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Continuing the NJOY modernization

W. Haeck, A. Lewis, J. Peterson, P. Sole, A. Golas, A. Kitamura

MCNP Symposium 2026, August 24 – August 26, 2026

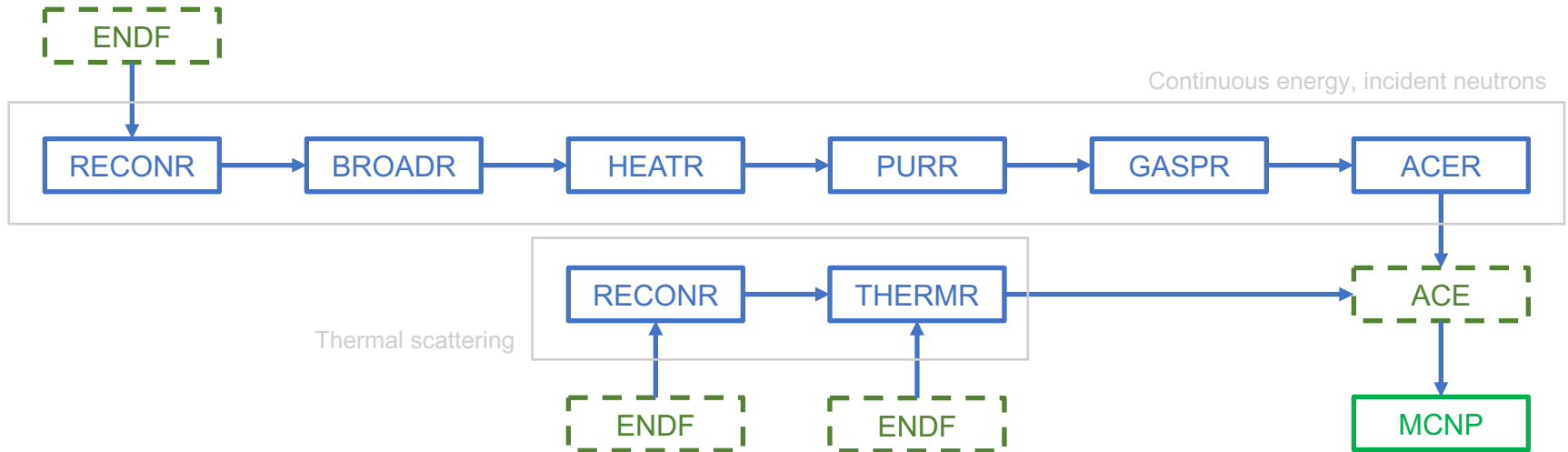
Outline

- Introduction
- A format agnostic data interface
- The first modern NJOY libraries : eprdata25
- Overview of new features
 - Covariance data structures
 - Thermal scattering data
- Conclusions and future developments



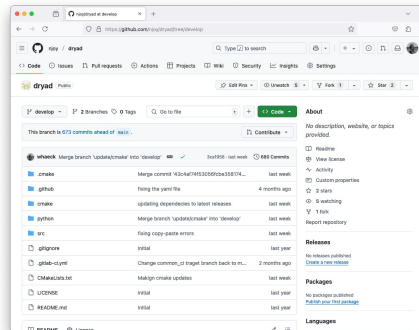
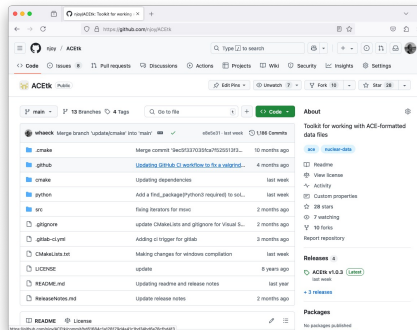
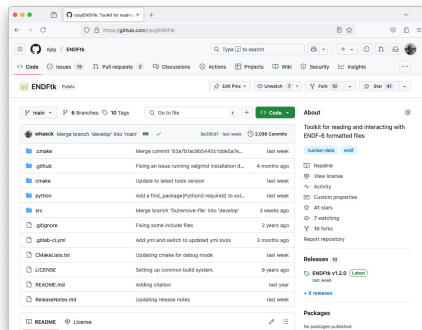
NJOY

- 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

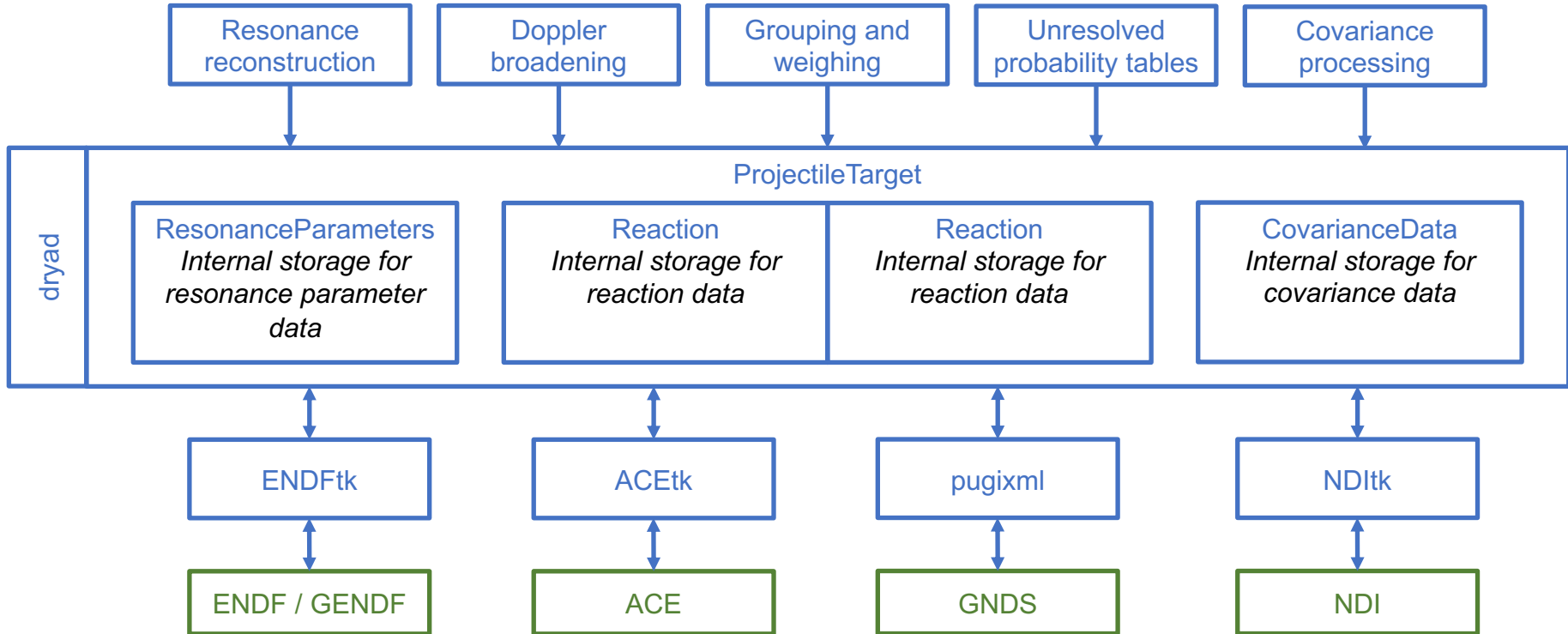


A component based modernization strategy

- Modernized modules are built from components
 - Format components: `ENDFtk`, `ACEtk`, `NDItk`
 - Mathematical operations and generic data representation: `scion`
 - Format agnostic nuclear and atomic data access and interpretation: `dryad`
 - Modernized modules like `reconr`, `broadr`, etc. will interact with the `dryad` interface
- Components can be developed and deployed faster than modules
 - Entirely developed in C++ and with Python bindings

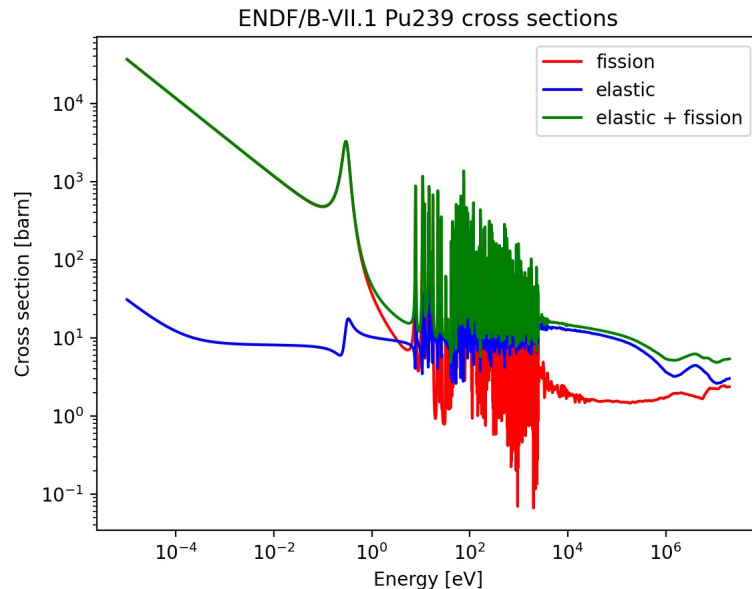


A component based modernization strategy



Format agnostic data interface and structures

- As a nuclear data user, you should not have to worry about format details
- `dryad` represents nuclear data in its most generic form using consistent units
- `dryad` is more than just an interface
 - Linearisation of tables and series
 - Operations on tables and series (+, -, *, /)
 - Calculation of mean values from a distribution
 - Data normalisation on demand
 - Resonance reconstruction at a given energy



```
from njoy.dryad import ProjectileTarget
from njoy.dryad.id import ReactionID

pt = ProjectileTarget.from_endf_file( '94239.endf' )

elastic_id = ReactionID( 'n,U235->n(0)' )
fission_id = ReactionID( 'n,U235->fission' )

elastic = pt.reaction( elastic_id ).cross_section
fission = pt.reaction( fission_id ).cross_section
sum = elastic + fission
```



Data format support in modern NJOY

Photoatomic and electroatomic data	ENDF	GNDS	ACE	GENDF
Atomic relaxation data			N/A	N/A
Cross section data				
Products, energy and angular distribution data				
Incident neutron, charged particle and photonuclear data	ENDF	GNDS	ACE	GENDF
Resonance parameters			N/A	N/A
Cross section data				
Products, energy and angular distribution data				
Covariance data			N/A (?)	
Other data types	ENDF	GNDS	ACE	GENDF
Radioactive decay data and fission yield data			N/A	N/A
Thermal scattering data				



eprdata25 has been released – we hope ...

It should appear here

LA-UR-26-27338



Memorandum

XCP-5 Materials and Physical Data

Subject: Release of eprdata25: ENDF/B-VIII.1-Based ACE Data Files for Photo- and Electro-atomic Transport

Introduction

On August 30, 2024, the National Nuclear Data Center (NNDC) released the ENDF/B-VIII.1 nuclear data library. The library was released in the standard Evaluated Nuclear Data File (ENDF) format. These files can be accessed on the NNDC's website (www.nndc.bnl.gov). The incident neutron and thermal scattering sub-libraries provided by the ENDF/B-VIII.1 nuclear data library have already been processed into ACE file for use with the MCNP code, respectively named the Lib81 and ENDF81Sab libraries. The current memo deals with the production of another MCNP library based on ENDF/B-VIII.1, this time for the photo-atomic, electro-atomic and atomic relaxation sub-libraries. The photo-atomic and electro-atomic sub-libraries provide the cross section data and secondary particle distribution data for atomic interactions of photons and electrons (including electron subshell ionization). The atomic relaxation sub-library supplements these two sub-libraries by providing the transition probabilities of vacancies in the electron subshells due to ionization, which allows us to calculate outgoing X-ray and Auger electron spectra.

To: Distribution
From: Wim Haecq, XCP-5
Mike Lively, XCP-3
Symbol: XCP-5:26-035
Date: August 4, 2026

The screenshot shows the Los Alamos National Laboratory website. The top navigation bar includes links for MISSION, SCIENCE & ENGINEERING, COLLABORATION, COMMUNITY, and ENVIRONMENT. The left sidebar contains a search bar and a list of libraries under the heading 'ACE LIBRARIES'. The main content area displays the title 'Electron/Photon/Relaxation Data Library—eprdata14' and the release date 'Released: 2015-07-02'. The text describes the library's origin from the EPICS2014 data and its processing into ACE format by H. Grady Hughes. It also mentions the library's coverage of elements from hydrogen (Z=1) to Fermium (Z=100) and provides examples of ZAIDS and their extensions.

Electron/Photon/Relaxation Data Library—eprdata14

Released: 2015-07-02

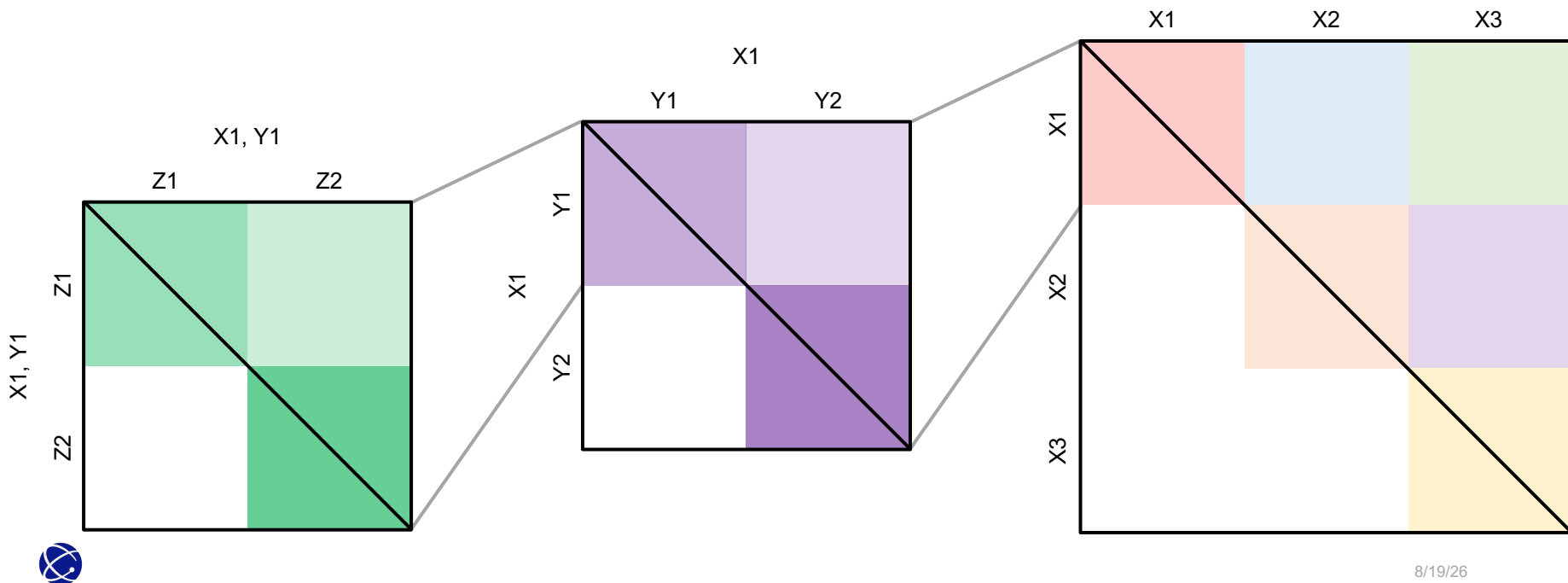
The eprdata14 library is based on the [EPICS2014](#) (Electron and Photon Interaction Cross Section) data from the IAEA, prepared Dermott E. "Red" Cullen. It was processed into ACE format by H. Grady Hughes at Los Alamos National Laboratory.

There is data for elements hydrogen (Z=1) to Fermium (Z=100). All of the ZAIDS are elemental and so the **A** is **000** for every data table. For example, the ZA **1000** is for hydrogen, **26000** for iron, **92000** for uranium, and similarly for all other elements. All of the ZAIDS in the eprdata14 library use the **.14p** extension.



Covariance data structures

- A new covariance data structure that can hold covariance matrices of any dimensionality and supports on- and off-diagonal submatrices



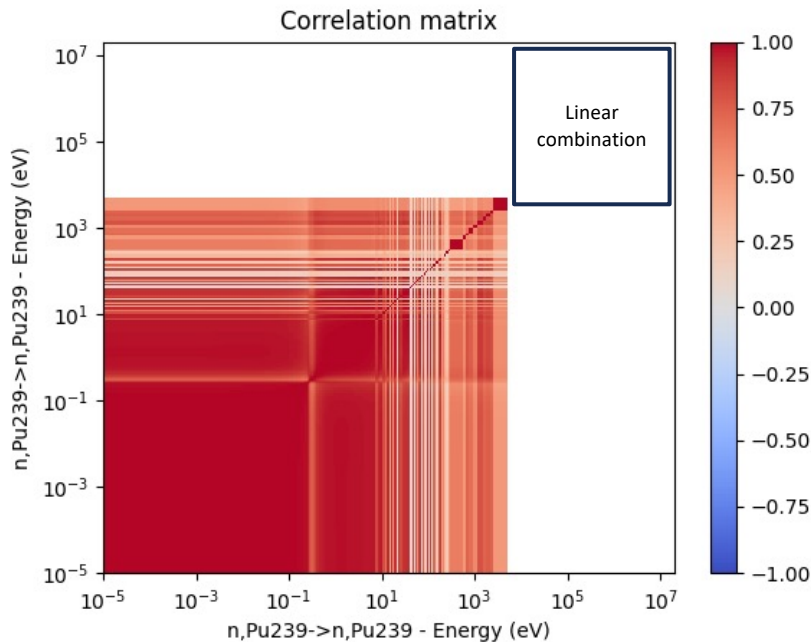
Covariance data structures

- Basic capabilities that are available in the covariance data structure:
 - Create data using covariance matrix or standard deviations and correlations
 - Derive data from the covariance matrix:
 - Covariance matrix
 - Standard deviations
 - Correlation matrix
 - Eigenvalues and eigenvectors
 - Extraction of submatrices
- Currently available for the following covariance types:
 - Cross section and angular covariance data
 - Product multiplicity covariance data (fission yield covariances)
- Populating these from ENDF, GNDS and GENDF



Covariance data structures

- Example: as-evaluated Pu239 elastic scattering correlations from ENDF/B-VIII.1



```
from njoy.dryad import ProjectileTarget
from njoy.dryad.id import ReactionID

# create some identifiers
id = ReactionID( 'n,Pu239->n(0)' )

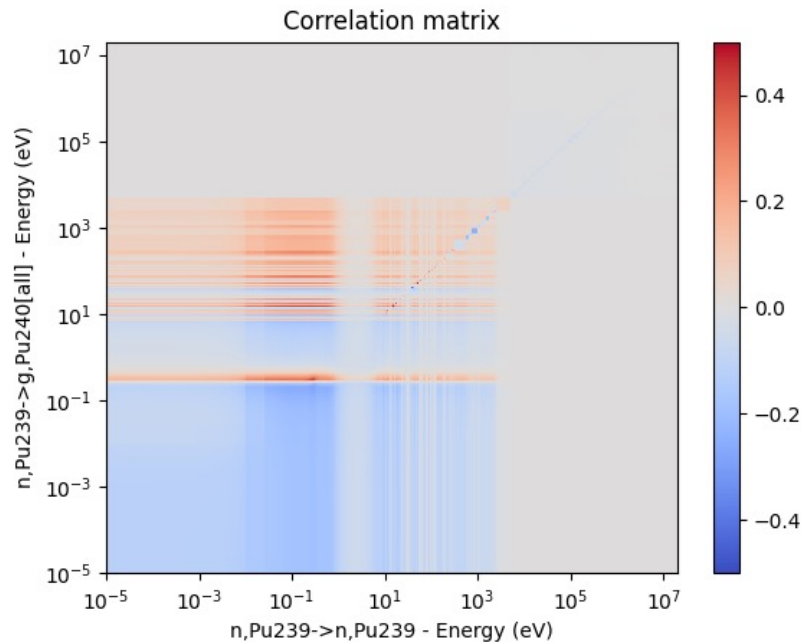
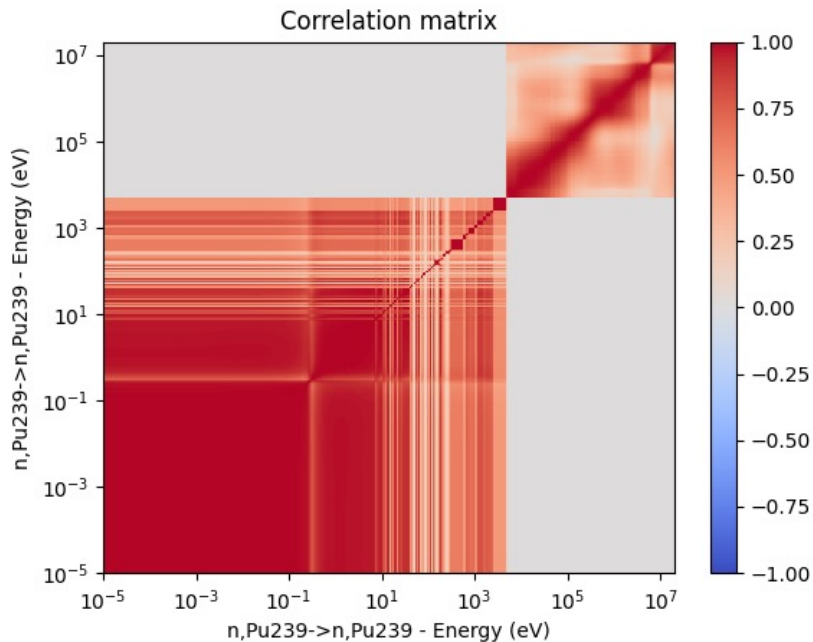
# open the GNDS file for Pu239
eval = ProjectileTarget.from_gnds_file( 'pu239.gnds' )

# get the covariance matrices (evaluated as 2 pieces)
cov = eval.covariance_data.cross_section.covariance_matrix( id )
```



Covariance data structures

- Example: NJOY2016 processed Pu239 correlation matrices from ENDF/B-VIII.1



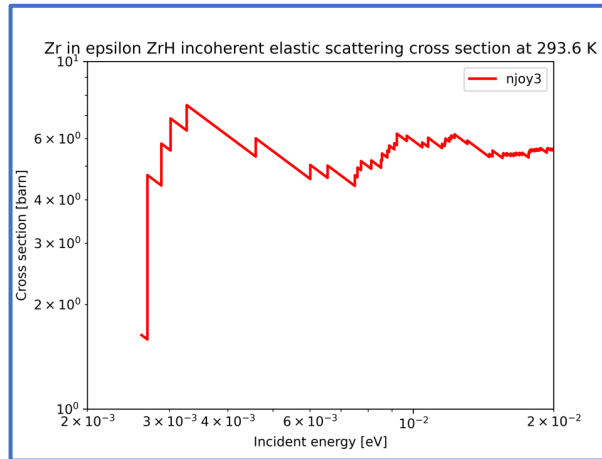
Thermal scattering data

- At low incident energies, molecular and crystalline bonds influence scattering
 - This is referred to as thermal scattering
 - Essentially related to material properties
- Multiple categories of thermal scattering exist:
 - Coherent elastic: important in crystalline solids (graphite, metals, etc)
 - Incoherent elastic: important in solids with hydrogen (polyethylene, ZrH, etc.)
 - Incoherent inelastic: all solid and liquid materials (hydrogen in water)
- NJOY2016 thermal scattering processing is done in THERMR
 - Fixed incident energy grid across all scattering categories
 - Angular distribution data is only given as equally probable discrete cosines

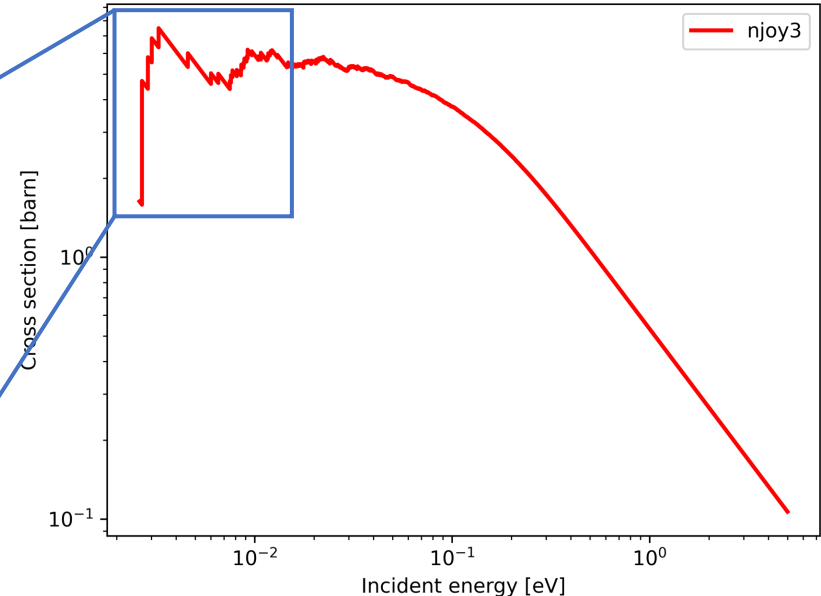


Thermal scattering data

- Coherent elastic is characterised by Bragg edges
 - Evaluated data consists of Bragg edge energies and associated magnitudes
 - Modern NJOY linearizes the cross section on demand



Zr in epsilon ZrH incoherent elastic scattering cross section at 293.6 K



Thermal scattering data

- Incoherent elastic
 - Evaluated data consists of the bound cross section and Debye-Waller integral values
 - Differential and integrated cross sections can be calculated analytically

$$\frac{d^2\sigma}{dE'd\mu}(E, E', \mu) = \frac{\sigma_b}{2} e^{2EW'(1-\mu)} \delta(E - E')$$

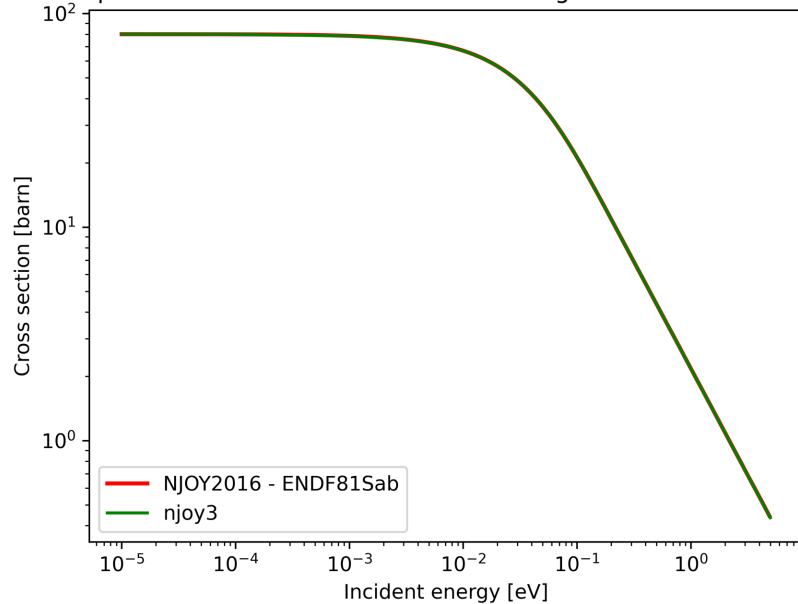
$$\frac{d\sigma}{d\mu}(E, \mu) = \frac{\sigma_b}{2} e^{-2EW'(T)(1-\mu)}$$

$$\sigma(E) = \frac{\sigma_b}{2} \frac{1 - e^{-4EW'}}{2EW'}$$

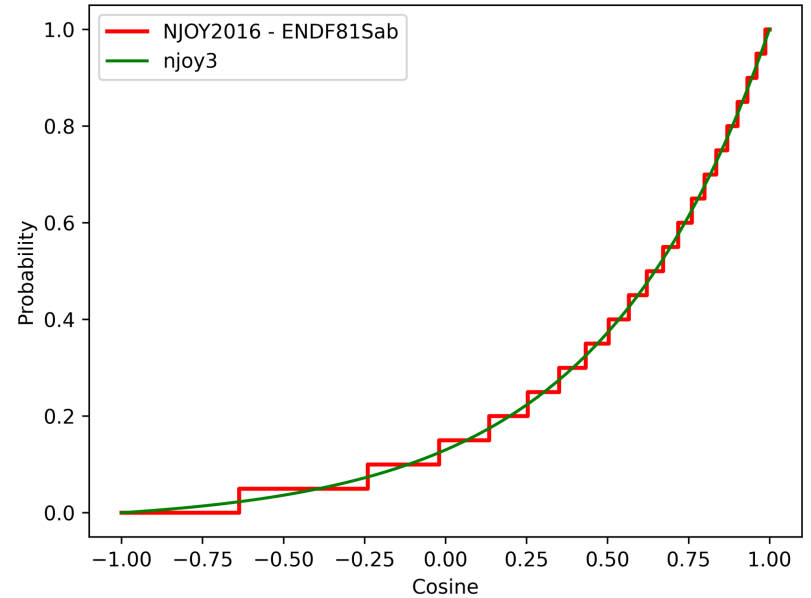


Thermal scattering data

H in epsilon ZrH incoherent elastic scattering cross section at 293.6 K



H in epsilon ZrH angular cdf for $E_{in} = 0.1035$ eV and 293.6 K



Thermal scattering data

- Incoherent inelastic: this is where it gets a lot more complicated
 - Evaluated data consists of a tabulated function of energy and momentum transfer

$$\frac{d^2\sigma}{dE'd\mu}(E, E', \mu) = \frac{\sigma_{bn}}{2kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta)$$

$$\beta = \frac{E' - E}{kT} \quad \alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{kT}$$

- Some approximation and tweaking is required to work with this data
 - Using the Short Collision Time (SCT) approximation outside the β grid and above the α grid
 - An approximation needs to be made small α values below the α grid
 - Log-linear interpolation cannot handle $S(\alpha, \beta) = 0$
 - NJOY2016 uses the SCT approximation inside the α, β grid for “low” values of $S(\alpha, \beta)$

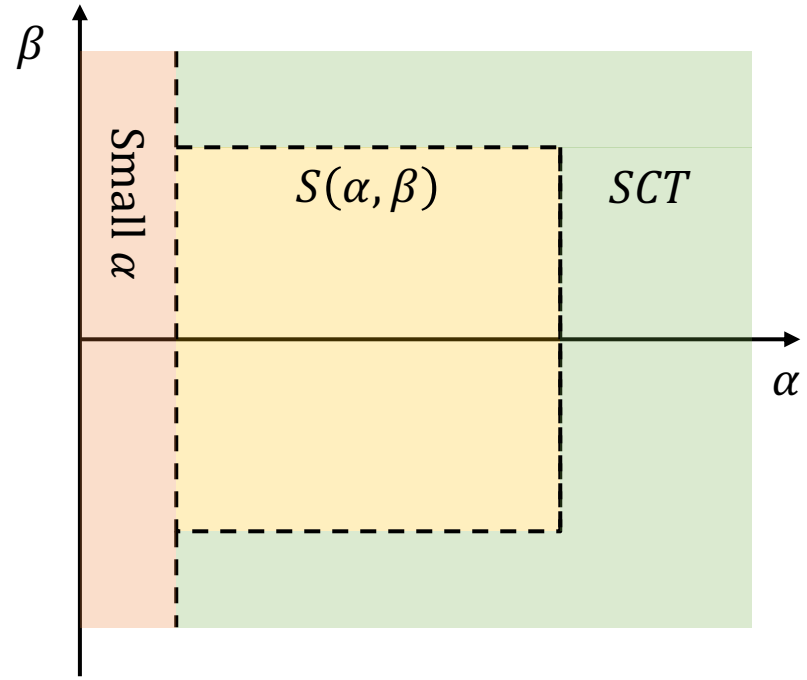


Thermal scattering data

- The cross section and distributions are calculated through integration
 - Adaptive linearization to obtain an appropriate grid along the primary dimension
 - Integration across the secondary dimension
 - Gauss-Lobatto adaptive quadrature
 - Integration of linearized distributions

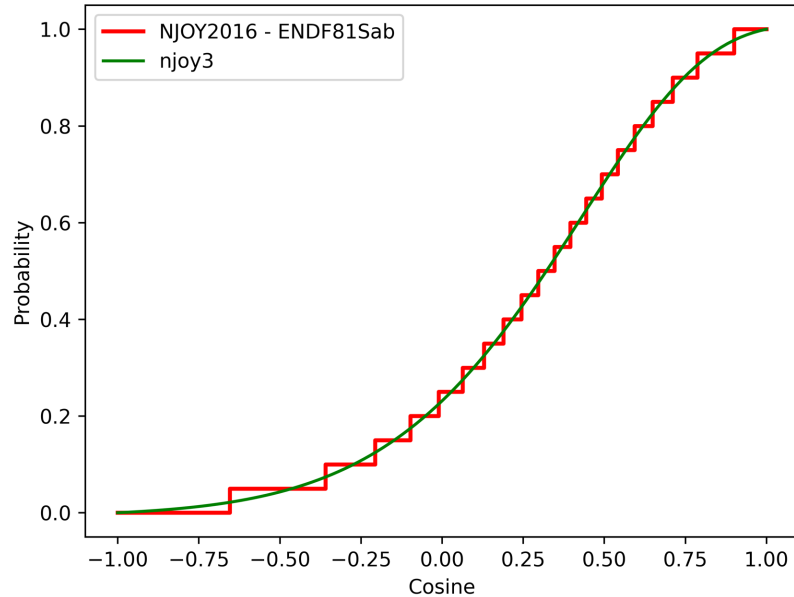
$$\frac{d^2\sigma}{dE'd\mu}(E, E', \mu) = \frac{\sigma_{bn}}{2kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta)$$

$$\beta = \frac{E' - E}{kT} \quad \alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{kT}$$

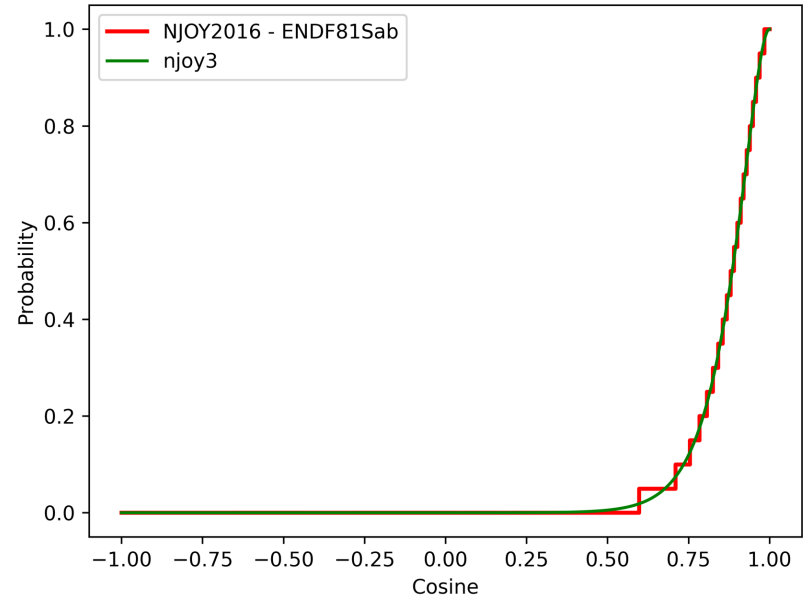


Thermal scattering data

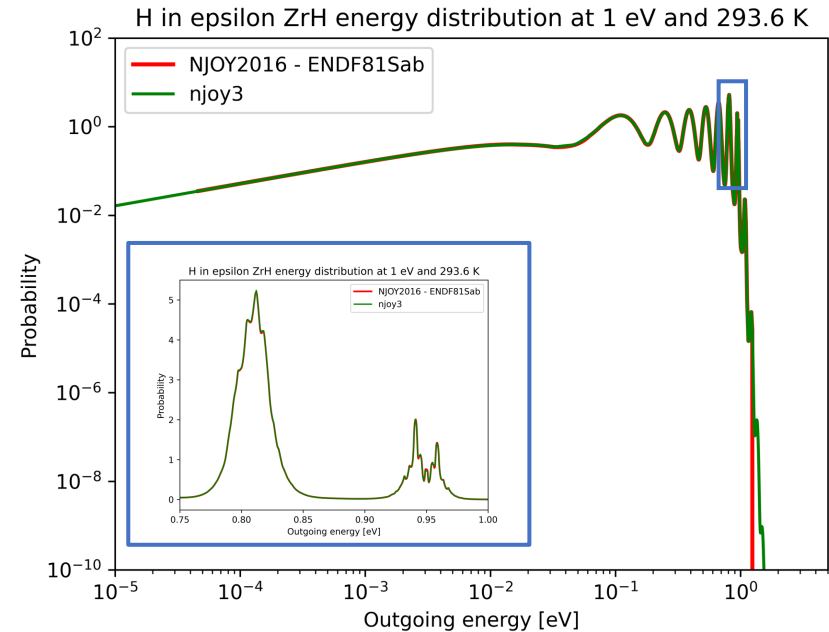
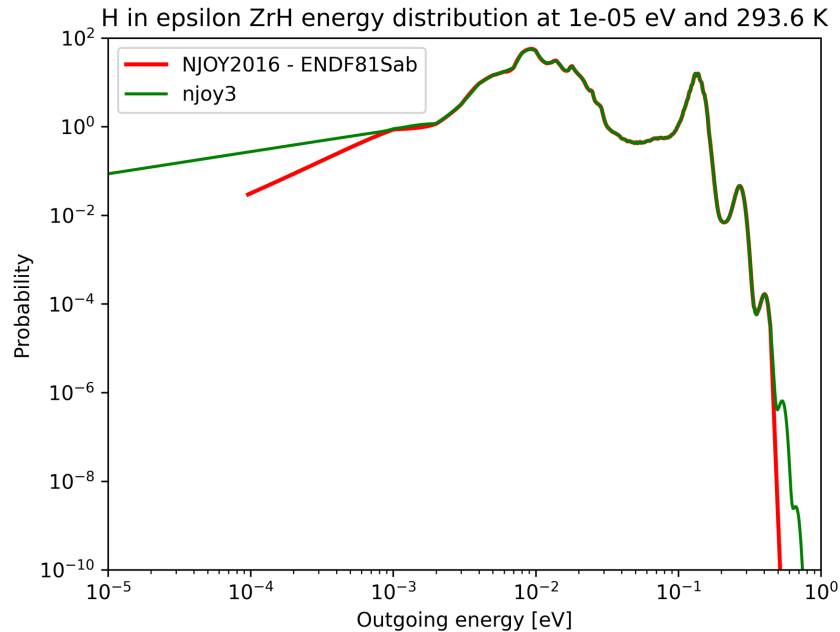
H in epsilon ZrH angular cdf for $E_{in} = 0.95$ eV, $E_{out} = 0.2$ eV and 293.6 K



H in epsilon ZrH angular cdf for $E_{in} = 0.95$ eV, $E_{out} = 0.95$ eV and 293.6 K

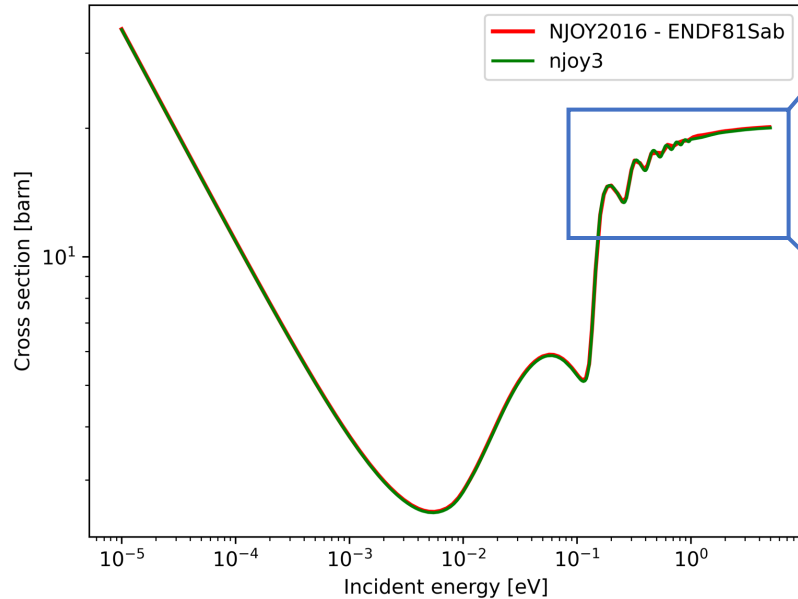


Thermal scattering data

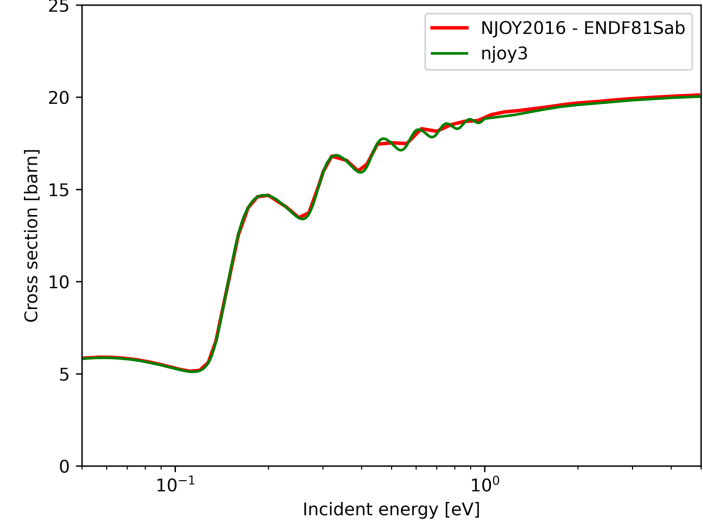


Thermal scattering data

H in epsilon ZrH incoherent inelastic scattering cross section at 293.6 K



H in epsilon ZrH incoherent inelastic scattering cross section at 293.6 K

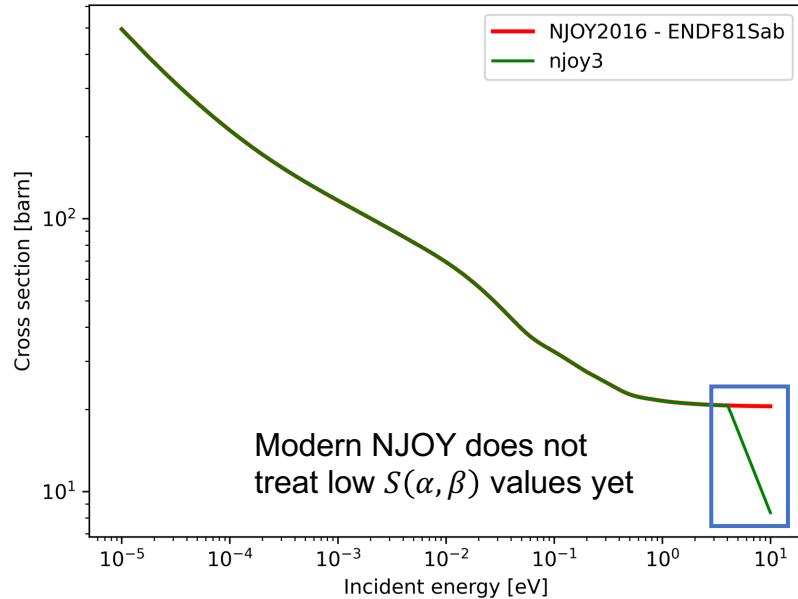


Adaptive linearization solves
this long outstanding problem!

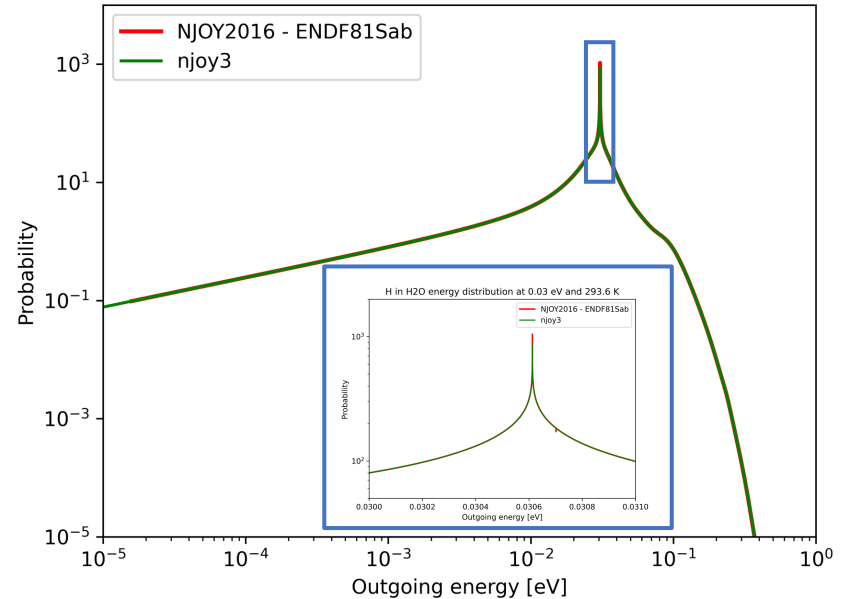


Thermal scattering data – some outstanding issues

H in H2O incoherent inelastic scattering cross section at 293.6 K



H in H2O energy distribution at 0.03 eV and 293.6 K



Conclusions and future work

- We are making great progress on the modernization
 - We have – hopefully – released the first library produced with modern NJOY
 - A format agnostic data interface serves the backbone of modern NJOY
 - Supporting ENDF and GNDS evaluation formats at the same time
 - Thermal scattering data processing is almost complete
- Current major development focus:
 - Resonance reconstruction
 - Covariance data processing
- Future developments we may start looking into:
 - Data testing and verification
 - More secondary particle distribution data structures

