NJOY for ENDF/B-VIII.1 and ENDF/B-IX

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Outline

- NJOY2016 updates
- ENDF/B-VIII.1 libraries for MCNP
  - Lib80 and ENDF81SaB
  - eprdata24
- A modernization update
  - Why modernize
  - Format components
  - The math core and a format agnostic interface
  - Putting it all together
- Conclusions

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

- Over the last 5 years we have worked towards this goal
  - This represents 26 updates to NJOY2016

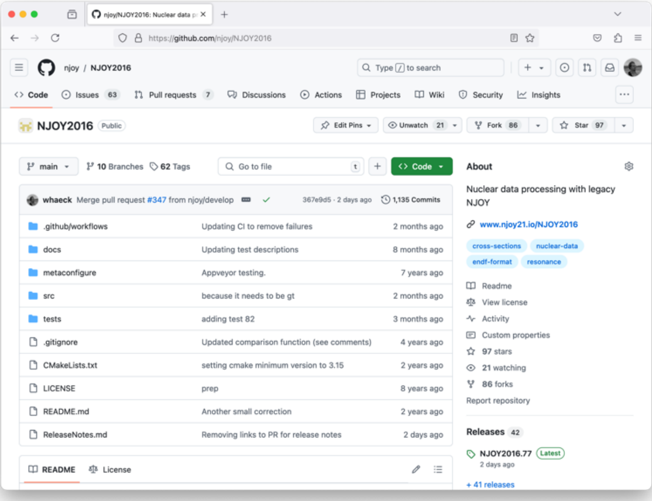
- Every ENDF/B generation makes changes and so did ENDF/B-VIII.1
  - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
  - Thermal scattering information in MF7 MT451
  - Background R-matrix elements for resonance parameters in MF2 MT151

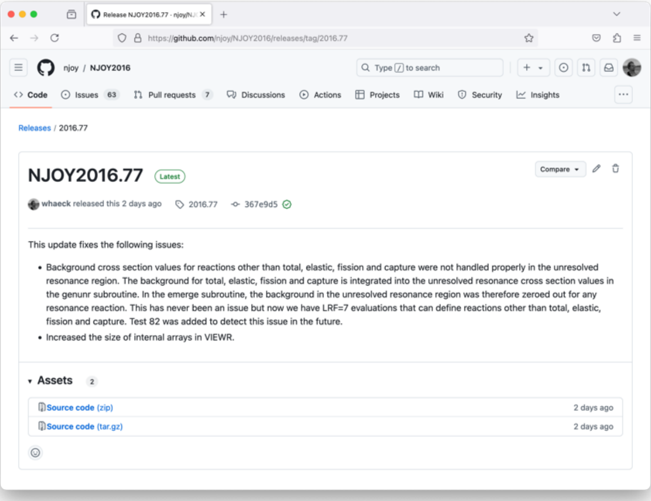
- New features that require changes in MCNP have been prioritized
  - We can say that MCNP6.3 is now ENDF/B-VIII.1 ready

Our new objective: smooth processing of ENDF/B-IX.0

Maintaining our production version

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





- Latest version is NJOY2016.77 (October 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

Noteworthy updates to NJOY2016

- NJOY2016.77:
  - Fixed an issue where cross sections for some reactions in the URR where zero for evaluations with both a RRR using LRF=7 and URR
    - Only when the RRR has resonances for a reaction other than elastic, capture and fission
    - This does NOT occur in ENDF/B-VIII.1

- NJOY2016.75:
  - ACE file updates:
    - Adding isomeric state S, atom number Z and mass number A to the NXS array
    - MCNP ZA naming conventions for metastable states (e.g. 95642 for Am242g)

- NJOY2016.74
  - Corrected value for the Euler-Mascheroni constant (impacts Coulomb wave functions)

MCNP libraries for ENDF/B-VIII.1

- Lib81 : incident neutron files
  - 557 targets
  - 8 temperatures : 293.6 K, 600 K, 900 K, 1200 K, 2500 K, 0.1 K, 233.15 K, 273.15 K
  - Extensions : 10c to 17c

- ENDF81SaB : thermal scattering files
  - 103 materials
  - Extensions : 70t to 89t depending on the material
  - 70t will either be room temperature or the lowest available temperature
  - This is a big library at over 40 GB

- We foresee a release of these files before the end of the year

MCNP libraries for ENDF/B-VIII.1

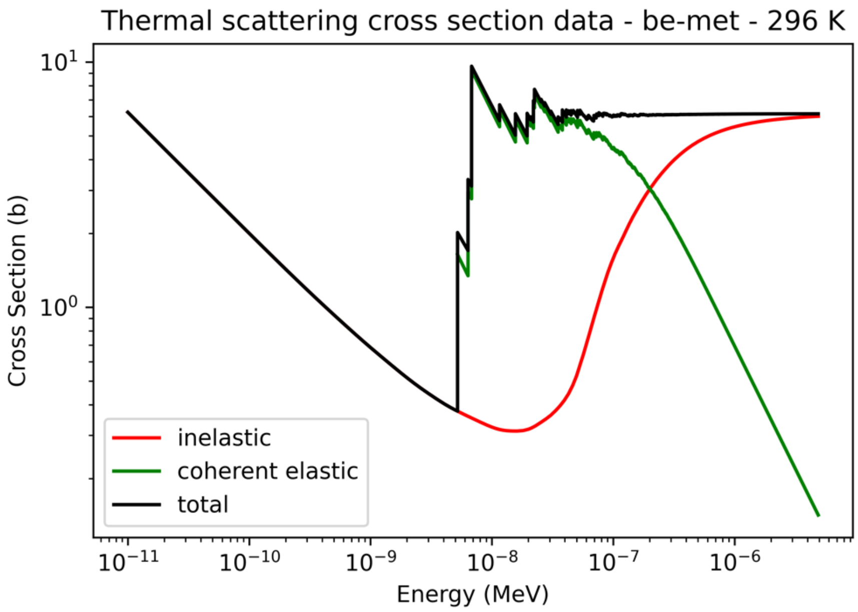
- Important notes concerning the content of Lib81
  - Neutron on neutron is not included
  - We may add Am239 as an extension to Lib81

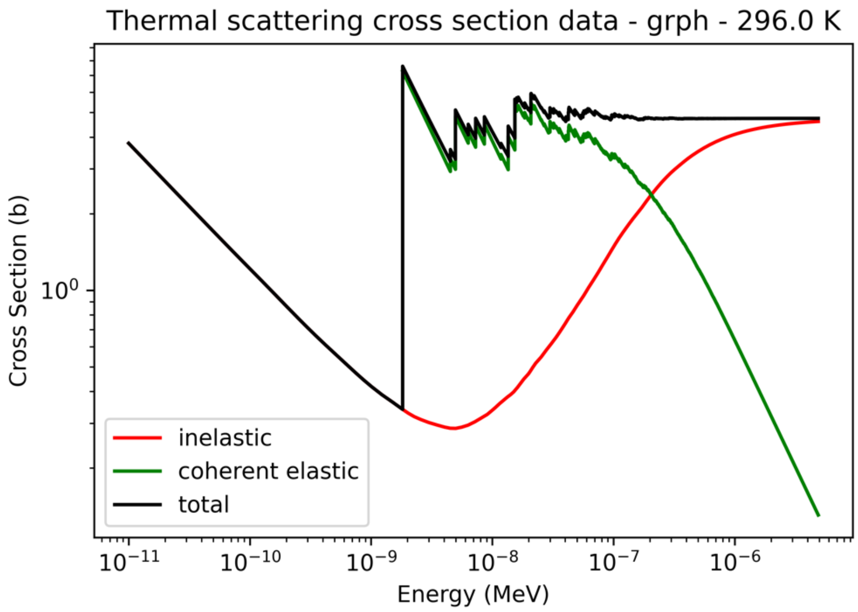
- Important notes concerning the content of ENDF81SaB
  - H in H2O : only 19 out of 94 temperatures (ENDF/B-VIII.0 temperatures + 273.15 K)
  - Only the graphite and Be with Sd effects are included (consultation with ORNL)
  - H and Zr in ZrH : only the epsilon and delta phase ZrH materials are included
  - SiO2 is replaced with O and Si in SiO2 (alpha quartz)
  - No CaH2 materials are included
  - Older mixed moderators like benzene, liquid and solid methane are not included

MCNP libraries for ENDF/B-VIII.1

Name	Description	Name	Description	Name	Description	Name	Description
al-27	Aluminium	orthod	Ortho-D	c-zrc	C in ZrC	n-un1 – n-un6	N in UN
fe-56	Iron	orthoh	Ortho-H	d-7ld	D in 7LiD	o-sap	O in sapphire (Al2O3)
be-met	Be metal	parad	Para-D	f-bef	F in BeF2	o-mgo	O in MgO
be-beo	Be in BeO	parah	Para-H	f-ptfe	F in teflon (CF2)	o-puo	O in PuO2
c-sic	C in SiC	grph10	10% porous graphite	f-flb	F in FLiBe	o-aqu	O in alpha quartz (SiO2)
d-d2o	D in heavy water	grph30	30% porous graphite	f-hf	F in HF	o-uo1 – o-uo6	O in UO2
h-luci	H in lucite	7l-7ld	7Li in 7LiD	f-mgf	F in MgF2	pu-puo	Pu in PuO2
h-poly	H in polyethylene	7l-7lh	7Li in 7LiH	h-7lh	H in 7LiH	si-aqu	Si in alpha quartz (SiO2)
h-h2o	H in light water	al-sap	Al in sapphire (Al2O3)	h-styr	H in styrene (C8H8)	u-met1 – u-met6	U in U metal
h-ice	H in ice	be-bec	Be in Be2C	h-hf	H in HF	u-uc1 – u-uc6	U in UC
h-yh2	H in YH2	be-bef	Be in BeF2	h-poil	H in paraffinic oil	u-un1 – u-un6	U in UN
o-beo	O in BeO	be-flb	Be in FLiBe	h-uh3	H in UH3	u-uo1 – u-uo6	U in UO2
o-d2o	O in heavy water	c-bec	C in Be2C	h-ezh	H in epsilon ZrH2	zr-zrc	Zr in ZrC
o-ice	O in ice	c-luci	C in lucite (C5O2H8)	h-dzh	H in delta ZrHx	zr-ezh	Zr in epsilon ZrH2
si-sic	Si in SiC	c-styr	C in styrene (C8H8)	li-flb	Li in FLiBe	zr-dzh	Zr in delta ZrHx
y-yh2	Y in YH2	c-ptfe	C in teflon (CF2)	mg-mgf	Mg in MgF2	grph20	20% porous graphite
grph	Graphite	c-uc1 – c-uc6	C in UC	mg-mgo	Mg in MgO		

MCNP libraries for ENDF/B-VIII.1





Future MCNP libraries for ENDF/B-VIII.1

- eprdata24 : photoatomic and electroatomic files
  - NJOY2016 does not process this type of ACE library
  - We are using this as a first application for a modern NJOY

- Incident charged particle and photonuclear files
  - We processed these for beta4 but may release these as a regular MCNP library
  - Photonuclear files will need work in NJOY2016
    - Y89, Rh103, Tb159, Ho165, Tm169, Ta181 fail with inconsistent XSS locators

- We foresee a release of the eprdata24 library next year

Why do we need to modernize our processing code?

- New nuclear data features are hard to introduce in NJOY2016
  - Energy dependent fission yield data
  - Incident charged particle resonance parameters
  - Thermal scattering covariance data

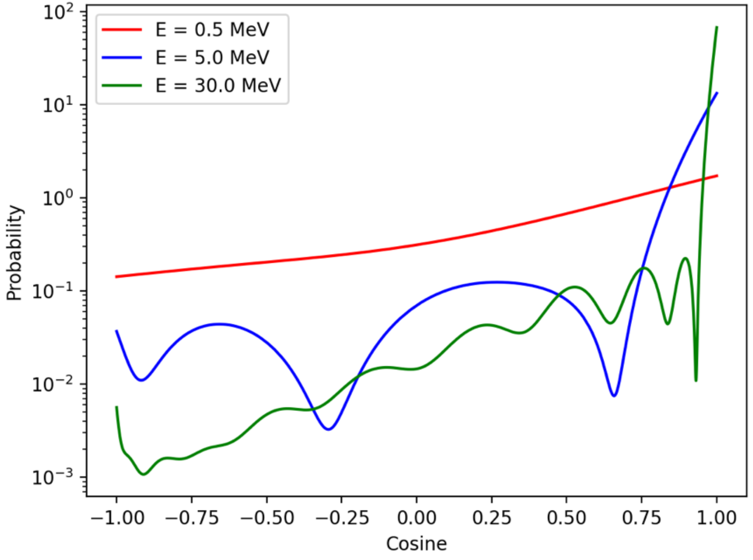
- Better knowledge of implemented methods
  - Modernization allows us to explore different methods and identify shortcomings

- NJOY 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

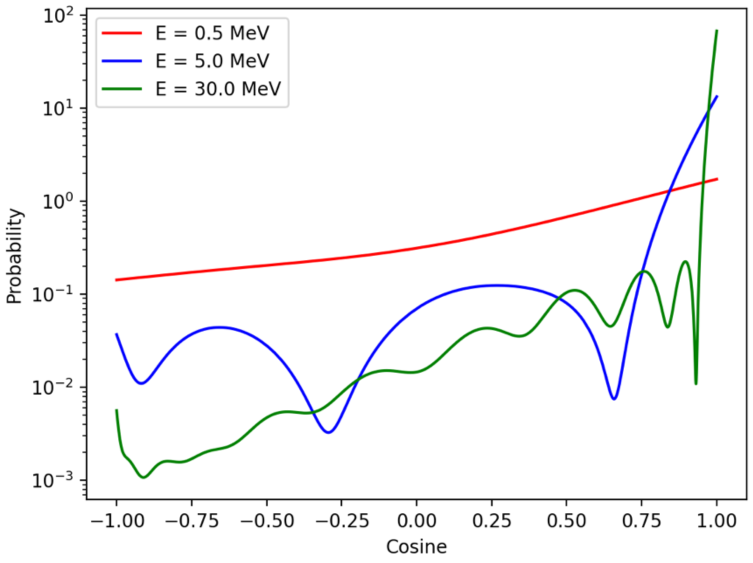
Example: linearize a Legendre angular distribution

- The general process of linearization:
  - Generate the initial grid
    - Ideally the minima, maxima and inflection points
    - Any points to ensure the interpolation does not intersect with the function
  - For each interval in the grid:
    - Evaluate the function at a point in the interval
      - This is generally the midpoint of the interval
    - Verify convergence:
      - If converged: move to the next interval
      - Else: add the point to the grid and move to the previous interval
    - Repeat until there are no intervals left



Example: linearize a Legendre angular distribution

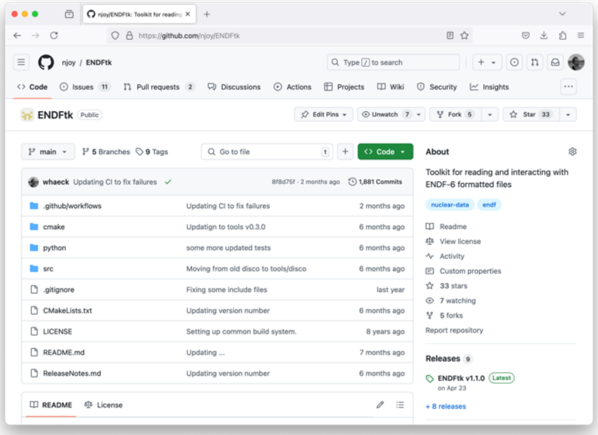
- Potential shortcomings in NJOY2016:
  - Only -1 and 1 are chosen for the initial grid
    - This can cause potential false convergence
    - Alleviated by using a smaller tolerance (0.02%) and thinning the final grid using a 0.2 % tolerance
  - Tolerances cannot be changed by the user
  - Legendre series evaluation is not as efficient as it could be

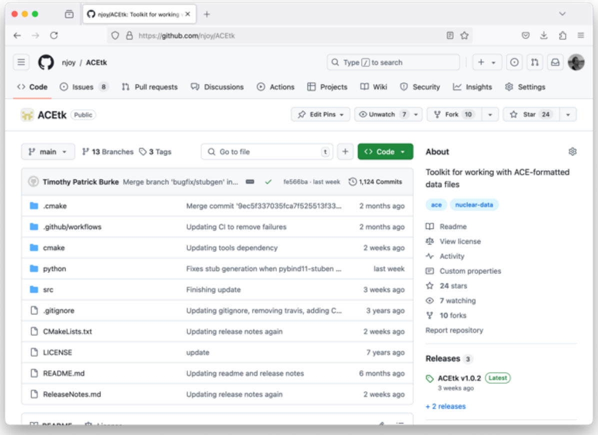


- Improvements in a modern NJOY:
  - Use minima, maxima and inflection points
  - Use Clenshaw recursion for series evaluation
  - Minimize grid size by optimizing panel splitting

A component based modernization strategy

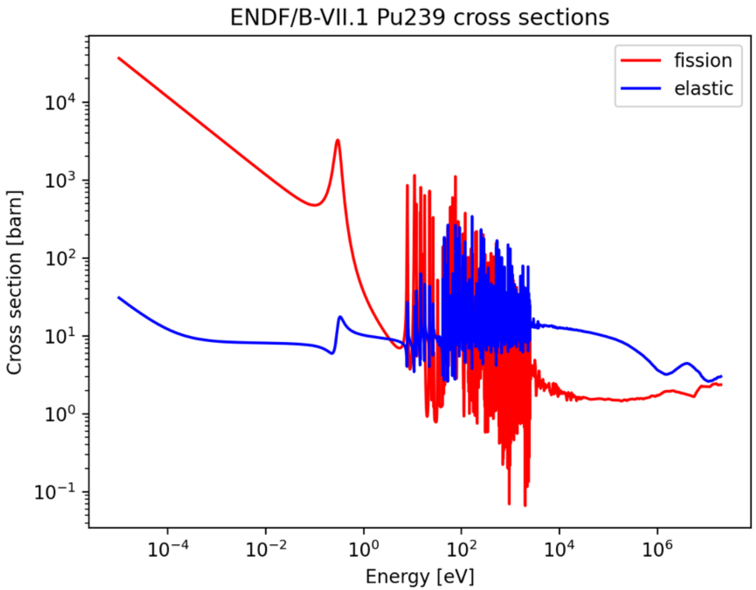
- Modernized modules are built from components
  - Format components: ENDF, ACE, GNDS, NDI, etc.
  - Processing components: resonance reconstruction, linearization, etc.
- Components can be developed and deployed faster than modules
  - Using a C++ and Python API at the same time





`ENDFtk` : an ENDF format component

- Latest release is `ENDFtk` v1.1.0
  - Fixing a parser issue where numbers are sometimes off by a very small value
  - Parsing ENDF files is now 10-20% faster
  - https://github.com/njoy/ENDFtk
- `ENDFtk` v1.2.0 will be released soon
  - Significantly faster compilation
  - Reduced memory usage during compilation
  - Several bug fixes and interface extensions



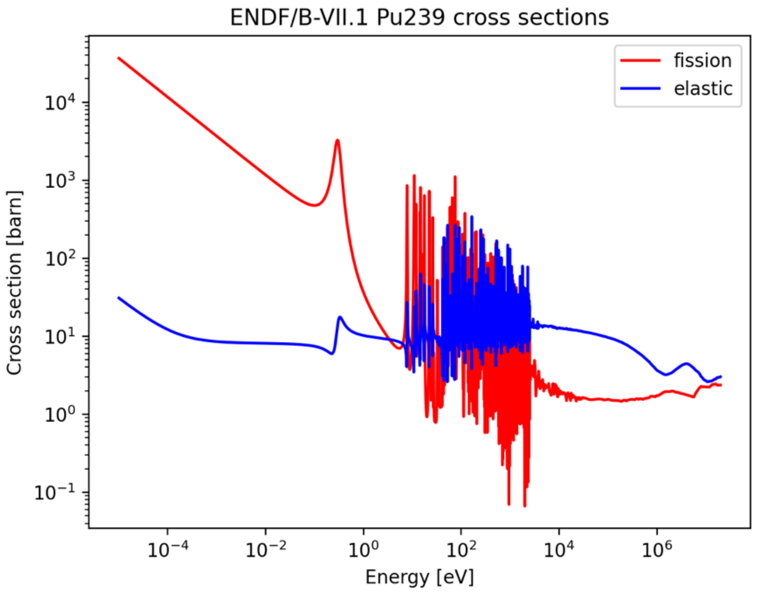

```
import ENDFtk

# open an endf file and extract elastic and fission
tape = ENDFtk.tree.Tape.from_file( '94239.pendf' )

elastic = tape.materials.front().section( 3, 2 ).parse()
fission = tape.materials.front().section( 3, 18 ).parse()
```

W. Haeck, N. Gibson, P. Talou, “ENDFtk: A robust tool for reading and writing ENDF-formatted nuclear data,” Comp. Phys. Comm., 303 (2024), DOI: 10.1016/j.cpc.2024.109245

ACEtk : an ACE format component

- Latest release is ACEtk v1.0.2
  - Several bug fixes and interface extensions
  - https://github.com/njoy/ACEtk

- Supported ACE format types:
  - neutron and charged particles files
  - photonuclear files
  - thermal scattering files
  - photoatomic and electroatomic files (eprdata)
  - dosimetry files



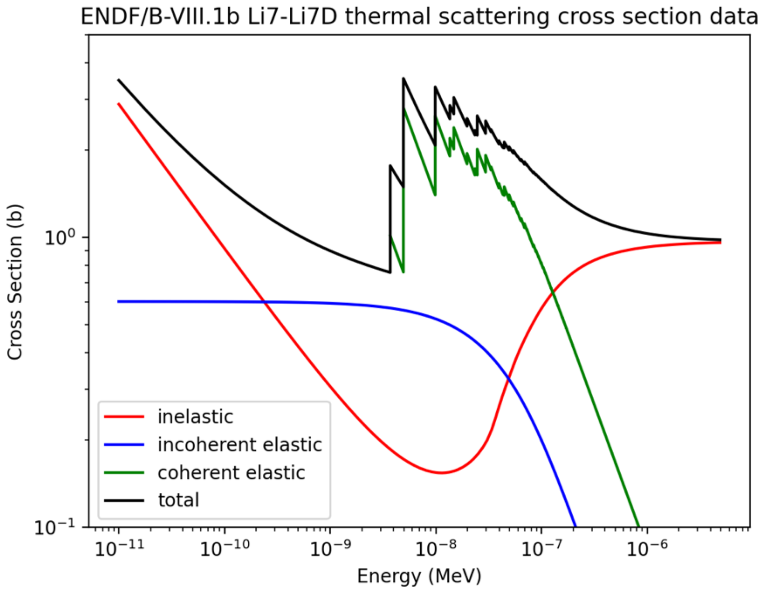

```
import ACEtk

# open an ace file and extract elastic and fission
table = ACEtk.ContinuousEnergyTable.from_file( '94239.710nc' )

index = table.reaction_number_block.index(18)
energies = table.principal_cross_section_block.energies
elastic = table.principal_cross_section_block.elastic
fission = table.cross_section_block.cross_sections(index)
```

`scion` : the mathematical core of a modern NJOY

- 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
  - Differentiation and integration of the data

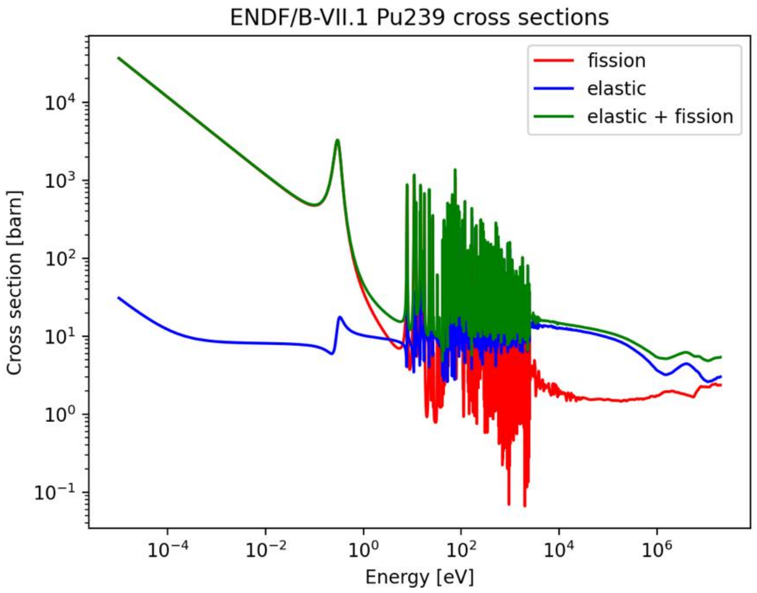
- New capabilities since last year:
  - Analytical integration of $f(x)$ and $xf(x)$ (mean or first raw moment) for tabulated data
  - Tabulated two-dimensional data $z = f(x, y)$

- The basis for our format agnostic interface



`dryad` : a format agnostic data interface

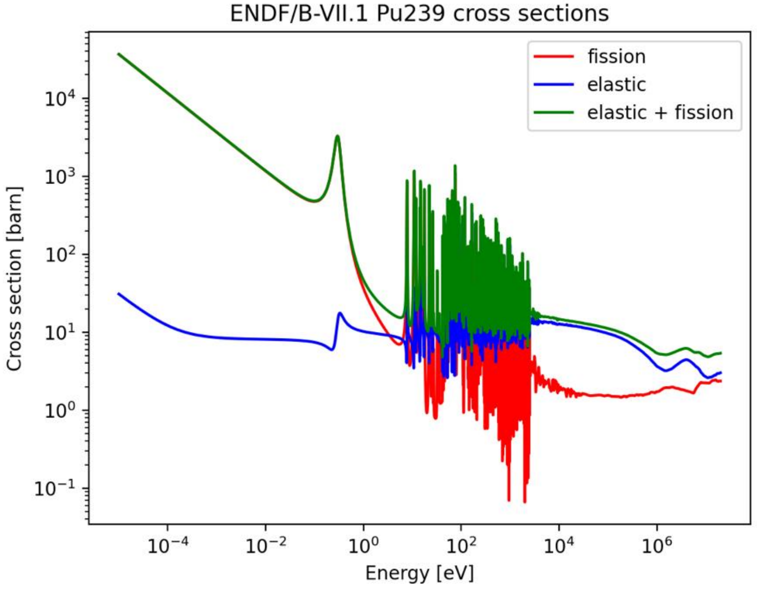
- As a nuclear data user, you should not have to worry about format details
- Nuclear data is represented in its most generic form using consistent units
  - Conversion at read time to the base units
  - ACE files in MeV and ENDF in eV
- `dryad` classes built upon `scion` classes
  - Makes basic operations available
  - Linearization of Legendre distributions
  - Operations on tabulated data




```
import dryad

# open an endf file and extract elastic and fission
pt = dryad.ProjectileTarget.from_endf_file( '94239.pendf' )

elastic = pt.reaction('2').cross_section
fission = pt.reaction('18').cross_section

sum = elastic + fission
```

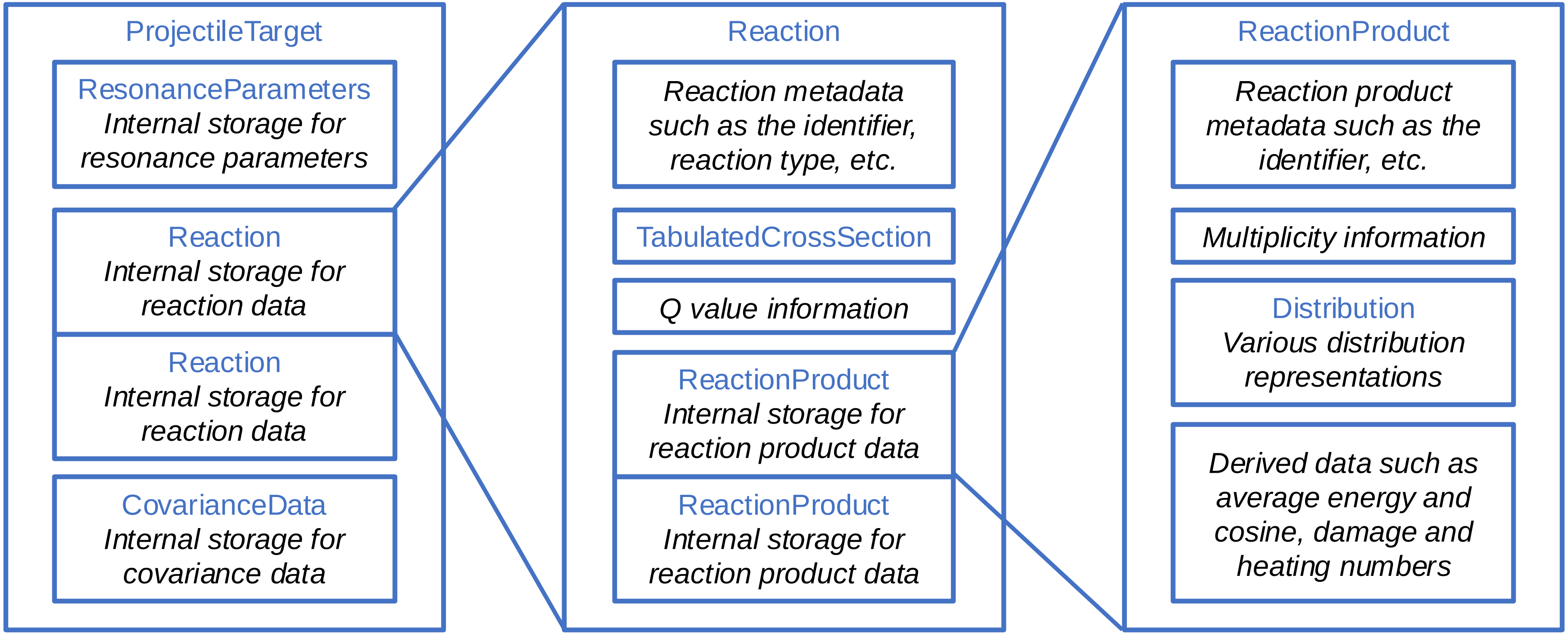
`dryad` : a format agnostic data interface

- Neutron, charged particles and photonuclear data
  - Reading from ENDF only
  - Cross section data
  - Limited outgoing particle distribution support
- Atomic relaxation data
  - Reading from ENDF only
  - Full capability
- Photoatomic and electroatomic data
  - Reading from both ENDF and ACE
  - Cross section data
  - Full distribution data



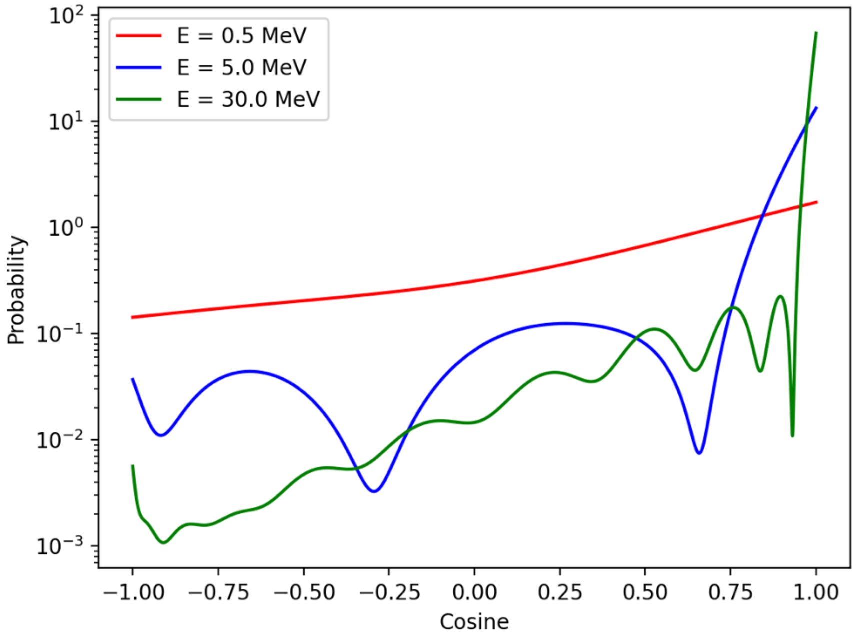

```
import dryad

# open an endf file and extract elastic and fission
pt = dryad.ProjectileTarget.from_endf_file( '94239.pendf' )

elastic = pt.reaction('2').cross_section
fission = pt.reaction('18').cross_section

sum = elastic + fission
```

`dryad` : a format agnostic data interface

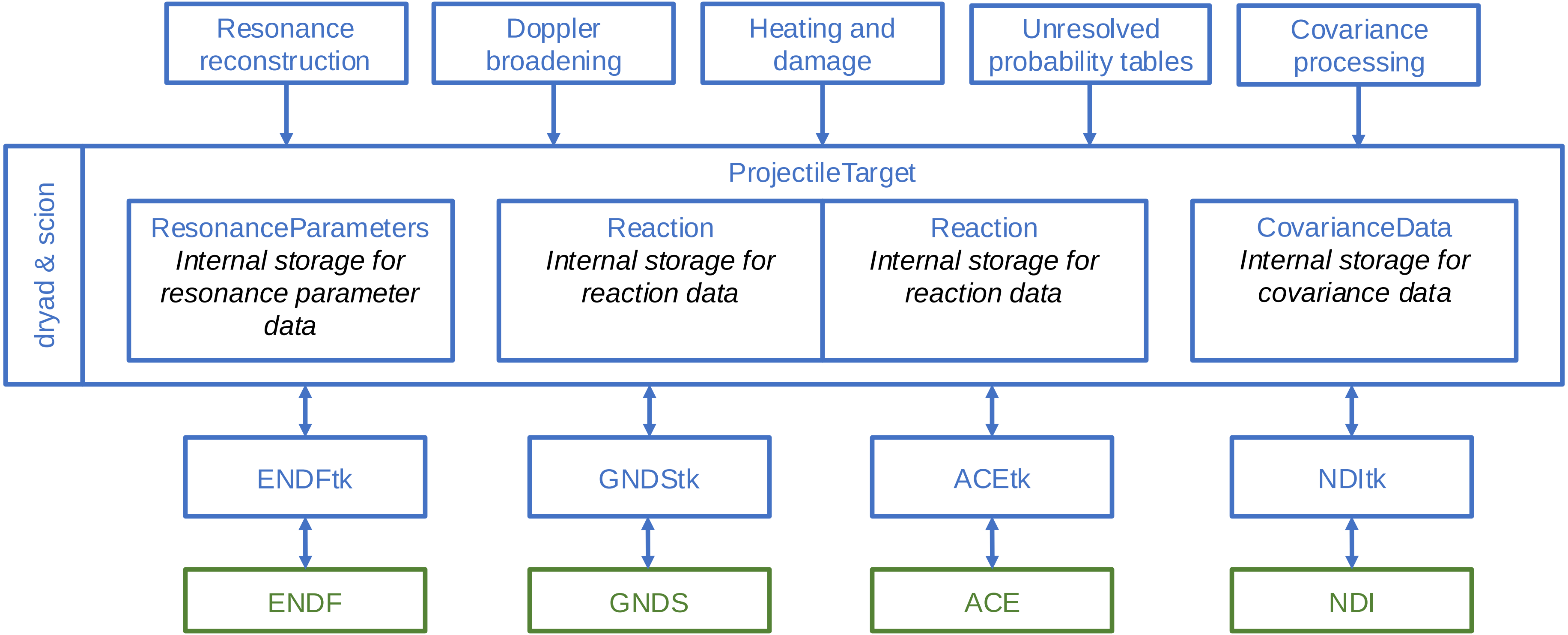


dryad : a format agnostic data interface

```
import dryad

# ENDF/B-VIII.1 Pu239 data
pt = dryad.ProjectileTarget.from_endf_file( 'n-094_Pu_239.endf' )

# get elastic angular distribution data
elastic = pt.reaction('2')
angular = elastic.products[0].distribution_data.angle

# linearise the distribution pdf at 0.5, 5 and 30 MeV
linearised1 = angular.distributions[8].pdf.linearise()
linearised2 = angular.distributions[22].pdf.linearise()
linearised3 = angular.distributions[-1].pdf.linearise()

# plot the distributions
plot.figure()
plot.plot( linearised1.cosines, linearised1.values )
plot.plot( linearised2.cosines, linearised2.values )
plot.plot( linearised3.cosines, linearised3.values )
plot.xlabel( 'Cosine' )
plot.ylabel( 'Probability' )
plot.show()
```



Putting it all together



Conclusions and future work

- NJOY2016 can process ENDF/B-VIII.1
  - Fix issues in NJOY2016 as soon as they become apparent
  - Known issues: some photonuclear data processing

- We continue our work on NJOY modernisation
  - A format agnostic data interface developed for photoatomic and electroatomic data
  - Identified potential improvements in photoatomic physics in MCNP

- Future work
  - A first modern NJOY version to process eprdata ACE files
  - Further development of the `dryad` interface (secondary distribution types)
  - A new physics testing module for a modern NJOY