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What's up with NJOY?

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Outline

Introduction: what is NJOY and how does it relate to MCNP?
 NJOY modernisation

3. NJOY related topics MCNP users should be aware of



Introduction

- What is NJOY and how does it relate to MCNP?
- How is an MCNP ACE library file created?
- What verification and validation is performed on the ACE libraries?

What is NJOY and how does it relate to MCNP?

- 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
- NJOY is the nuclear data processing software develop 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

$$M + 1 = N$$

 $I + 1 = J$
 $N + 1 = O$
 $X + 1 = Y$



How is an MCNP ACE library file created?

- NJOY provides a set of data processing modules that are called sequentially
 - Different processing paths for different library types
 - Incident neutron, incident charged particles, thermal scattering, photonuclear, etc.





What verification and validation is performed?

- Once processing is completed, library files should be verified
 - ACE checking codes test cross sections, probability tables, pdf and cdf values, etc.
 - Comparison to experiments: criticality benchmarks (ICSBEP), pulsed spheres, etc.



Which version should you use?

- NJOY has come been around for over 40 years now
 - Major versions: NJOY99, NJOY2012, NJOY2016, NJOY21
- NJOY2016 is the production code at LANL
 - The MCNP ENDF/B-VIII.0 library was produced using NJOY2016
 - Latest version is NJOY2016.64 (June 2021)
 - Get it at https://github.com/njoy/NJOY2016
- NJOY21 is currently a NJOY2016 wrapper with additional input verification
 - Latest version is NJOY21 v1.2.2 (January 2021)
 - Get it at https://github.com/njoy/NJOY21



What does the future bring?

- NJOY2016 will be maintained for the foreseeable future
 - NJOY2016 is essentially the production code at LANL
 - New formats for ENDF/B-VIII.1 will be supported:
 - Thermal scattering: mixed coherent and incoherent elastic scattering
 - External R-matrix elements used in some new resonance evaluations
- NJOY21: shift from a module based to a component based modernisation
 - Modernised modules are built from components
 - Components provide formats (ENDF, ACE) or processing operations (resonance reconstruction)
 - 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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NJOY modernisation

- NJOY21 components versus modules
- C++ and Python interfaces
- Processing components are format agnostic

NJOY21 components

	NJOY21 format components	
ENDFtk	Evaluated nuclear data format (the legacy one)	See N. Gibson's presentation
GNDStk	Evaluated nuclear data format (the new one)	
ACEtk	Application library format for MCNP	

NJOY21 processing components			
SCION	Functional interpretation, linearization, differentiation and integration		
R2	Resolved and unresolved resonance reconstruction		
No name yet	Doppler broadening of cross section data		
No name yet	Thermal scattering		
No name yet	Damage and heating		
No name yet	Unresolved resonance treatment and probability tables		
No name yet	Group collapsing and transfer matrices		
No name yet	Covariance data processing		



NJOY21 components versus modules

ENDFtk		RECONR	GROUPR	ACER	ERRORR
Neutron & CP data	\checkmark	×	×	×	×
Photons	\checkmark	×	×	×	
Resonances	\checkmark	×			×
Photonuclear data	×	×		×	
Covariance data	×				×

SCION		RECONR	GROUPR	ACER	ERRORR
Interpretation	×	×	×	×	×
Linearisation	×	×	×	×	
Unionisation	×	×			
Integration	×		×	×	
Differentiation	×				×



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Processing components are format agnostic

- In the beginning there was only ENDF ...
 - As a result, NJOY2016 is very closely linked to ENDF
 - Introducing the new GNDS format in NJOY2016 is practically impossible
- NJOY21 processing components MUST be format agnostic
 - Internal data structures that reflect generic data can be built from scratch
 - Build these data structures using ENDF or GNDS evaluated data, or other user data





C++ and **Python** interfaces for components

- Components are developed in C++ with Python bindings
 - C++ is great for performance

xs = reconstruct(1e-5)

- Python is great for deploying our components more quickly
- ENDFtk is the first component with a full Python interface
 - The R2 resonance reconstruction component is next

```
import ENDFtk, r2
# open the Pu239 ENDF file and extract the resonance parameters
tape = ENDFtk.tree.Tape.from_file( 'Pu239.endf' )
resonances = tape.materials.front().file( 2 ).section( 151 ).parse()
parameters = resonances.isotopes[0].resonance_ranges[0].parameters
# create a reconstructor from the resonance parameters
reconstruct = r2.fromENDF( parameters )
# reconstruct the cross sections at 1e-5 eV
```



Things MCNP users should be aware of



We need your help to make NJOY better

- When you see something, say something
- By posting on the MCNP forum
- By posting an issue on GitHub
 - https://github.com/njoy/NJOY2016/issues
- By sending us an email
 - njoy@lanl.gov

Sea	rch or jump to VIII requests Issues Marketplace Explore		<u></u> ф+•
oy / N	JOY2016	watch 👻 21 🖄 Star 🛛	80 V Fork
Code	🖸 Issues 58 🕮 Pull requests 4 💿 Actions 🔟 Projects 🖽 Wiki 🕕 Security 🗠 Insights 🛞	Settings	
TEN ⊙ci	IDL photonuclear processing issue for Ra226 #201 whatek opened this issue on May 24 - 3 comments	Edi	it New issue
8	whack commented on May 24 - edited + Member) 💿 …	Assignees	×
	An email was posted to the MCNP user forum concerning an issue with a photonuclear ACE file for Ra226 from TENDL 2019.	n whaeck	
	The length of the ACE file did not correspond to the length written to the xsdir entry, indicating an issue while printing the ACE file. When performing an ACER run for testing an existing ACE file, ACER crashes due to an expected end of file (again due to the ACE file being incomplete).	Labels None yet	Ŕ
	The following input and ENDF file illustrate the issue: input.txt g=fa226.tendl.txt	Projects None yet	Ŕ
	R what k self-assigned this on May 24	Milestone No milestone	ŧ
		Linked pull requests	Ę
8	whatek commented on May 24 (Member) (Author) ③ …	Successfully merging a pull re this issue.	quest may close
	I have put this through the feature/pn-iaea branch. That branch contains some diagnostics for checking the locator positions in the photonuclear ACE files when NJOY writes them out (these diagnostics were previously available for continuous energy	Ş⊶ Fix/tendl pn	
	neutron and charged particle files but this branch will extend it to the photonuclear data). When running this version of	Notifications	Customiz
	NJOY2016, I'm getting an error message on a mismatching locator (i.e. a locator points to a position before the current position in the xss array) which would lead to a malformed ACE file. This new version therefore errors out.	没 Unsubscr	
	I have now narrowed it down to the MF6 MT51 entry in the Ra226 photonuclear file. In this piece of the ENDF file, there are three reaction products: a neutron, a residual Ra225 and a photon. For some reason, ACER is not counting this reaction as a	You're receiving notifications watching this repository.	because you're
	photon producing reaction when it fills out the IXS array in the particle production blocks. However, when ACER Is filling in the MTRH, TYRH, LSIGH, SIGH, etc. blocks for the photon it does pick up the photon from MF6 MT51. Because this offsets the size of the MTRH, TYRH and LSIGH block, what is supposed to be the locator for the cross section of the first MT on the MTRH photon block is in fact the TYR value for a shifted reaction. Since TYR=-1, this results in a locator for that first reaction	2 participants	
	photon production cross section pointing to a position before the SIGH block.	A Lock conversation	
	Long story short: if you go into the evaluation, and set the LAW=0 for ZAP=88225 in MF6 MT51 (second subsection), then the issue goes away in the above mentioned branch. The diagnostics still warn about a locator mismatch later in the file (LANDH	🛠 Pin issue (i)	
	and ANDH for photons seem to be correct but the LDLWH block is shifted by ~100 values) which indicates a gap in the file.	→ Transfer issue	



Making a new ENDF/B library ...

- We like to change formats and add new data previously not available in each ENDF/B generation
- ENDF/B-VIII.0 added the following new format capabilities
 - Fission neutron and gamma probabilities in MF6/MT18
 - Sub-actinide and non-neutron induced "fission" in MF10/MT18
 - Tabulated fission energy release components in MF1/MT458
- ENDF/B-VIII.1 will not be an exception:
 - Thermal scattering: mixed coherent and incoherent elastic scattering
 - External R-matrix elements used in some new resonance evaluations
 - Photonuclear data evaluations no longer assume isotropic photons



Making a new ENDF/B library ...

- As a result, our work is never done ...
 - Update MODER so that we can toggle between ASCII and binary
 - Update RECONR for the external R-matrix elements
 - Update THERMR, GROUPR, ACER, etc. for the mixed mode elastic scattering
- This can have an impact on the ACE library format
 - New libraries might not be compatible with older MCNP version!
 - This will most likely be the case for the mixed mode elastic scattering



Conclusions

- NJOY is the nuclear data processing software used at LANL
- NJOY2016 is the production version
 - New formats for ENDF/B-VIII.1 will be supported
 - Get it at https://github.com/njoy/NJOY2016
- NJOY21 modernisation shift to components instead of pure modules
 - Format components: ENDFtk, GNDStk and ACEtk
 - Processing components: R2 and SCION
 - Providing a C++ and Python interface

