Resonance Reconstruction Capabilities in NJOY21

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NJOY21—NJOY for the 21st Century

- Modernization of NJOY
- Ground-up rewrite of NJOY2016
- Enable independent use of components
  - ENDFtk
  - Interpolation library
  - Resonance reconstruction
- Bindings to legacy Fortran code

Goals

1. Maintain NJOY's legacy of a gold standard processing code
2. Easier
3. Flexible
4. Maintainable
RECONR Module from NJOY2016

1. Resonance reconstruction
   - njoy::resonanceReconstruction
     - Single-Level Breit-Wigner
     - Multi-Level Breit-Wigner
     - Reich-Moore
     - R-Matrix Limited

2. Energy-grid unionization
   - njoy::twig

3. Linearization of tabulated cross sections
   - njoy::twig

4. Removal of negative cross sections

5. Removal of positive cross sections below the reaction $Q$-value
1. Resonance reconstruction \texttt{njoy::resonanceReconstruction}  
   - Single-Level Breit-Wigner  
   - Multi-Level Breit-Wigner  
   - Reich-Moore  
   - R-Matrix Limited  

2. Energy-grid unionization \texttt{njoy::twig}  

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4. Removal of negative cross sections  

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Resonance Parameters

Formalisms:

- Single-Level Breit-Wigner (SLBW) (LRF=1)
- Multi-Level Breit-Wigner (MLBW) (LRF=2)
- Reich-Moore (RM) (LRF=3)
- Adler-Adler (AA) (LRF=4)
- R-Matrix Limited (RML) (LRF=7)
Resonance Parameters—Single-Level Breit-Wigner

Trkov, Herman, and Brown, *ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files*, Appendix D

\[
\sigma_{n,n}(E) = \sum_{\ell=0}^{\text{NLS}-1} \sigma_{n,n}^\ell(E),
\]

(D.1)

\[
\sigma_{n,n}^\ell(E) = (2\ell + 1) \frac{4\pi}{\lambda^2} \sin^2 \phi^\ell
\]

potential scattering

+ \frac{\pi}{\lambda^2} \sum_J g_J \sum_{r=1}^{\text{NR}_J} \Gamma_{nr}^2 - 2\Gamma_{nr} \Gamma_r \sin^2 \phi^\ell + 2 (E - E_r') \Gamma_{nr} \sin (2\phi^\ell)

\frac{1}{4} \Gamma_r^2 (E - E_r')^2 + \frac{1}{4} \Gamma_r^2

(D.2)

Parameters in red are parameters given in the ENDF file (some assembly required).

**Note:** Resonance parameters are not (necessarily) given in order of \( J \) or \( \ell \).
Results

- NJOY2016 run through RECONR module.
- NJOY21 resonance reconstruction with energy grid from NJOY2016.
Results

- NJOY2016 run through RECONR module.
- NJOY21 resonance reconstruction with energy grid from NJOY2016.

```plaintext
 realtime function sigfig(x,ndig,idig)
 !----------------------------------------------------------------------
 ! Adjust x to have ndig significant figures. If idig is not zero,
 ! shade x up or down by idig in the last significant figure.
 !----------------------------------------------------------------------

sigfig(1.2345678901,7) → 1.234567
sigfig(1.2345678901,7,2) → 1.234569
```
Single-Level Breit-Wigner Formalism

$^{105}\text{Rh}$

![Graph showing cross sections and relative differences for elastic and capture processes.]
Multi-Level Breit-Wigner Formalism

$^{58}\text{Co}$

Energy (MeV)

Cross Section (b)

Relative Difference

- elastic
- capture
- fission

$10^{-5}$  $10^{-4}$  $10^{-3}$  $10^{-2}$  $10^{-1}$  $10^{0}$  $10^{1}$  $10^{2}$  $10^{3}$
Multi-Level Breit-Wigner Formalism

$^{168}\text{Tm}$

![Graph showing cross sections for elastic, capture, and fission processes as a function of energy. The graph plots cross section in barns (b) versus energy in MeV, with logarithmic scales on both axes.](image)
Multi-Level Breit-Wigner Formalism

\[ ^{238}\text{Np} \]

![Graph showing cross sections for elastic, capture, and fission reactions as a function of energy in MeV.](image)

- **Cross Section (b)**
  - Elastic
  - Capture
  - Fission

- **Energy (MeV)**
  - 10^{-5} to 10\(^{1}\)

- **Relative Difference**
  - 10^{-9} to 10^{-7}
Reich-Moore Formalism

Cross Section (b)
- Elastic
- Capture
- Fission

Energy (MeV)
- Relative Difference

235U

Graph showing cross sections and relative differences for different processes across energy levels.
Reich-Moore Formalism

$^{238}\text{U}$

Cross Section (b)

- elastic
- capture
- fission

Relative Difference

Energy (MeV)

10$^{-4}$, 10$^{-2}$, 10$^{0}$, 10$^{2}$, 10$^{4}$
Relative Differences

- Biggest difference: $6.4 \times 10^{-3} \%$
- Integral difference likely much smaller

$$\int_{E_{i-1}}^{E_i} \frac{\sigma_{21} - \sigma_{16} dE}{\int_{E_{i-1}}^{E_i} \sigma_{16} dE}$$

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<th>Form</th>
<th>Isotope</th>
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<th></th>
<th>capture</th>
<th>mean</th>
<th>max</th>
<th>average</th>
<th>fission</th>
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</table>
When resonance reconstruction is short, NJOY21 is comparable to NJOY2016. When resonance reconstruction takes a long time (>1 s) NJOY21 is clearly faster.
Conclusion

- Resonance reconstruction capabilities in NJOY21 for:
  - Single-Level Breit-Wigner
  - Multi-Level Breit-Wigner
  - Reich-Moore

- Timing:
  - Comparable when resonance reconstruction is easy
  - Faster when resonance reconstruction is difficult

- Future Work:
  - R-Matrix Limited (RML) Formalism (coming FY2018)
  - Removal of negative cross sections
  - Removal of non-zero cross sections below $Q$-value