

#### NJOY's road toward GNDS

W. Haeck, N. Gibson, M. Staley

May 16, 2023



## Agenda

A quick NJOY2016 update
 The NJOY modernisation progress
 GNDStk update



# Maintaining our production version

Get it at <a href="https://github.com/njoy/NJOY2016">https://github.com/njoy/NJOY2016</a>



- Latest version is NJOY2016.70 (April 2023)
  - 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



## **Overview of some of the latest NJOY2016 changes**

- ACER processing using multi-temperature PENDF files (NJOY2016.68)
  - PENDF files could contain multiple FEND records due to incorrect logic in RECONR
  - ACER sometimes picked the wrong temperature from a multi-temperature PENDF file
    - Only happens when the materials in the PENDF contained only linearised MF3 data (no MF10, MF12 or MF23 data was added by RECONR).
- Bondarenko cross sections from probability tables (NJOY2016.69)
  - The NJOY output file provides Bondarenko data calculated during the sampling process and calculated from the final probability tables
  - For low dilution values, the Bondarenko data calculated from the final probability tables are closer to the results from UNRESR so those are now written to MF2 MT152
  - Note: deterministic data processing should use UNRESR



# **Overview of some of the latest NJOY2016 changes**

- Heating values using MF6 LAW2 in MT5 (NJOY2016.69)
  - ACER assumed that the yield of the secondary particle is 1, which is correct in all cases except when MT5 is used as a lumped reaction
- Segmentation fault in ERRORR (NJOY2016.69)
  - Some ENDF/B-VIII.0 and ENDF/B-VIII.1 evaluations failed in ERRORR
  - ERRORR would segfault for LRF=7 resonance evaluations when MF33 was present without MF32
- Multiple calls to ERRORR for MF34 and MF35 data now work (NJOY2016.70)
  - ERRORR needs to be called for each sub-subsection and incident energy group
  - The issue was related to arrays being allocated but not deallocated in the previous ERRORR run in NJOY's Sammy routines for evaluations using MF2 LRF=7.



#### **NJOY modernisation strategy**

- NJOY21: shift 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 (e.g. scion)
    - 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

rjøy/ENDFtk: Tool	this for reading $\times$ +			o      o      rjoy/ACIItk at feature/table-ctor × +		
→ C @ 1	C A https://github.com/njoy/ENDFtk		E 🕁 🗢 🖉 =	← → C @ ○ A https://github.com/	njoy/ACEtk/tree/feature/table-ctor	E 🕁 🗢 🎱
Search or jump to	7 Pull requests Issues Mark	etplace Explore	₽ +• ∰•	Search or jump to / Pull r	equests Issues Marketplace Explore	₽ +• Ø•
njoy/ENDFtk Public	c 🛇 Edit Pins 👻	⊙ Unwatch 6	• ♀ Fork 2 • ☆ Star 16 •	Injoy/ACEtk Public	🛇 Edit Pins + 💿 Unwatch 7	▼ ♥ Fork 5 ▼ ☆ Star 9 ▼
Code 📀 Issues 14	11 Pull requests 8 🖓 Discussions 💿	Actions 🗄 Proje	ncts 🖽 Wiki 🛈 Security \cdots	↔ Code ⊙ Issues 5 11 Pull requests 28	🖓 Discussions 🕞 Actions 🖽 Proj	jects 🖽 Wiki 🛈 Security \cdots
² master 🗸 🗜 17 bra	anches 🛇 4 tags Go to file Add f	ile * Code -	About ®	\$7 feature/table →     \$7 42     branches     tags	Go to file Add file * Code -	About ®
whack Merge pull request #135 f 🦂 🗸 c3cb844 on Jul 26, 2021 🗿 1,360 commits			Toolkit for reading and interacting with ENDF-6 formatted files This branch is 357 commits ahead of develop.		11 #73	Toolkit for working with ACE-formatted data files
.github/workflows	Update to latest develop	17 months ago	endf			ace nuclear-data
cmake	Updated build system files	2 years ago	Readme	whack Fixed a few typos 🗸 f111985 21 days ago 🕚 718 commits		Readme
python	Merge pull request #129 from njoy/update/nlsc	16 months ago	4₫8 View license	.github/workflows Updating OS to remove	deprecation warnings/ 2 months ago	s ago 🚯 View license
src	Updating ENDFtk.hpp	15 months ago	☆ 16 stars	cmake Adding the 2.0.1 heade	r 2 months ago	☆ 9 stars
.gitignore	Added x(), y() and regions() functions to MF3,	2 years ago	¥ 2 forks	python Fixed a few typos	21 days ago	¥ 5 forks
CMakeLists.txt	Updated build system files	2 years ago		src Fixing pybind11 issue	2 months ago	
LICENSE	Setting up common build system.	6 years ago	Releases 4	_gitignore Updating gitignore, rem	noving travis, adding CI 15 months ago	Releases
README.md	ADME.md Added comment on using -DPYTHON_EXECU 2 years ago		© ENDFtk v0.3.0 (Latest) on Jul 26, 2021	CMakeLists.txt Updating python bindin	igs 2 months ago	No releases published
				LICENSE update	5 years ago	Create a new release
README.md		0	+ 3 releases	Cleaning up a bit	15 months ago	Dackages
Continuous Integration passing			Daakagaa			No packages published

5/14/23



# **ENDFtk and ACEtk development is almost completed**

- ENDFtk: <u>https://github.com/njoy/ENDFtk</u>
  - We now have full support for all data, including covariance data
  - We have added functionality for manipulating ENDF files
    - Inserting, replacing and removing materials, files and sections
    - Updating the directory of the ENDF file
- ACEtk: <a href="https://github.com/njoy/ACEtk">https://github.com/njoy/ACEtk</a>
  - 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
    - Dosimetry ACE files
- Look out for v1.0 releases of both toolkits soon!



#### So we can read and write data, now what?

- 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.
  - Differentiation and integration of the data
- This will be the job of SCION
  - SCientific interpretatION, linearisatION, differentiatION, integratION and more IONs
  - It will provide a format agnostic data interface

This one's important, more on this later





# **Current capabilities in SCION**

- Functional interpretation of tabulated data using various interpolation schemes
- Functional interpretation of polynomial based expansions
  - Normal power series, Legendre series and Chebyshev series
  - Root finding for the general case f(x) = a using the companion matrix
  - Integration and differentiation can be performed using a functional interface
- Generic linearisation of functions
  - Extensible interface for convergence and panel splitting
- Common mathematical capabilities
  - Horner and Clenshaw recursion for polynomial evaluation
  - Newton-Raphson for root finding
  - Special mathematical functions



### **Current capabilities in SCION**

import scion import ENDFtk import matplotlib.pyplot as plot

```
# convert to the proper Legendre coefficients
def convert( data, index ) :
    coefficients = data.angular distributions[index].coefficients
    converted = [0.5]
    for i in range( 1, len( coefficients ) + 1 ) :
        converted.append( ( 2 * i + 1 ) / 2 * coefficients[i - 1] )
    return converted
```

# open the H1 data and extract the elastic angular distribution data u235 = ENDFtk.tree.Tape.from file( 'h1.endf' ) elastic = u235.materials.front().file( 4 ).section( 2 ).parse()

# retrieve the angular distributions at different energies d1 = scion.math.LegendreSeries( convert( elastic, 0 ) ).linearise() d2 = scion.math.LegendreSeries( convert( elastic, -11 ) ).linearise() d3 = scion.math.LegendreSeries( convert( elastic, -1 ) ).linearise()

```
# plot the data
plot.figure()
plot.plot( d1.x, d1.y, label = 'E \{in\} = 1e-5 eV', color = 'red' )
plot.plot(d3.x, d2.y, label = '\{in\} = 20 MeV', color = 'blue')
plot.xlabel( 'Cosine' )
plot.ylabel( 'Angular distribution' )
plot.show()
```

#### ENDF/B-VIII.0 H1 elastic angular distribution data 0.55 $E_{in} = 1e-5 eV$ $E_{in} = 15 \text{ MeV}$ 0.54 $E_{in} = 20 \text{ MeV}$ 0.53 Angular distribution 0.52





# A format agnostic nuclear data interface in SCION

- 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
- How to achieve format abstraction?
  - Solution 1: there can be only ONE!

This is a really short-sighted solution

- Translate every format to the one you use
- Solution 2: an interface capable of using any format
  - Data is represented in its native format but extracted using a common interface
- Solution 3: format agnostic data structures
  - Data is represented in its most generic form and can be translated to/from different formats

This is the one we should use



#### **Example in resonance reconstruction**





# A format agnostic nuclear data interface in SCION





# **Current status of GNDStk**

- GNDStk core interface
  - A standard independent generic tree and node based interface
  - Using the core interface requires an almost perfect knowledge of the GNDS structure
  - Queries can be verbose due to GNDS complexity
- GNDStk standard interface
  - A simpler high-level interface linked to GNDS standards
  - It provides a simpler and less verbose interface (both C++ and python)
  - It can be generated automatically and can be customised later
  - Non-standard GNDS hierarchies still require the core interface



### **Current status of GNDStk**

- Autogenerating the standard interface has proven to be quite difficult
  - The GNDS specifications were not written for this type of use
  - Circular dependencies in the original GNDS specifications
- We now have a GNDS 2.0 "compliant" interface in C++ and Python
  - The original GNDS 2.0 specifications had to be rewritten
  - It should be able to read all existing GNDS 2.0 files
- · There are outstanding issues that we need to solve
  - Compilation time is currently prohibitive
  - Documentation is missing because of the autogeneration



## Conclusions

- NJOY2016 will be maintained for the foreseeable future
  - ENDF/B-VIII.1 processing is our current goal
  - More changes on photonuclear data processing are coming
- NJOY modernisation is on track
  - ENDFtk and ACEtk v1.0 releases are "imminent"
  - Development of SCION has started and a format agnostic interface is in the works
- GNDStk development continues but it's ... complicated
  - We now have a GNDS 2.0 "compliant" interface in C++ and Python
  - Outstanding issues need to be solved before we can formally release it

