LA-UR-25-26362

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Title:	Photoatomic and electroatomic data for MCNP
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Intended for:	2025 MCNP® User Symposium, 2025-07-07/2025-07-10 (Los Alamos, New Mexico, UNITED STATES)
Issued:	2025-07-03

Photoatomic and electroatomic data for MCNP

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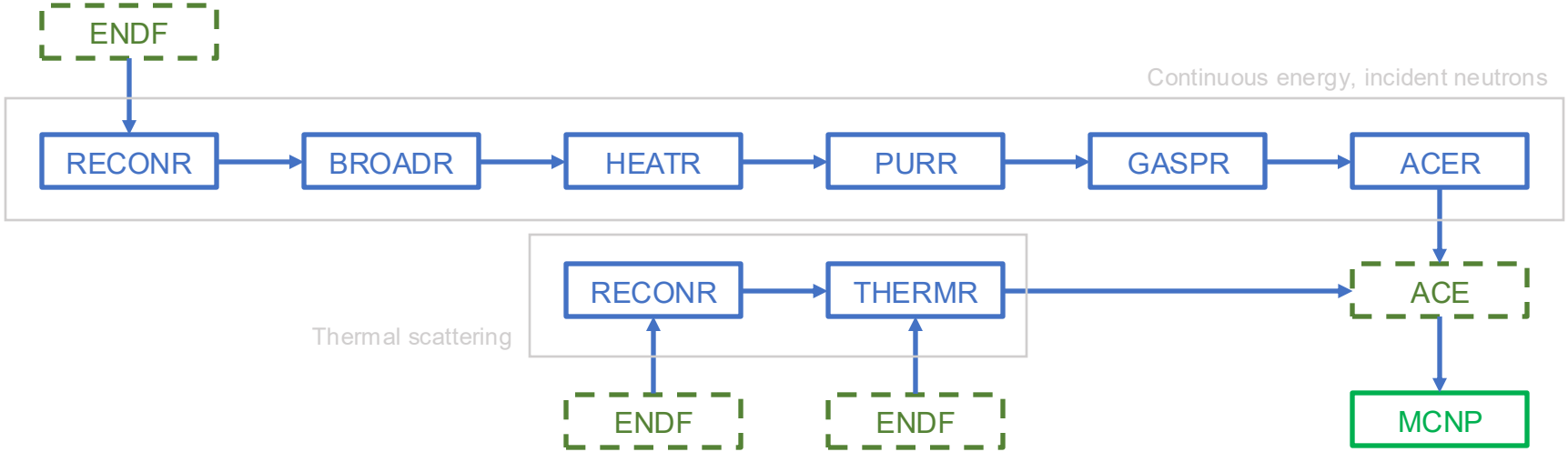
MCNP User Symposium, Los Alamos, July 7 – July 10, 2025

Outline

- Introduction
- Overview of the history of photoatomic and electroatomic data for MCNP
- Comparing photoatomic and electroatomic data

NJOY

- NJOY is the nuclear data processing software developed at Los Alamos
  - Main processing code to produce nuclear data application libraries for MCNP
  - Widely used for multigroup cross section generation for reactor analysis codes



Why do we need to modernise our processing code?

- New nuclear data features are hard to introduce in NJOY2016
  - Energy dependent fission yield data
  - Incident charged particle resonance parameters
- Better knowledge of implemented methods
  - Modernisation allows us to explore different methods and identify shortcomings

- NJOY2016 is too closely linked to the ENDF format
  - Introducing new evaluation formats like GNDS is “impossible” in NJOY2016
- Our users have needs that NJOY2016 does not provide
  - NJOY2016 does not linearise MF9 data
  - NJOY2016 cannot produce the photoatomic and electroatomic ACE files (eprdata)

Photoatomic data for MCNP

- `mcplib` is the oldest photoatomic library still being distributed with MCNP
  - Original release date: 1982
  - Energy range: 1 keV to 15 Mev (for a few selected elements) or 1 keV to 100 MeV
  - Form factor data (coherent and incoherent scattering) taken from ENDF/B-IV

- `mcplib02` was released in 1993 and extends `mcplib`
  - Energy range range extension to 100 GeV
    - Data below 10 MeV are identical to `mcplib`
    - Data above 10 MeV are taken from the LLNL Evaluated Photon Data Library (EPDL)
  - Form factor and fluorescence data are identical to `mcplib`

- ENDF/B evaluated data (other than form factors) have not been used

Photoatomic data for MCNP

- `mcplib03` is another extension of the `mcplib`/`mcplib02` generation libraries
  - Original release date: 2002
  - Cross section, form factor and fluorescence data are identical to `mcplib02`
  - Compton Doppler Broadening Data (CDBD) was added
- `mcplib04` is an alternative mcplib library based on “evaluated ENDF/B” data
  - Original release date: 2002
  - Cross Section data, form factors and fluorescence data taken from ENDF/B-VI.8
    - Photoatomic data in ENDF/B-VI.8 were in turn taken from the LLNL EPDL97 library
  - Compton Doppler Broadening Data (CDBD) is identical to `mcplib03`
  - This is the only library produced using NJOY99
- `mcplib63` and `mcplib84` are minor updates to `mcplib03` and `mcplib04`
  - Released in 2012 to correct data interpretation issues in MCNP5 (pdf to cdf)

Photoatomic and electroatomic data for MCNP

- `eprdata12` adds electroatomic data to the libraries
  - Original release data: 2013
  - All data taken from ENDF/B-VI.8 (thus equivalent to `mcplib84` for photoatomic data)
  - Compton Doppler Broadening Data (CDBD) equal to `mcplib63`/`mcplib84`

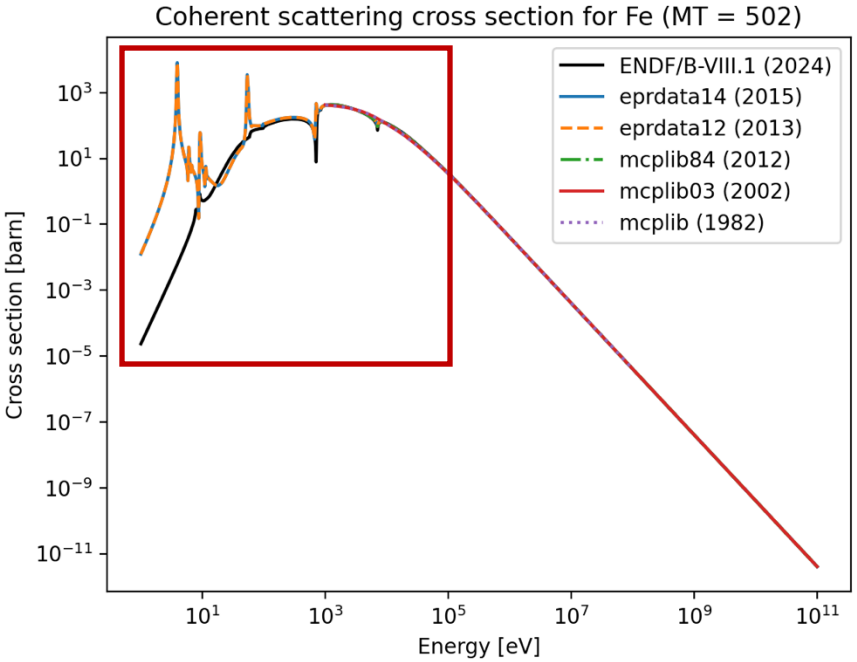
- `eprdata14` updates the format and supersedes `eprdata12`
  - Original release data: 2015
  - All data taken from EPICS2014
  - Compton Doppler Broadening Data (CDBD) is identical to `eprdata12`

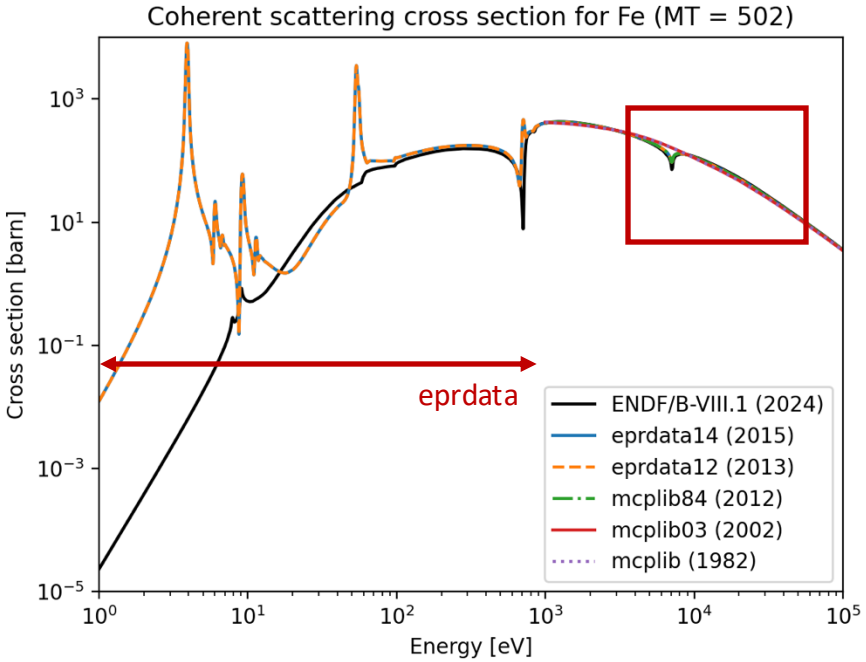
- With `eprdata14` we went back to “not using” evaluated ENDF/B data
  - It should be noted EPICS2017 was later adopted for ENDF/B-VIII.0

New photoatomic and electroatomic data : `eprdata25`

- The first application for modernised NJOY
- Source of the data is ENDF/B-VIII.1 (which is EPICS2023) whenever possible
- We have to do reverse engineering to figure out how eprdata files were made
  - Compton Doppler Broadening Data (CDBD) will be copied over from `eprdata14`
  - Fluorescence data can be derived from atomic relaxation data
  - Transport corrected elastic scattering cross section for electroatomic data
- Current status of the new library
  - We have prototype files with all new electroatomic data
  - We foresee a release of a prototype library by the end of July 2025

Photoatomic data comparison





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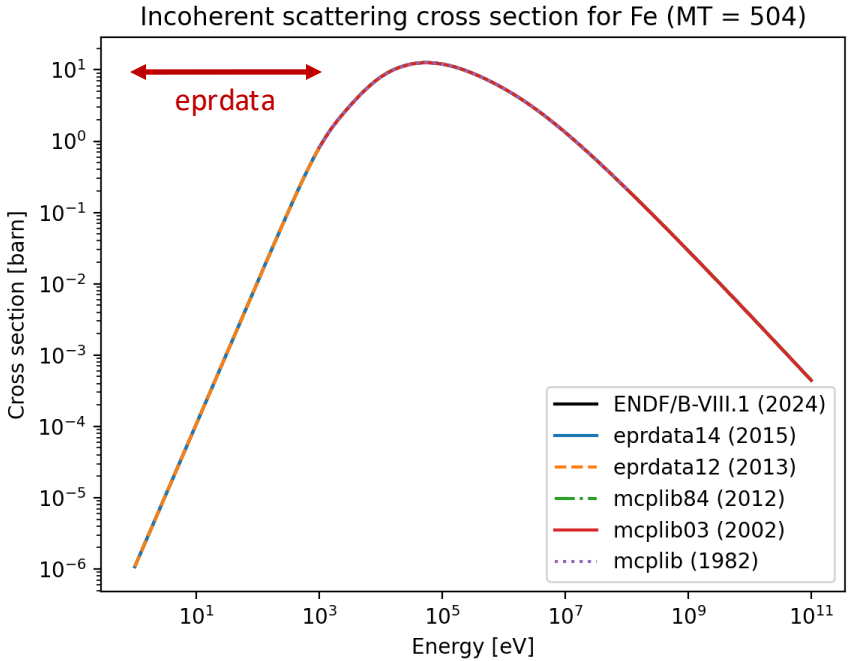

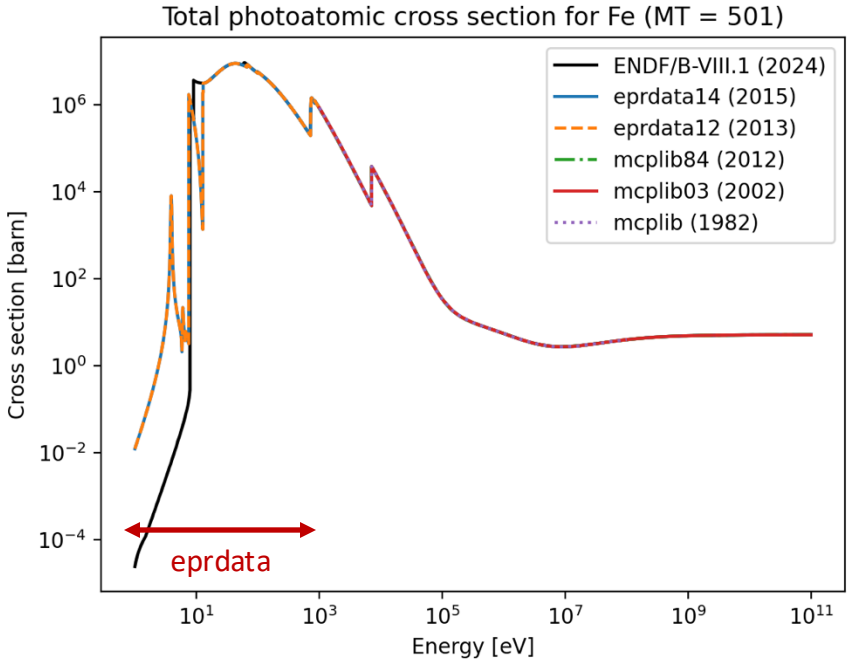

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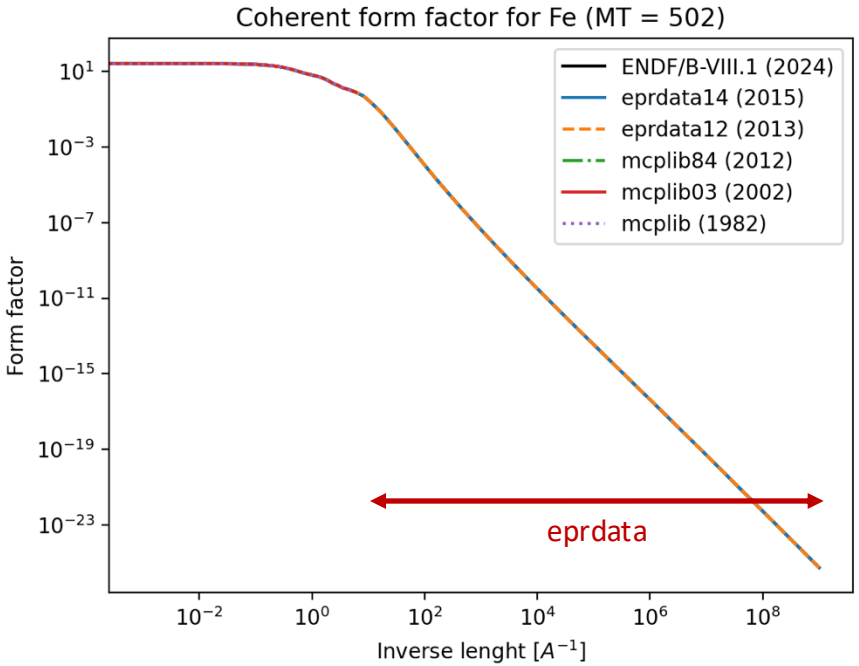
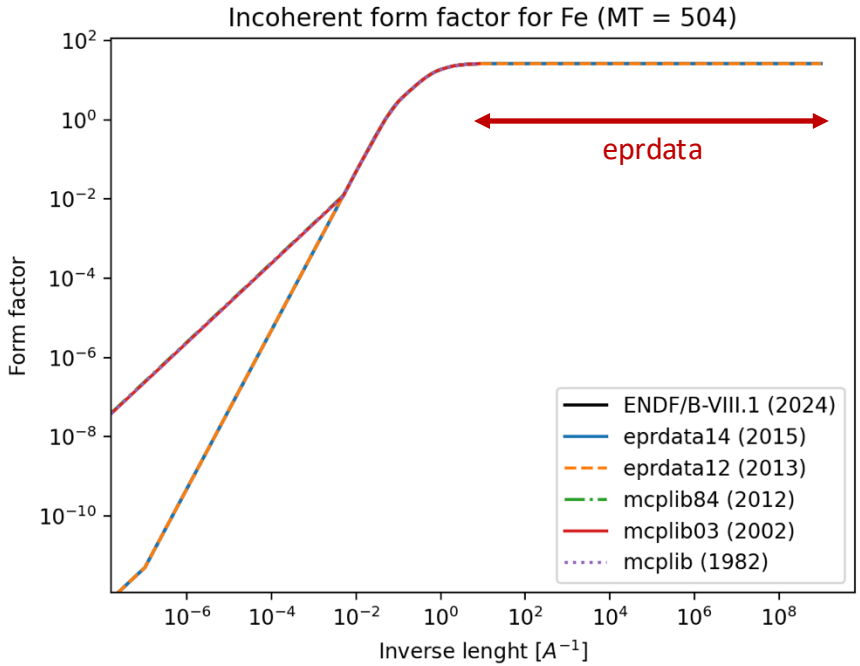




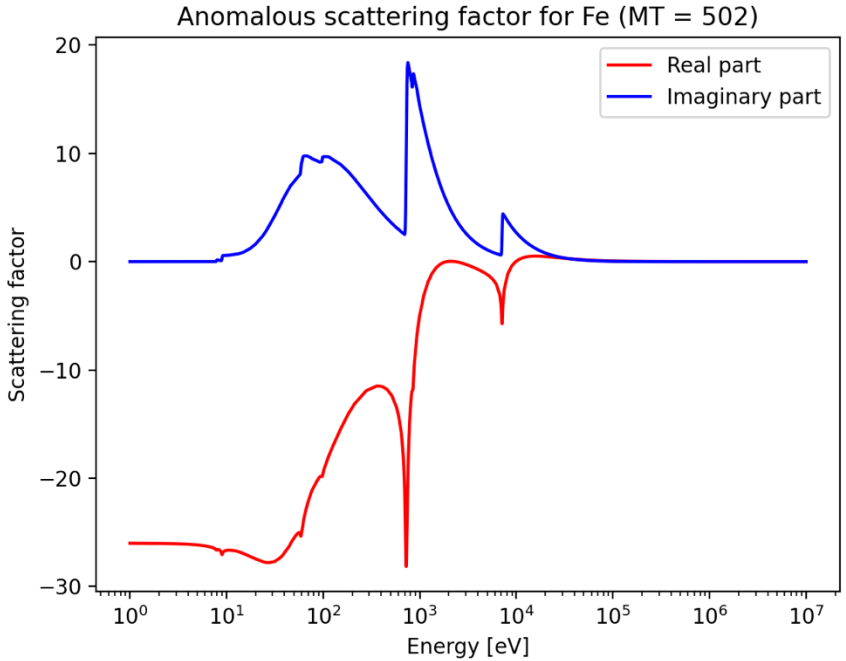
Using the anomalous scattering factor?

- Coherent scattering is proportional to the Thompson cross section:

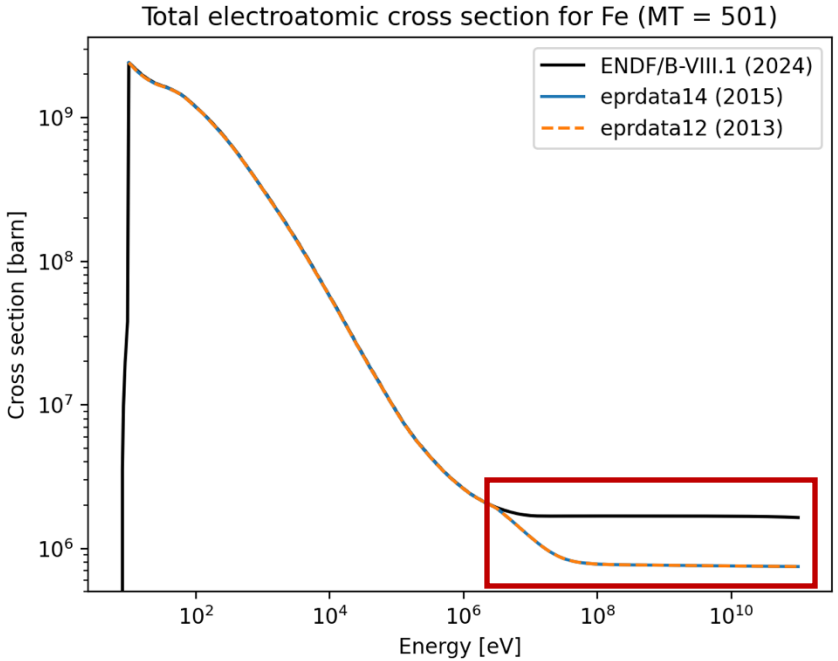
$$\frac{d\sigma_{coh}(E,\mu)}{d\mu} = \frac{d\sigma_T(E)}{d\mu} \|F(x,Z) + G(E)\|^2$$

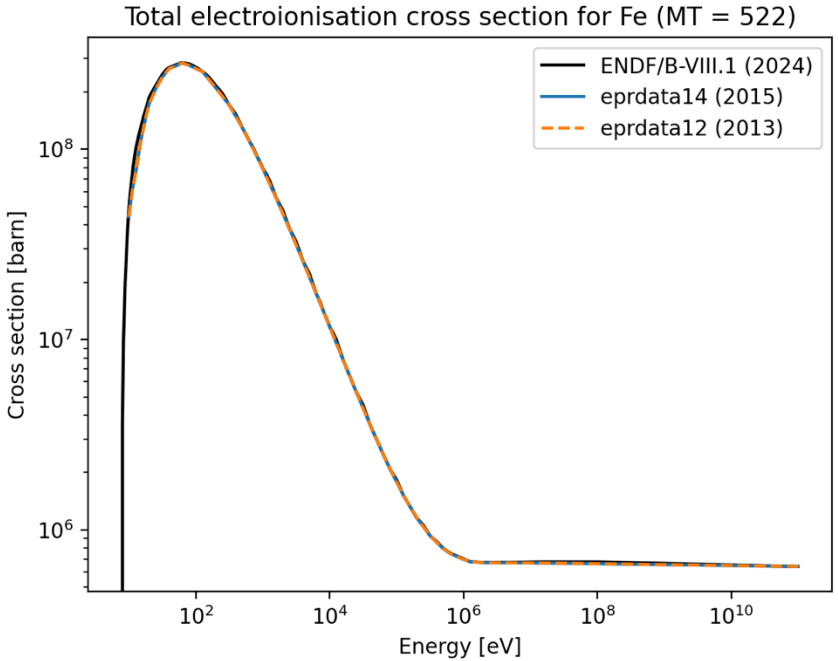
  - $F(x,Z)$ is the coherent form factor
  - $G(E)$ is the anomalous scattering factor

- These coherent anomalous scattering factors are not stored in the ACE files

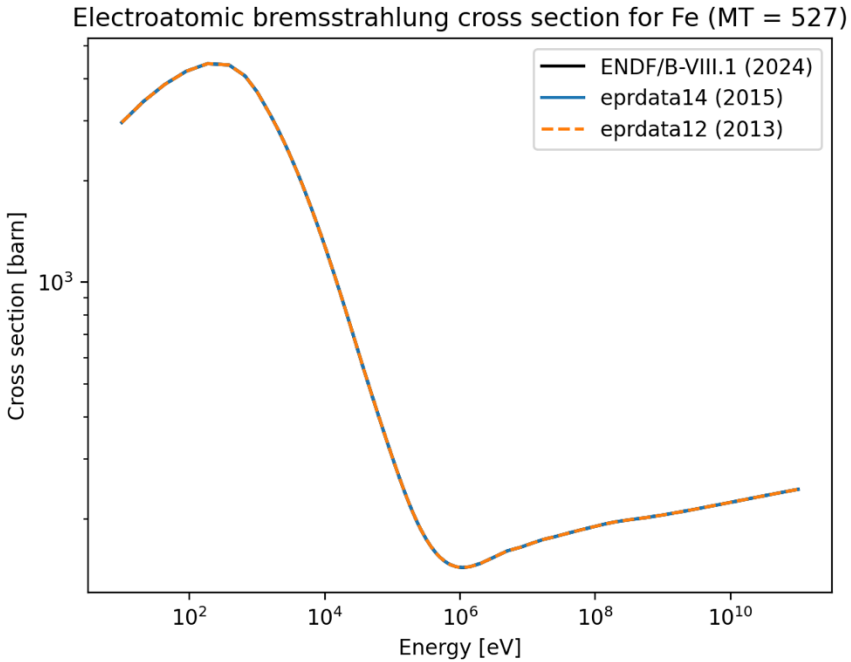


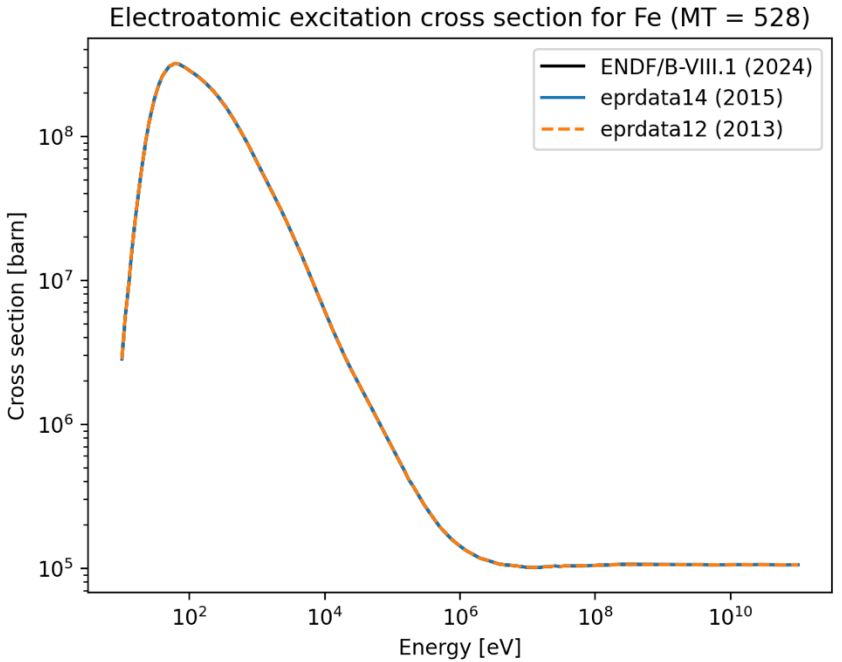
Electroatomic data comparison





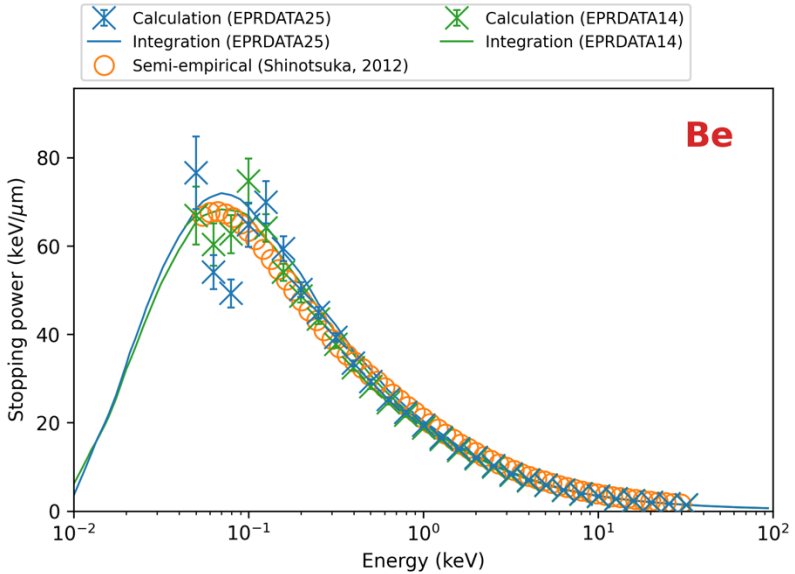
Electroatomic data comparison

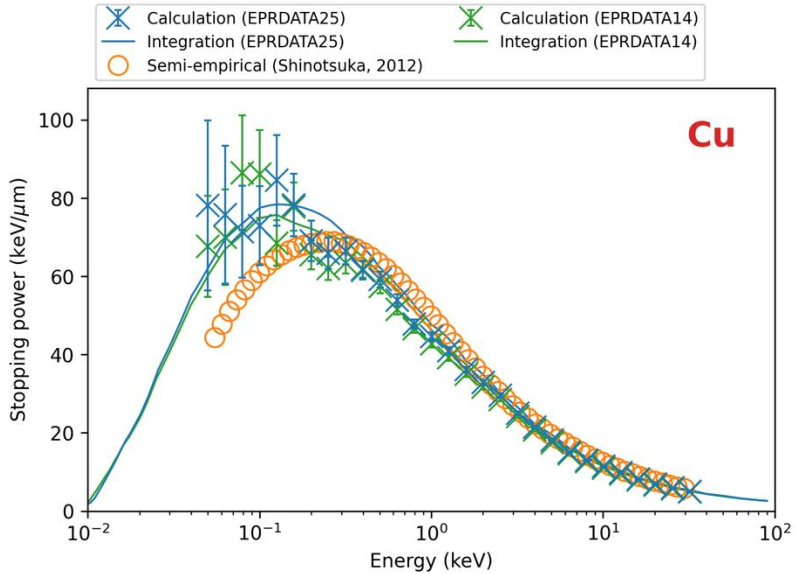




Verification and validation of `eprdata25`

- The first results for electron stopping power calculations with MCNP
  - See also M. Lively's talk in this session





Conclusions and future work

- A new photoatomic and electroatomic data library for MCNP : `eprdata25`
  - We talked about it a lot over the last 2 years but it is finally happening
  - A release candidate for the library will be available by the end of July 2025

- The first application for modern NJOY
  - Only `mcplib04` was produced with NJOY99 and the format has diverged since
  - A lot of reverse engineering – and head scratching
  - And just for kicks: we will use GNDS files to produce the library