Just a little NJOY update

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Agenda

1. Getting NJOY2016 ready for ENDF/B-VIII.1
   1. Overview of features to be supported
   2. ACE format changes
   3. NJOY2016.66
2. Modernisation updates
   1. ENDFtk
   2. ACEtk
   3. GNDStk

Making a new ENDF/B library …

- 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)
  - Background R-matrix elements for resonance parameters in MF2 MT151
  - Improved photonuclear data

- If these changes 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
- MCNP6.3 will have experimental support for these new ENDF/B-VIII.1 features

Thermal scattering

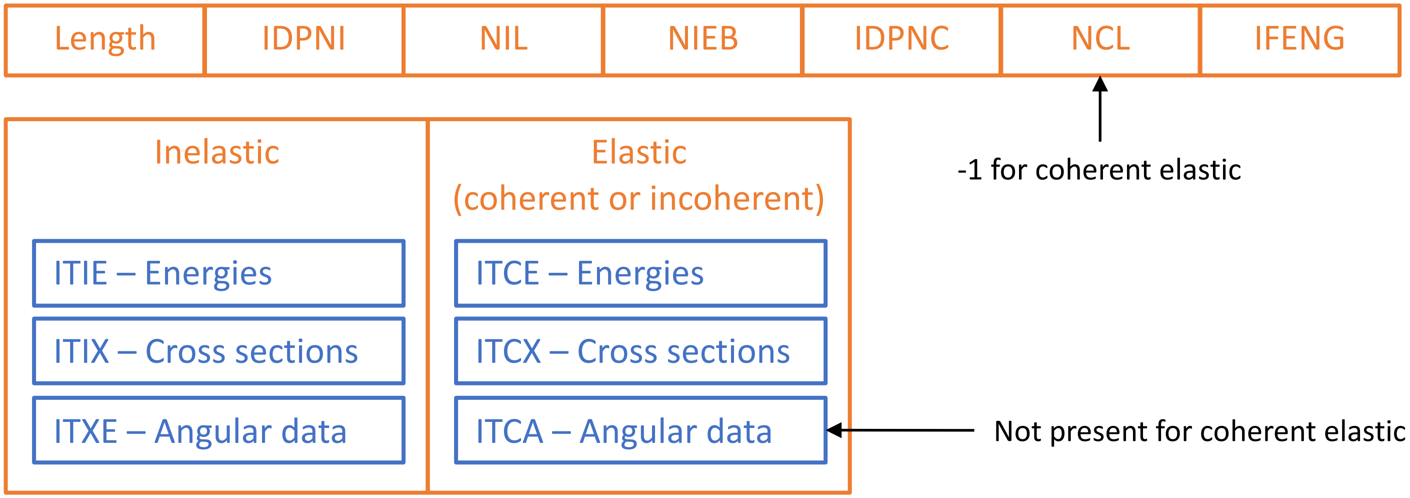
- Nuclear data evaluations identify multiple categories of thermal scattering:
  - Coherent elastic: important in crystalline solids (graphite, metals, etc)
  - Incoherent elastic: important in solids with hydrogen (polyethylene, ZrH, etc.)
  - Coherent and incoherent inelastic: all solid and liquid materials (hydrogen in water)

- Prior to ENDF/B-VIII.1: either coherent or incoherent elastic scattering
  - Coherent and incoherent are not exclusive and neglecting one is an approximation
  - ENDF/B-VIII.1 will introduce mixed mode elastic scattering

- This feature is reflected in the ACE format itself
  - Only one elastic thermal scattering data block, which is either coherent or incoherent
  - We needed to add an optional second block when both are given

The original thermal scattering format in ACE

- The thermal scattering format is relatively simple
  - Two main blocks: one for inelastic and one for elastic
  - The elastic block is either coherent (IDPNC=4) or incoherent (IDPNC=3)
  - Formatting parameters given in the NXS array



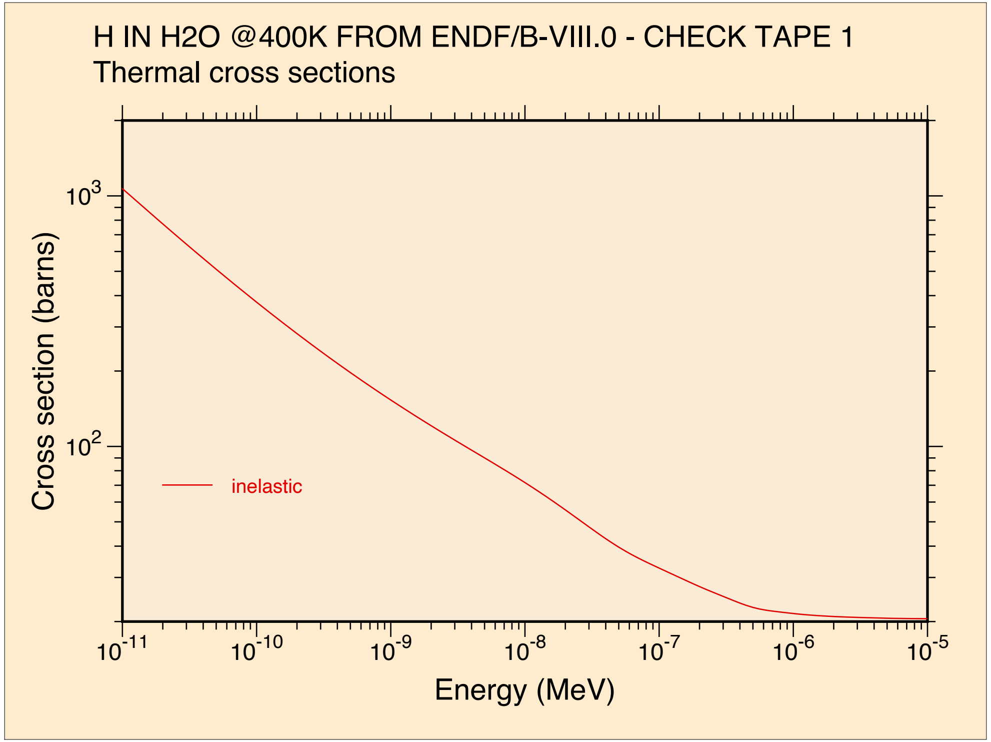
The original thermal scattering format in ACE

- The old format is still VALID
  - When mixed mode is used, there will be an additional elastic block (IDPNC=5)
  - Coherent elastic is always given first, incoherent elastic is given after that
  - An additional formatting parameter: NCLI for the second elastic block only
    - NCL will always be -1 for IDPNC=5

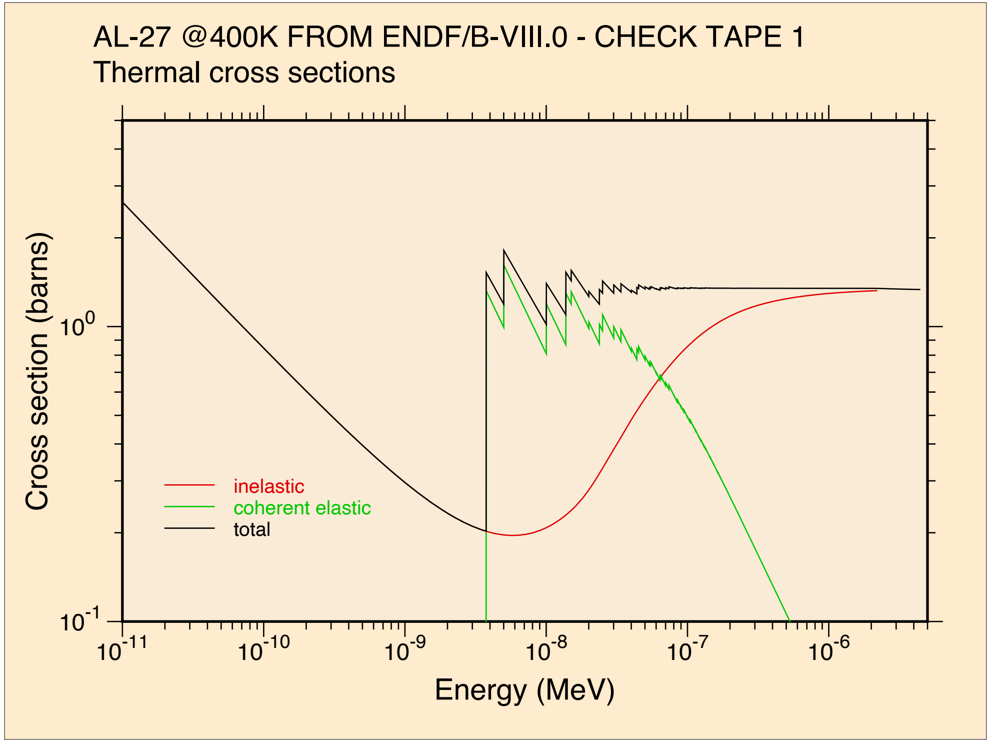
Length	IDPNI	NIL	NIEB	IDPNC	NCL = -1	IFENG	NCLI

Inelastic	Coherent elastic	Incoherent elastic
ITIE – Energies	ITCE – Energies	ITCEI – Energies
ITIX – Cross sections	ITCX – Cross sections	ITCXI – Cross sections
ITXE – Angular data	ITCA – Angular data	ITCAI – Angular data

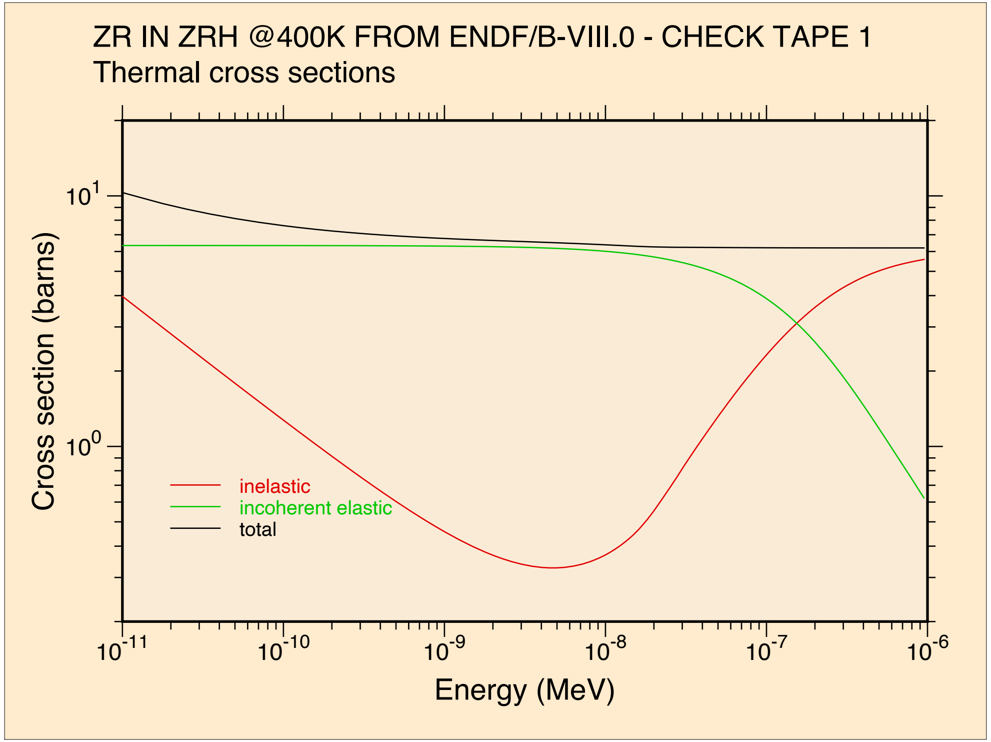
Example: H-H2O - inelastic only



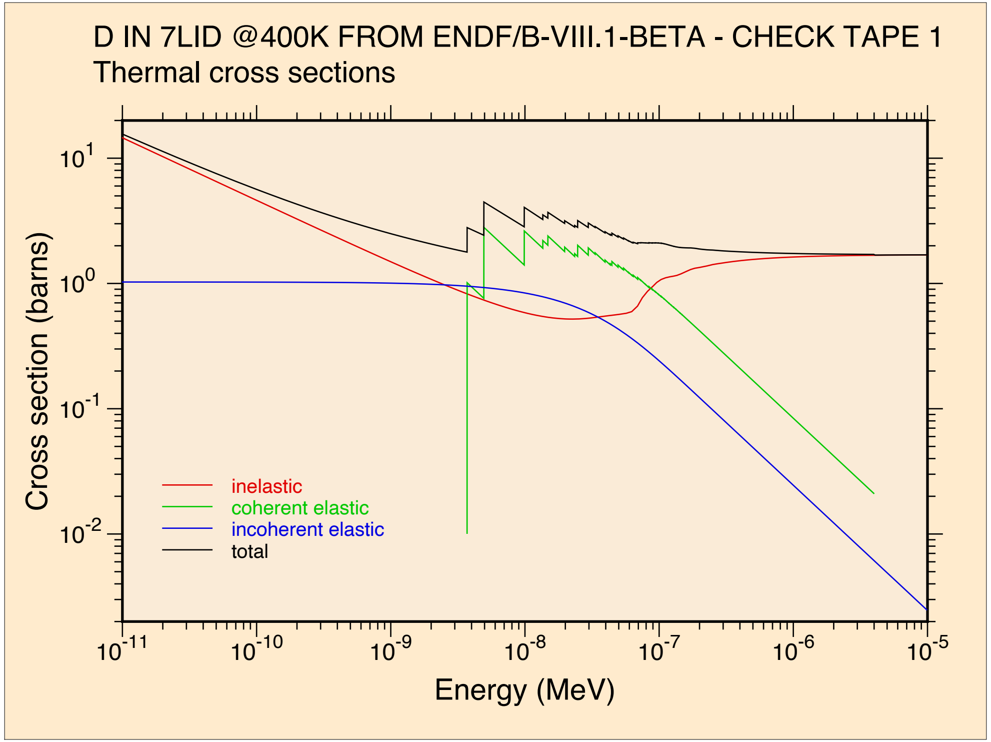
Example: Al27 metal – coherent elastic and inelastic



Example: Zr-ZrH – incoherent elastic and inelastic



Example: D-^{7}LiD – mixed mode elastic and inelastic



Photonuclear data

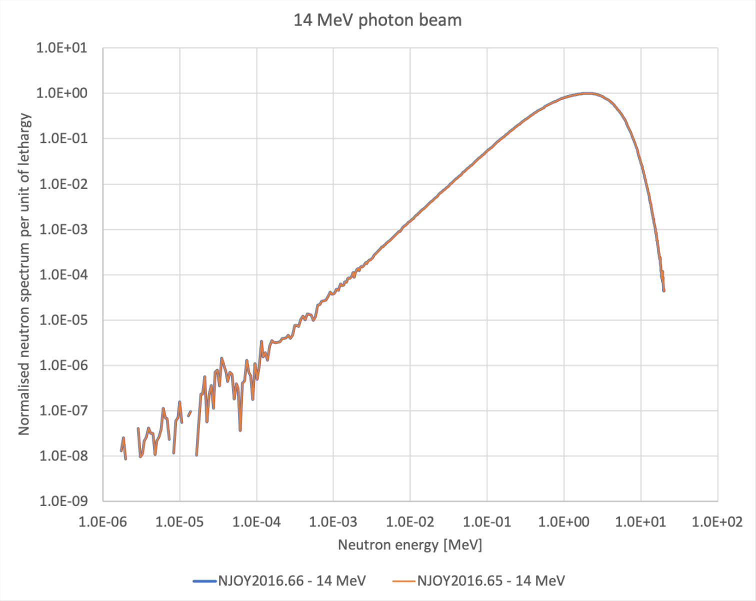
- Traditional photonuclear data
  - Secondary photon distributions traditionally given using the LAW=1 LANG=1 format
  - Traditionally using a single Legendre coefficient (i.e. isotropic distribution)
  - This assumption was hardcoded in NJOY2016's ACER module

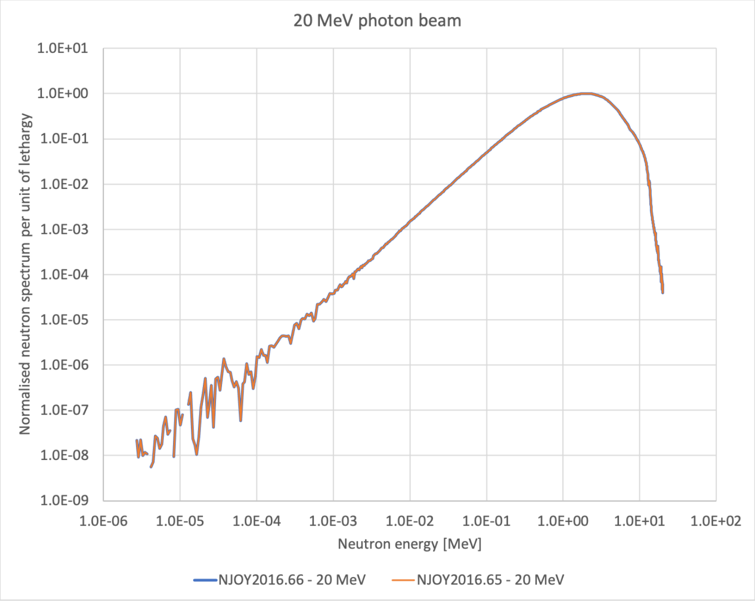
- And then the IAEA-2019 library was released (August 2020)
  - Secondary distributions are using anisotropic Legendre expansion

- NJOY2016 had to be updated
  - A temporary fix was introduced to keep the distributions isotropic
  - A permanent fix now translates the distributions properly into ACE LAW=61
  - Only MCNP6.3 is capable of using these new photonuclear files

Example: Mono-energetic photon beam on a Pu239 disk

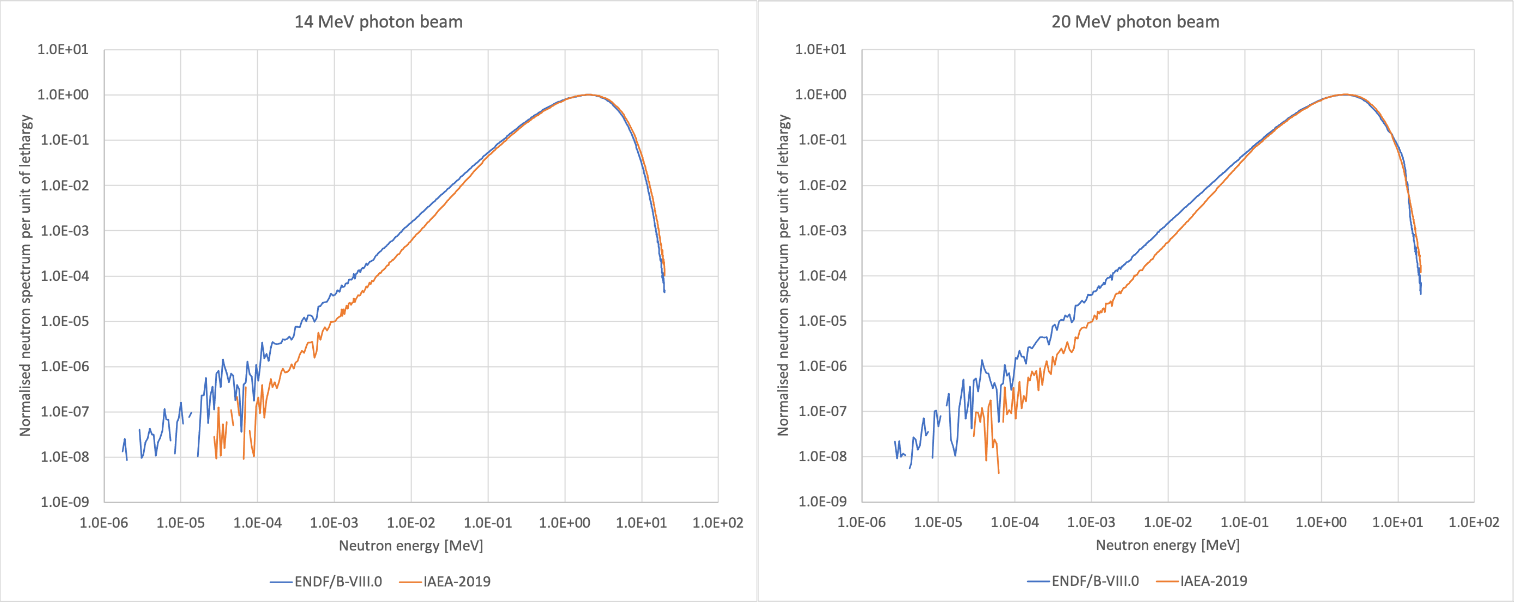
- Neutron spectrum tallied outside the disk in a 0.1 mm sphere
  - Using ENDF/B-VIII.0 photonuclear data





Example: Mono-energetic photon beam on a Pu239 disk

- Comparing ENDF/B-VIII.0 with IAEA-2019
  - Only MCNP6.3 can run the IAEA-2019 ACE files



NJOY2016.66

- This is a big update, the major changes are:
  - The photonuclear data format changes (ACE LAW 44 to 61)
  - Mixed mode elastic scattering in thermal scattering laws
- ACER
  - Photonuclear ACE format update (including plots and output file)
  - Formatting/processing the thermal scattering data (including plots and output file)
  - The XSS array and its size is now set in the common acecm module
  - Added locator checking and unknown law checking when writing out ACE files
    - NJOY2016 will now error out when locators are inconsistent or when an unknown law is used
    - Previously only for incident neutron and charged particle CE files
    - Extended to photonuclear and thermal scattering files
  - Some changes in the input file for mixed mode elastic (card 9: ielas=2)
  - Charged particle updates

When this happens, there is an issue that can cause MCNP problems. These things previously went undetected.

NJOY2016.66

- MODER
  - MF7 and MF28 update
- THERMR
  - Most of the thermal scattering processing happens here
  - Between 1 and 3 thermal scattering MT numbers are added to the PENDF file
- ERROR
  - Fixed a crash caused by MF34 covariances using multiple subsections
  - Each subsection is now processed but we are still working on outputting the results
- Additional non-regression tests
  - There are now 71 cases in the NJOY2016 test suite
  - Tests 67-70 provide tests for all combinations of thermal scattering data

What does the future bring?

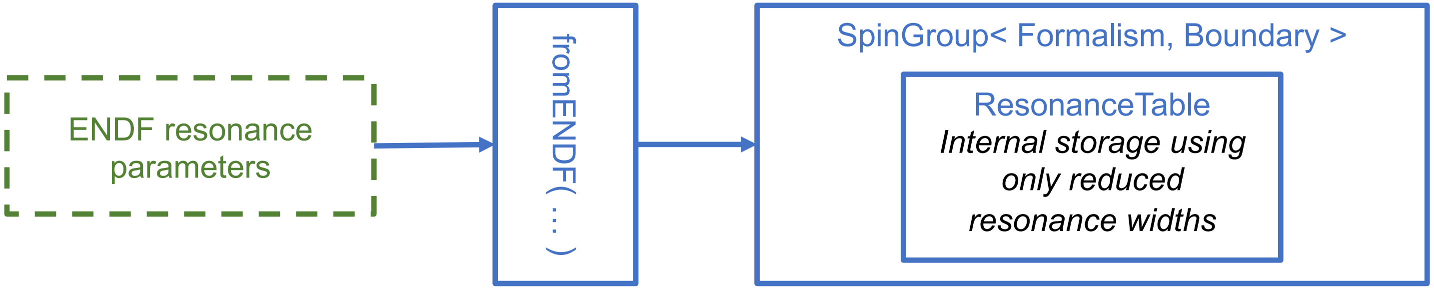
- NJOY2016 will be maintained for the foreseeable future
  - NJOY2016 is essentially the production code at LANL
  - New formats for ENDF/B-VIII.1 will be supported:
    - Thermal scattering: mixed coherent and incoherent elastic scattering
    - External R-matrix elements used in some new resonance 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
    - Components provide features that modules do not provide
  - Using a C++ and Python API at the same time

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



NJOY21 formatting 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

- ENDFtk: almost everything in the ENDF format, including internal NJOY sections
  - Some of the covariance sections are still missing
  - GENDF support (for GROUPR and ERRORR) will be added soon
  - https://github.com/njoy/ENDFtk
- ACEtk and GNDStk will be our focus for FY22
  - https://github.com/njoy/ACEtk
  - https://github.com/njoy/GNDStk

Current status of ACEtk

Incident neutron and charged particle continuous energy files			
Block	Description	C++	Python
ESZ	Energy grid and principal cross sections (total, elastic, absorption, heating)	Yes	Yes
NU	Average number of neutrons per fission	Yes	Yes
MTR, MTRP, MTRH	Available reactions (excluding elastic)	Yes	Yes
LQR	Reaction Q values	Yes	Yes
TYR, TYRH	Reference frame and multiplicity	Yes	Yes
SIG	Cross section data	Yes	Yes
SIGP, SIGH	Particle production cross sections	No	No
AND, ANDP, ANDH	Angular distribution data for secondary particles (no correlated angular)	Yes	Yes
DLW, DLWP, DLWH	Secondary particle energy distribution data (includes correlated angular)	Yes/No	Yes/No
GPD, HPD, YP, YH	Total secondary particle production cross section and multiplicities	No	No
PTYPE, NTRO, IXS	Auxiliary arrays for secondary particle production	Yes/No	Yes/No
UNR	Unresolved resonance probability tables	No	No

Current status of GNDStk

- The GNDStk development approach
  - A tree/node based core interface that is GNDS standard agnostic
  - A GNDS standard interface layer
    - An autogenerated interface that follows the GNDS standard specifications
    - Both a C++ and python interface is generated
    - Allowing for customization to produce a slimmed down and abstracted interface

- GNDStk v0.1.0 is a prototype using a slimmed down GNDS 1.9 standard

- We’re in the process of implementing the GNDS 2.0 standard
  - The autogenerated interface should be ready by now (at least I hope it is)
  - Customisation will begin for resonance parameters and cross section data

A first application: plotting

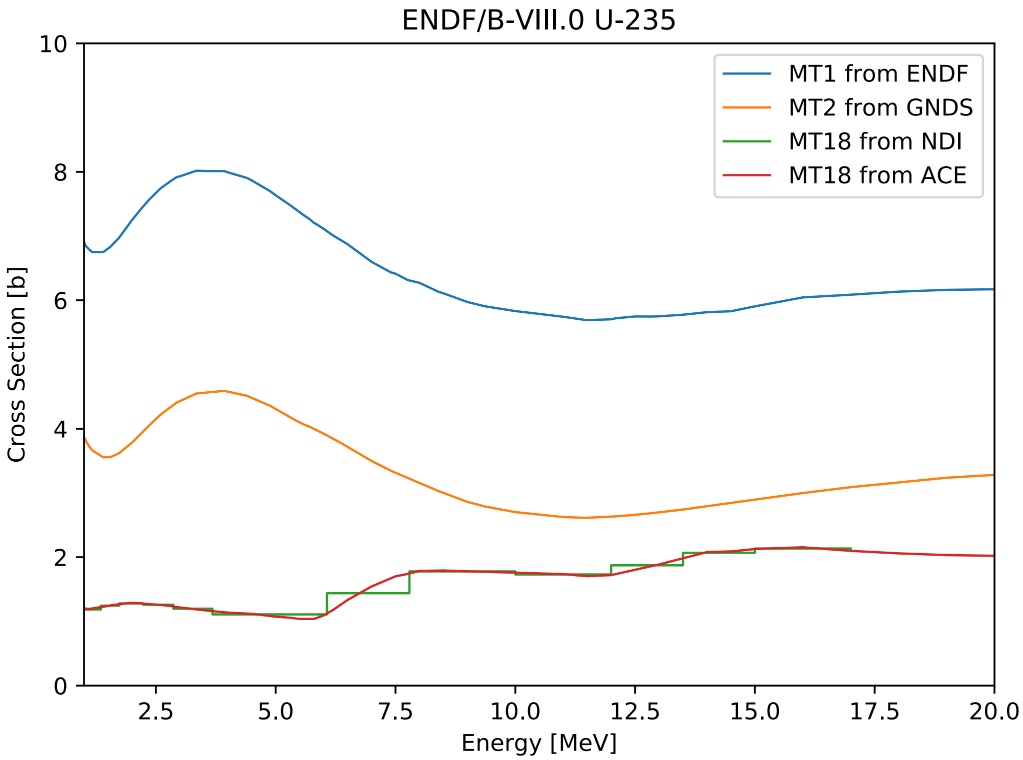
```
import ENDFtk, ACEtk
import matplotlib.pyplot as plot

# open an Pu239 ENDF file and extract the total cross section
tape = ENDFtk.tree.Tape.from_file( 'U235.endf’ )
section = tape.materials.front().file( 3 ).section( 1 ).parse()
energies1 = section.energies
total = section.cross_sections

# open the associated Pu239 ACE file and extract the total cross section
ace = ACEtk.ContinuousEnergyTable.from_file( 'U235.ace' )
index = ace.MTR.index( 18 )
energies2 = [ energy * 1e+6 for energy in ace.ESZ.energies ]
fission = ace.SIG.cross_sections( index )

# plot the cross sections
plot.plot( energies1, total )
plot.plot( energies2, fission )
plot.xscale( 'log' )
plot.yscale( 'log' )
plot.xlabel( 'Incident neutron energy [eV]' )
plot.ylabel( 'Cross section [barn]' )
plot.show()
```

A first application: plotting



Conclusions

- NJOY2016 will be maintained for the foreseeable future
  - New formats for ENDF/B-VIII.1 will be supported
  - NJOY2016.66 already implements a few of these
  - Experimental support for the ACE format changes in MCNP6.3

- NJOY21 modernisation
  - Component based versus module based
  - C++ and python interfaces
  - Currently focus is on format components: ENDFtk, ACEtk, GNDStk