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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 = OX + 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.





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Maintaining our production version

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

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whaeck Merge pull request #3	40 from njoy/develop 🚥 🗸 cd1cd21 - last mont	h 🕚 1,120 Commits	Nuclear data processing with legacy NJOY		
.github/workflows	Update ContinuousIntegration.yml	last month	∂ ² www.njoy21.io/NJOY2016		
docs	Updating test descriptions	6 months ago	cross-sections nuclear-data		
metaconfigure	Appveyor testing.	7 years ago	endf-format resonance		
src src	Update vers.f90	last month			
tests	Updating ce zaid values with zaoption	6 months ago	-∿ Activity		
.gitignore	Updated comparison function (see comments)	4 years ago	Custom properties		
CMakeLists.txt	setting cmake minimum version to 3.15	2 years ago	 21 watching 		
LICENSE	prep	8 years ago	V 84 forks Report repository		
README.md	Another small correction	2 years ago			
ReleaseNotes.md	Update ReleaseNotes.md	last month	Releases 41		
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README Hucense		0 =	on Jul 3		



- 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
- An ORNL Sr88 evaluation now uses the SAMMY parametrisation option
- NJOY2016.73 (November 2023) is required for background R-matrix elements

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ight| \delta_{JJ'}.$



(D.76)

Background R-matrix elements in MF2 MT151





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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

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P main → P 9 Branches ⊘9 Ta	gs Q. Go to file It	+ Code -	About (8) Toolkit for reading and interacting with	P main ▼ P 13 Branches ⊘2 Tags	Q. Go to file	↔ Code •	About
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.github/workflows	Updating CI	last month	nuclear-data endf	.github/workflows	Update ContinuousIntegration.yml	last month	ace nuclear-data
cmake	Updatign to tools v0.3.0	4 months ago	Readme	Cmake	Updating release deps	last month	D Readme
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ignore	Fixing some include files	last year	☆ 31 stars		Updating gitignore, removing travis, adding Cl	3 years ago	☆ 22 stars
takeLists.txt	Updating version number	4 months ago	¥ 5 forks	CMakeLists.txt	Update ACEtk version number in cmake	last month	 7 watching 10 forks
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README.md	Updating	5 months ago	Releases 9	README.md	Updating readme and release notes	4 months ago	Releases 2
ReleaseNotes.md	Updating version number	4 months ago	S ENDFtk v1.1.0 Latest	ReleaseNotes.md	Update ReleaseNotes.md	last month	C ACEtk v1.0.1 (Latest)
README DE License		1 =	+ 8 releases	🖾 README 🛛 🙅 License		1 =	+ 1 release



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: <u>https://github.com/njoy/ENDFtk</u>
- 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: <u>https://github.com/njoy/ACEtk</u>
- 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

	Projecti	leTarget	
ResonanceParameters Internal storage for resonance parameter data	Reaction Internal storage for reaction data	Reaction Internal storage for reaction data	CovarianceData Internal storage for covariance data



Putting it all together



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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

