Resonance Reconstruction Capabilities in NJOY21

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Jeremy Lloyd Conlin[1] Austin P. McCartney[1] Wim Haeck[1] Amelia Jo Trainer[2,1]

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[1]Los Alamos National Laboratory
PO Box 1663, Los Alamos, NM 87545

[2]Department of Nuclear Science & Engineering
Massachusetts Institute of Technology
77 Massachusetts Avenue, 24-107
Cambridge, MA, 02139

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

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

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

$$\sigma_{n,n}(E) = \sum_{\ell=0}^{\mathrm{NLS}-1} \sigma_{n,n}^{\ell}(E), \tag{D.1}$$

$$\sigma_{n,n}^{\ell}(E) = \underbrace{(2\ell+1)\,\frac{4\pi}{k^2}\sin^2\phi_\ell}_{\text{potential scattering}} + \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{{\Gamma_{nr}}^2 - 2\Gamma_{nr}\Gamma_r \sin^2\phi_\ell + 2\,(E-E_r')\,\Gamma_{nr}\sin(2\phi_\ell)}{(E-E_r')^2 + \frac{1}{4}{\Gamma_r}^2} \tag{D.2}$$

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 ℓ.

Results

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

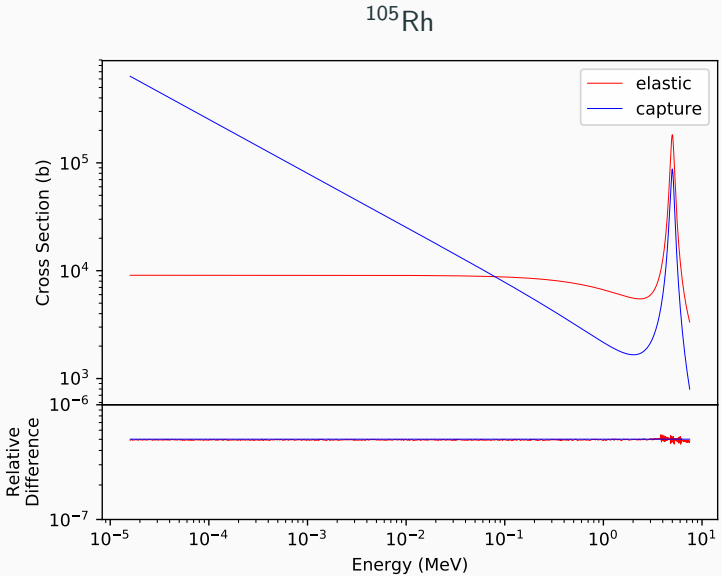
Results

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

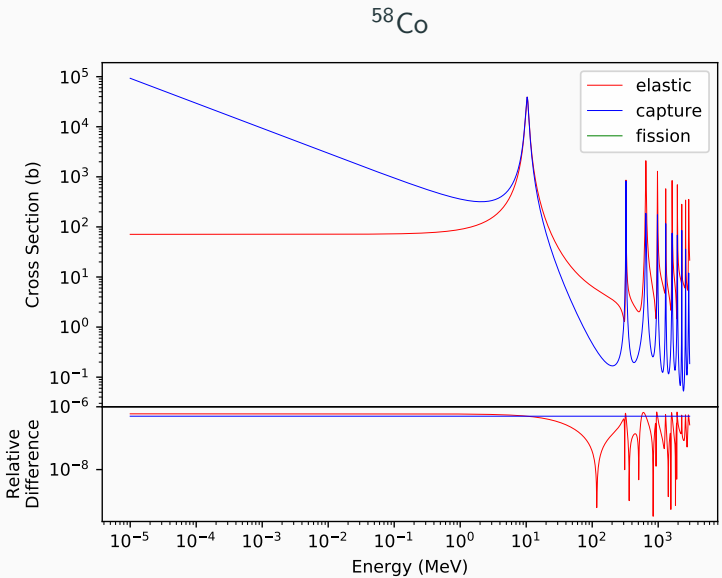
```
real(kr) function sigfig(x,ndig,idig)
!--------------------------------------------------------------------
! Adjust x to have ndig signficant figures.  If idig is not zero,
! shade x up or down by idig in the last significant figure.
!--------------------------------------------------------------------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

sigfig(1.2345678901,7) → 1.234567
sigfig(1.2345678901,7,2) → 1.234569

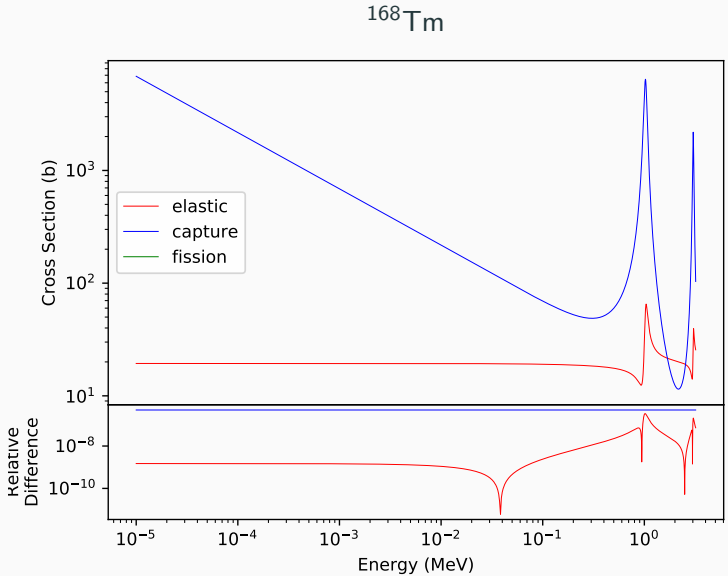
Single-Level Breit-Wigner Formalism



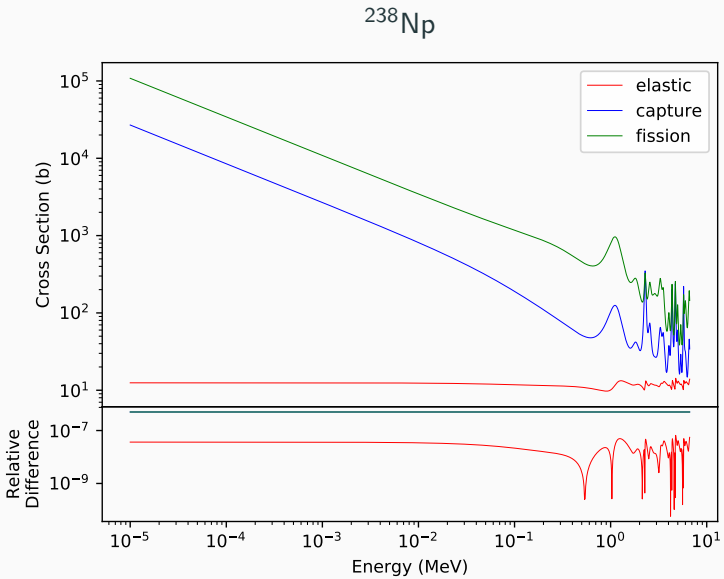
Multi-Level Breit-Wigner Formalism



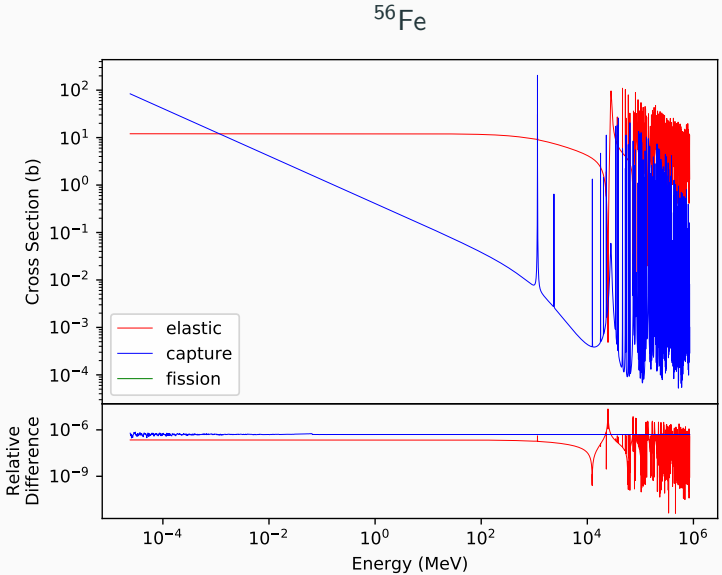
Multi-Level Breit-Wigner Formalism



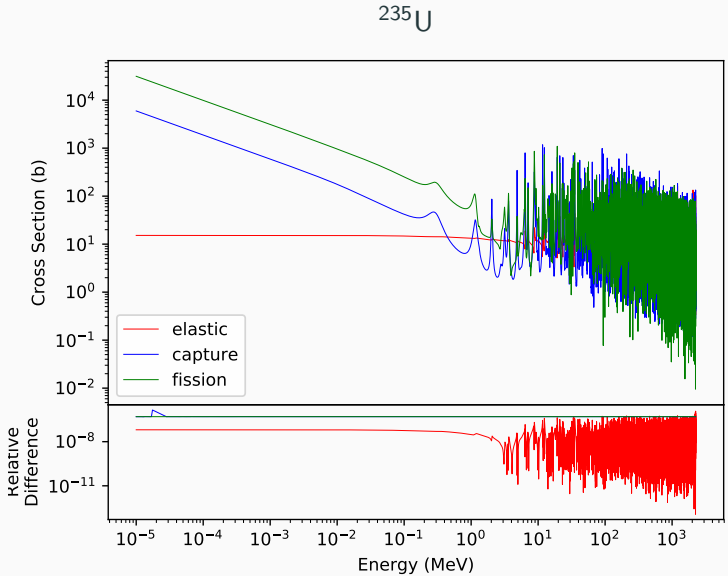
Multi-Level Breit-Wigner Formalism



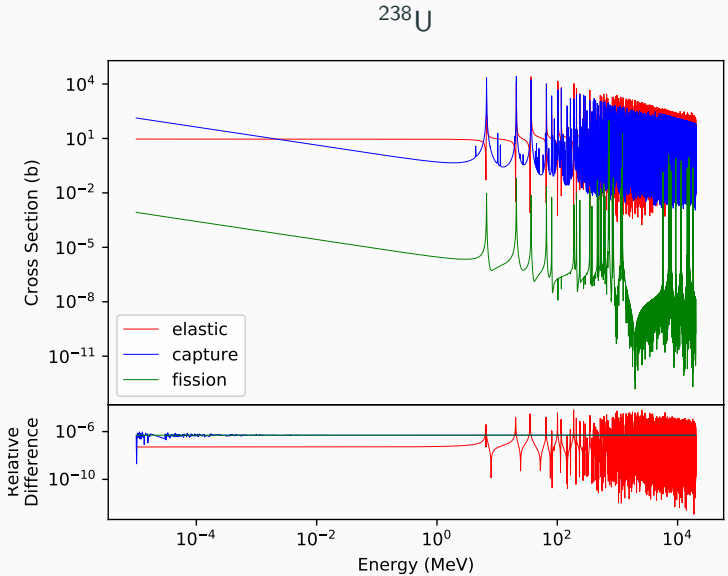
Reich-Moore Formalism



Reich-Moore Formalism



Reich-Moore Formalism



Relative Differences

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

$$\frac{\int_{E_{i-1}}^{E_i} \sigma_{21} - \sigma_{16} \mathrm{d}E}{\int_{E_{i-1}}^{E_i} \sigma_{16} \mathrm{d}E}$$

		Relative Difference (1×10^{-7})					
		elastic		capture		fission	
Form	Isotope	max	mean	max	mean	max	mean
SLBW	^{105}Rh	5.5	5.0	5.0	5.0		
MLBW	^{58}Co	6.8	3.9	5.0	5.0		
MLBW	^{168}Tm	0.66	0.25	5.0	5.0	5.0	5.0
MLBW	^{238}Th	3.4	0.57	5.0	5.0		
RM	^{56}Fe	220	3.7	7.2	5.0		
RM	^{235}U	12.0	0.67	14.0	5.0	5.0	5.0
RM	^{238}U	640	4.7	9.5	5.0	5.0	5.0

Timing Results

Formalism	Isotope	NJOY2016 (ms)	NJOY21 (ms)	NJOY21 Speedup
SLBW	^{105}Rh	0.256	0.122	2.1
MLBW	^{58}Co	2.69	1.37	1.97
	^{238}Np	0.196	0.574	0.883
	^{168}Tm	0.311	0.283	1.10
		(s)	(s)	
RM	^{56}Fe	0.648	0.135	4.80
	^{235}U	82.7	13.6	6.07
	^{238}U	144	14.7	8.12

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