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Title: What's up with NJOY?

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Los Alamos NATIONAL LABORATORY

What's up with NJOY?

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Outline

1. Introduction: what is NJOY and how does it relate to MCNP?
2. 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?

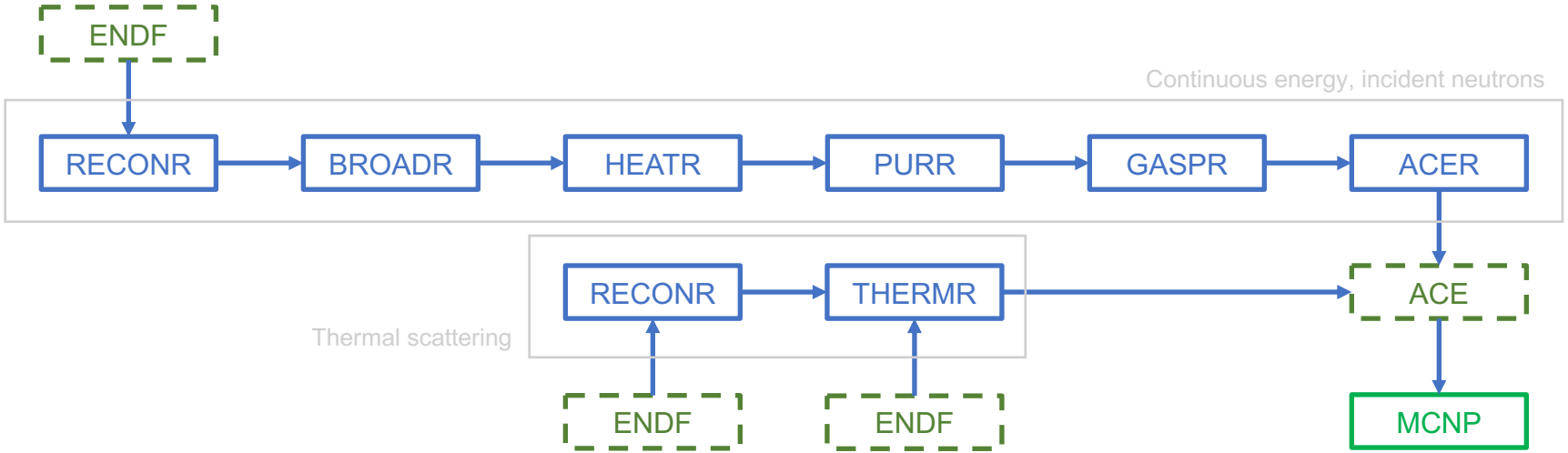
- Some of the main tasks of the XCP-5 Nuclear Data Team at LANL:
  - Maintain nuclear data libraries for LANL simulation codes (MCNP, PARTISN, etc.)
  - Verify and validate new data libraries when they become available

- 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
```

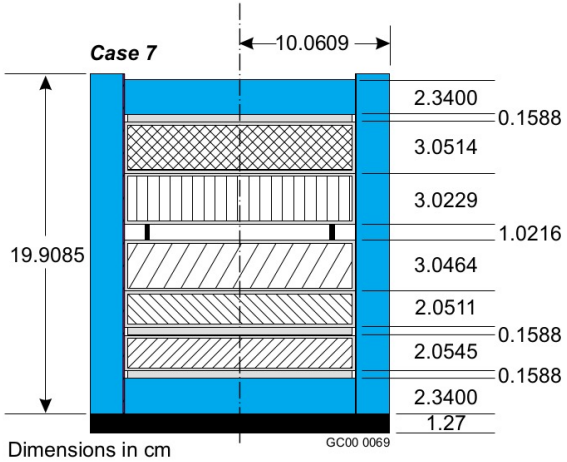
How is an MCNP ACE library file created?

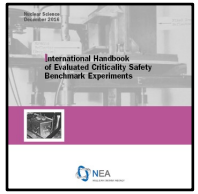
- NJOY provides a set of data processing modules that are called sequentially
  - Different processing paths for different library types
  - Incident neutron, incident charged particles, thermal scattering, photonuclear, etc.



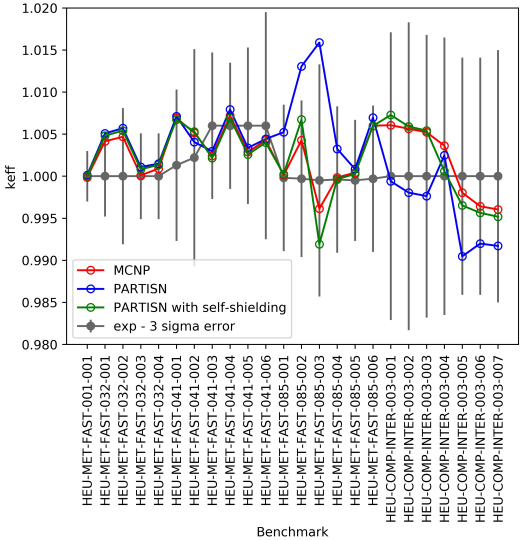
What verification and validation is performed?

- 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.





Depleted Uranium
Beryllium
SAE 1020 Steel
Aluminum
Iron



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

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)
GNDStk	Evaluated nuclear data format (the new one)
ACEtk	Application library format for MCNP

← See N. Gibson's presentation

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

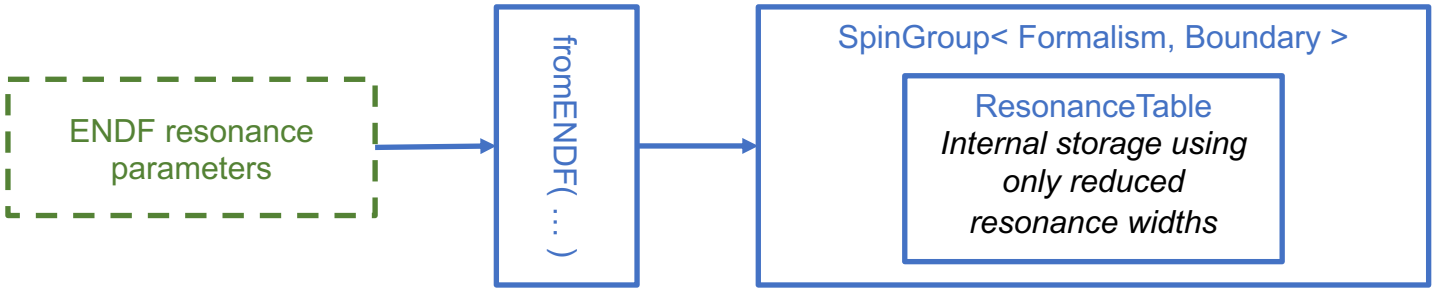
ENDFtk		RECONR	GROUPR	ACER	ERRORR
Neutron & CP data	✓	×	×	×	×
Photons	✓	×	×	×	
Resonances	✓	×			×
Photonuclear data	✗	×		×	
Covariance data	✗				×

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

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
  - Python is great for deploying our components more quickly

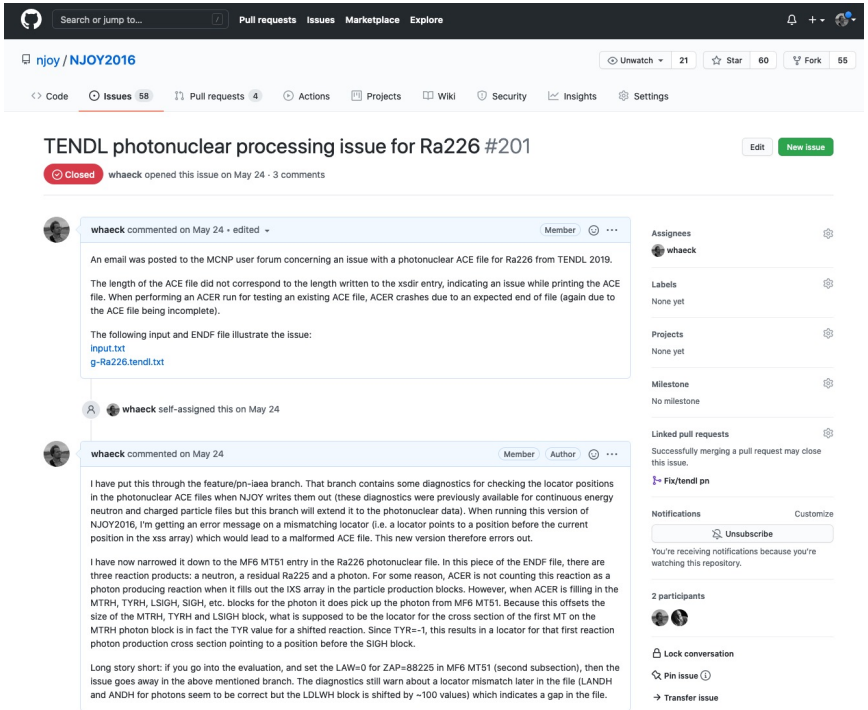
- ENDFtk is the first component with a full Python interface
  - The R2 resonance reconstruction component is next

```
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
xs = reconstruct( 1e-5 )
```

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



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