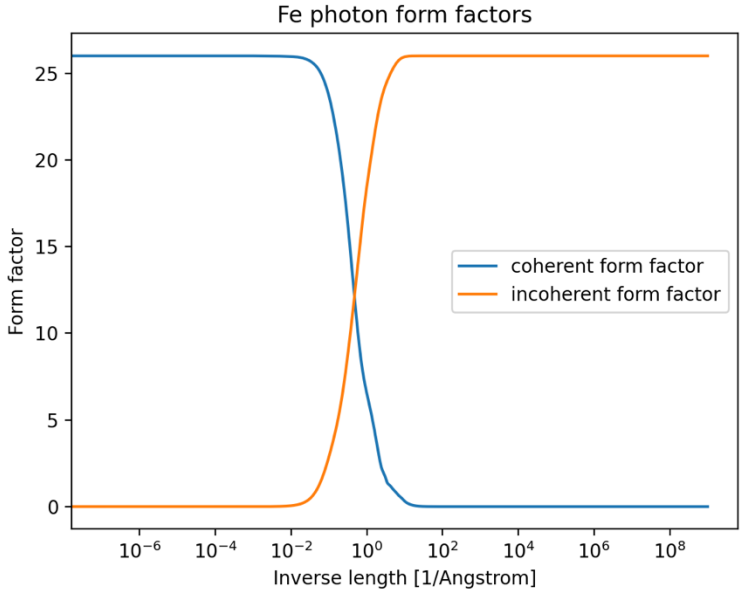
- NJOY2016 cannot process this type of ACE files so we are using this as a first application in a modernised NJOY

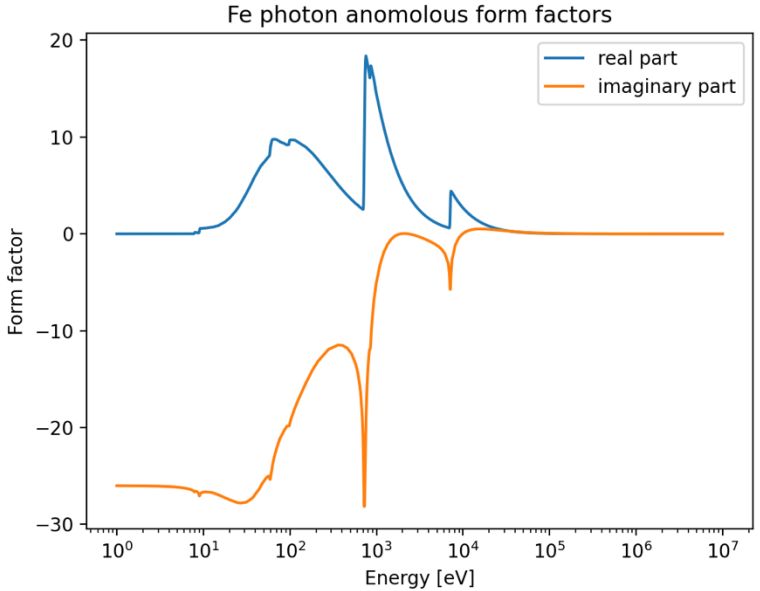




A first application: photo- and electro-atomic ACE files

- The current ACE files do not contain the anomalous form factors for coherent scattering so we are looking into adding these as well

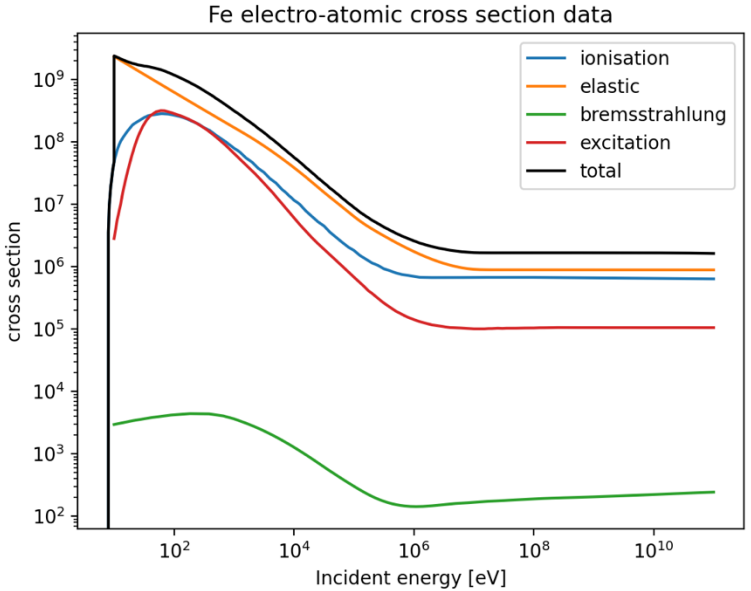




A first application: photo- and electro-atomic ACE files

- We have made significant progress towards completing this task

- Completed:
  - Reading photo-atomic data into dryad
  - Reading electro-atomic data into dryad
- In progress:
  - RECONR module implementation
    - Linearisation and unionisation
    - Photo- and electro-atomic data only
- Up next:
  - ACER module implementation
  - Input file and Python toolkit interface



Conclusions

- We continue to maintain and improve NJOY2016 for ENDF/B-VIII.1
  - Implement new ENDF features (e.g. background R-matrix elements)
  - Fix issues in NJOY2016 as soon as they become apparent

- New ENDF/B-VIII.1 nuclear data libraries will be processed
  - A multi-temperature incident neutron and thermal scattering data library
  - A new photo-atomic and electro-atomic (eprdata) library
  - We might also release a photonuclear and incident charged particle data library

- We continue our work on NJOY modernisation
  - A format agnostic data interface
  - New ACE files for photo-atomic and electro-atomic data
  - Potential improvements in photo-atomic physics in MCNP