

Overview of NJOY work for NCSP FY23

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Outline

- Updates to NJOY2016 related to ENDF/B-VIII.1
 - MF7 MT451
 - Background R-matrix elements
 - Other notable changes
- Update on the NJOY modernisation
 - ENDFtk, ACEtk
 - scion

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 (somewhere in 2024)
 - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
 - Improved photonuclear data
 - Thermal scattering information in MF7 MT451
 - Background R-matrix elements for resonance parameters in MF2 MT151
- NJOY2016 should be able to handle or at the very least be able to read these
 - New features that require changes in MCNP have been prioritised
 - As a result, MCNP6.3 already supports these new ENDF/B-VIII.1 features



Maintaining our production version

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

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- Latest version is NJOY2016.74 (January 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



Thermal scattering information in MF7 MT451

- MF7 MT451 was approved as a format option this year
 - It provides composition and other relevant data on the molecule or crystal unit cell
 - A number of LIST elements per element
 - Each list gives isotopes, isomeric state, abundance, AWR and cross section values
- NJOY2016 does not use this data but can handle its presence in an ENDF file
 - Modifications were made to MODER only
 - We will make use of this in a modernised version of NJOY
- NJOY2016.71 (July 2023) is required when MF7 MT451 is present



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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Background R-matrix elements in MF2 MT151

- Changes were required in the following NJOY2016 modules:
 - MODER:
 - read over the background R-matrix element information
 - RECONR:
 - Add a few requirement tests to protect against NJOY2016 limitations
 - Background R-matrix elements are only allowed in LRF=7, KRM=3 (Reich-Moore)
 - NJOY2016 does not handle reduced resonance widths (IFG=1)
 - Add the background R-matrix element to the R-matrix
 - All options are supported although we only validated the SAMMY parametrisation
 - This new capability was tested in collaboration with ORNL
 - ERRORR:
 - Add derivatives to the background R-matrix elements
 - This currently only supports the SAMMY parametrisation and has not been validated



Background R-matrix elements in MF2 MT151





Other noteworthy updates to NJOY2016

- NJOY2016.70:
 - Primarily fixes in HEATR that may lead to differences with previous versions
- NJOY2016.72:
 - ERRORR now allows for the selection of the MF34 sub-subsection to be calculated
 - By default, the L=1,L1=1 sub-subsection will be calculated which in almost all cases will correspond to the first sub-subsection in the MF34 data
- NJOY2016.73:
 - Fixes in LEAPR to properly run some of the input files used for the ENDF/B-VIII thermal scattering files



When you see something, say something

- We try to fix issues in NJOY2016 as soon as they become apparent
 - Sr88 R-matrix background elements
 - LEAPR input files segfaulting
 - IAEA updates

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	I have put this through the feature/pn-iaea branch. That branch contains some diago	sitions	⊱ Fix/tendl pn		
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	I have now narrowed it down to the MF6 MT51 entry in the Ra226 photonuclear file. three reaction products: a neutron, a residual Ra225 and a photon. For some reason	e are n as a	You're receiving notifications because you're watching this repository.		
	photon producing reaction when it fills out the IXS array in the particle production b MTRH, TYRH, LSIGH, SIGH, etc. blocks for the photon it does pick up the photon fre are of the MTRH_TYRH and I SIGH before which is environment the balance for the	g in the the	2 participants		
	MTRH photon block is in fact the TYR value for a shifted reaction. Since TYR=-1, this	s results in a locator for that first re	action	**	
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So what about the NJOY modernisation?

- 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

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ENDFtk and ACEtk development is almost completed

- ENDFtk: <u>https://github.com/njoy/ENDFtk</u>
 - ENDFtk v1.0.0 (February 5, 2024): now with full ENDF compatibility
- ACEtk: https://github.com/njoy/ACEtk
 - ACEtk v0.1.0:
 - Incident neutron and charged particle ACE files
 - Photoatomic (including eprdata files) and photonuclear ACE files
 - Thermal scattering ACE files
 - Dosimetry ACE files
- Look out for v1.0 releases of both toolkits soon!
 - Updating cmake build systems and unit test framework update
 - Add an installation option
 - Updating dependencies



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

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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





Current capabilities in SCION





Our focus for next year

- Continue maintenance of NJOY2016 with respect to ENDF/B-VIII.1
 - This includes updating the NJOY2016 dependency in NJOY21 for those who use it
- NJOY modernisation:
 - Covariance related work (codex)
 - Resonance reconstruction overhaul
 - Processing the latest photoatomic and electron (EPICS) data into ACE files for MCNP

