OAK RIDGE National Laboratory

Isotope Effects in Thermal Neutron Scattering

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Background

- AMPX links Thermal Scattering Law (TSL) libraries to isotopes in the resolved resonance region
  - TSL eval explicitly names isotope, we only bind TSL data to that isotope
    - tsl-013_Al_027, tsl-026_Fe_056
  - Otherwise, assumes all isotopes can apply the TSL eval
    - tsl-reactor-graphite-10P -> ^{12}C-10p-graphite, ^{13}C-10p-graphite
    - Zr-ZrH -> ^{90}ZrH + ^{91}ZrH + ^{92}ZrH + …
    - U-UO_2 -> $^{233}UO_2$ + $^{234}UO_2$ + $^{235}UO_2$ + …
- No guidance is given in the TSL files or the ENDF format if this is acceptable or advised
- This can lead to some issues…

Different Scattering Lengths

- Isotopes of the same element can have significantly different scattering lengths and, therefore, different bound/free scattering cross sections
- Element-specific bound/free scattering cross section given in File 7, but not sub-divided into isotopic distribution
- User must rely on either description in the ENDF file or references, which may not provide necessary description
- Different from issue in incoherent elastic bound scattering cross section issue

Different Scattering Lengths – Comparison of Elemental and Isotopic Free Scattering Cross Sections

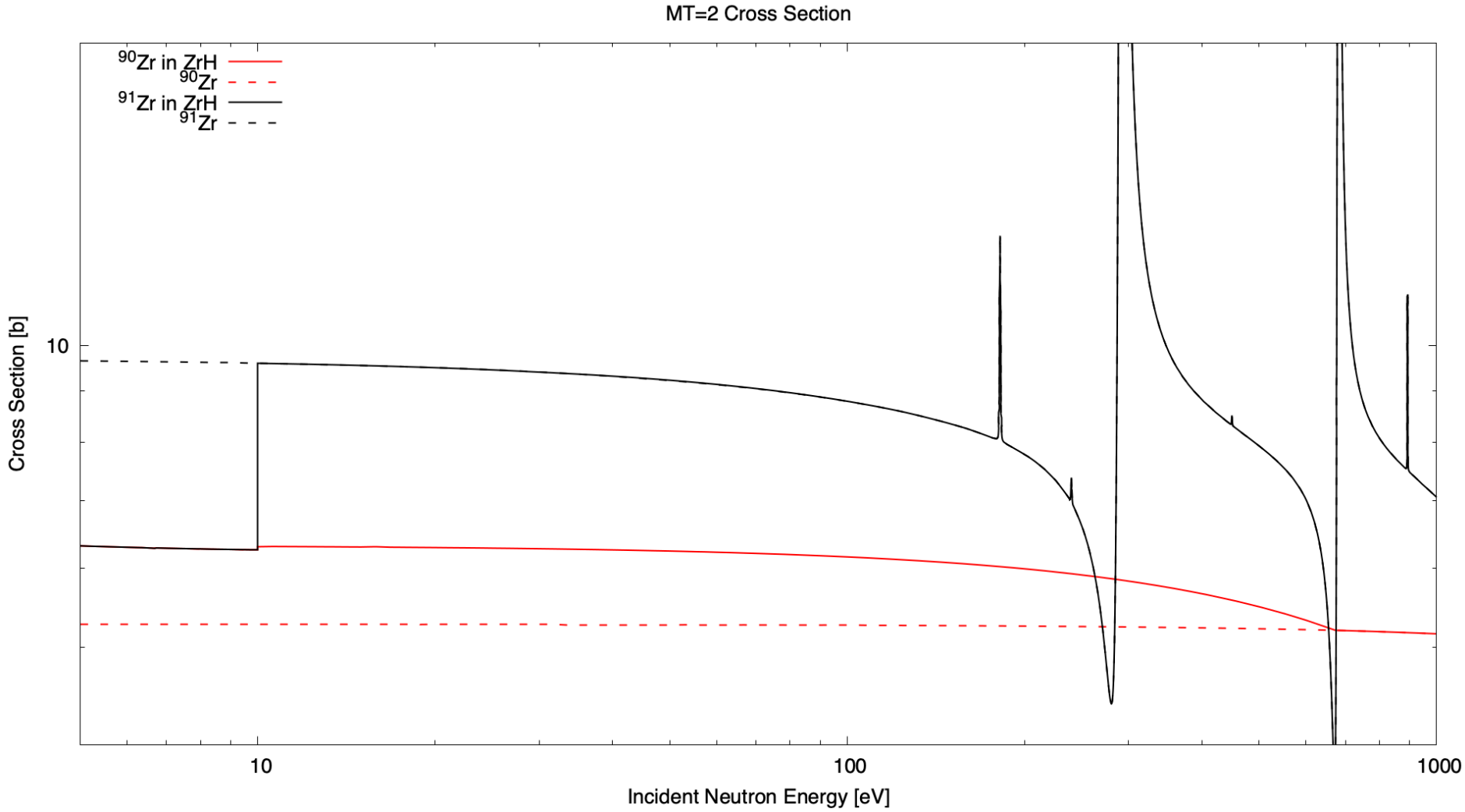
- Examples [1]:

Isotope/ Material	Weight pct.	Free Scattering xs [b]
^{90}Zr	51.45	4.99
^{91}Zr	11.32	9.49
^{92}Zr	17.19	6.75
^{94}Zr	17.28	8.22
^{96}Zr	2.76	3.72
^{nat}Zr		6.32
Zr-ZrH		6.34

Isotope/ Material	Weight pct.	Free Scattering xs [b]
^{28}Si	92.23	1.98
^{29}Si	4.67	2.60
^{30}Si	3.1	2.47
^{nat}Si		2.02
Si-SiC		2.042

- Up to 50% difference between isotopic & elemental scattering xs

Different Scattering Lengths



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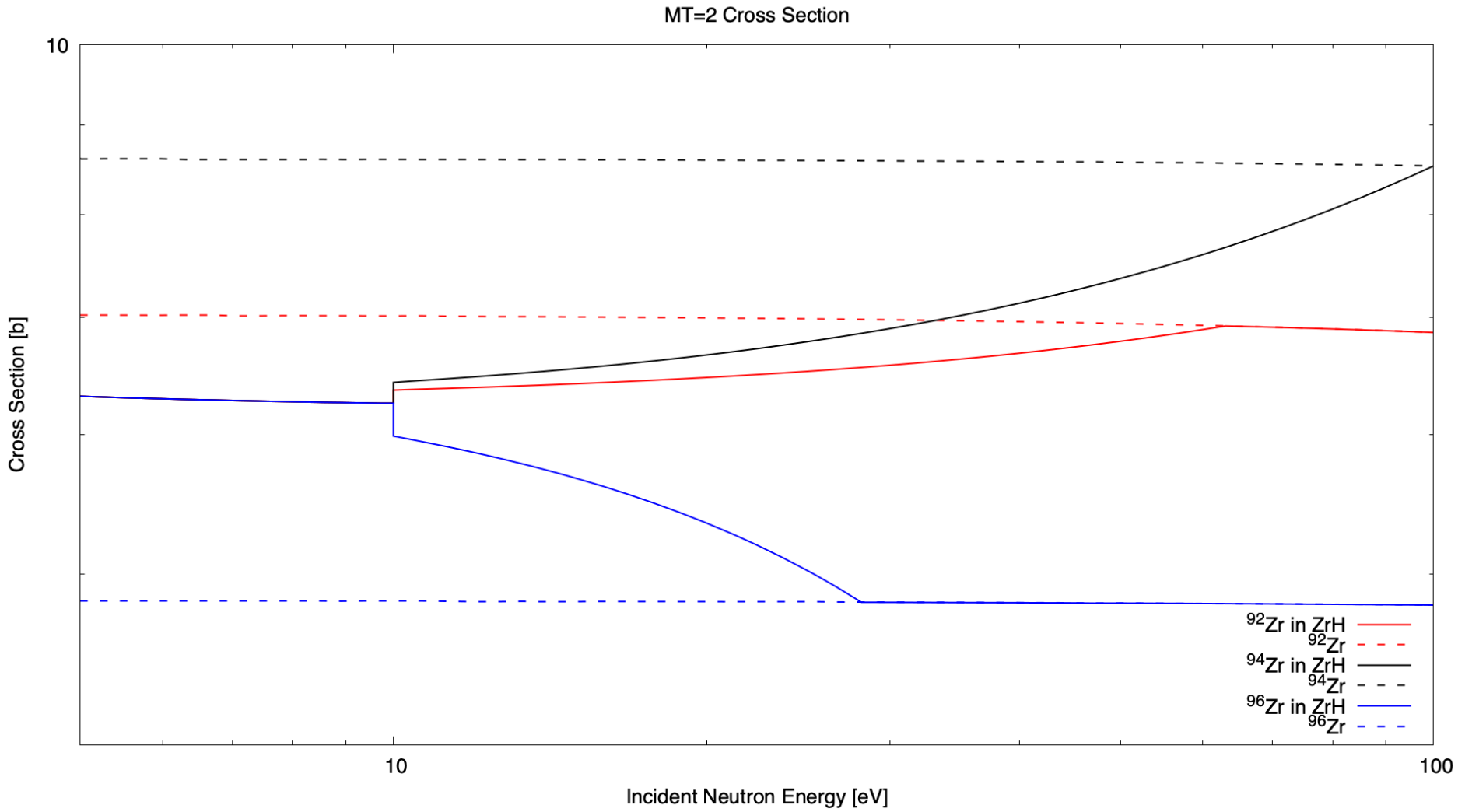
Different Scattering Lengths



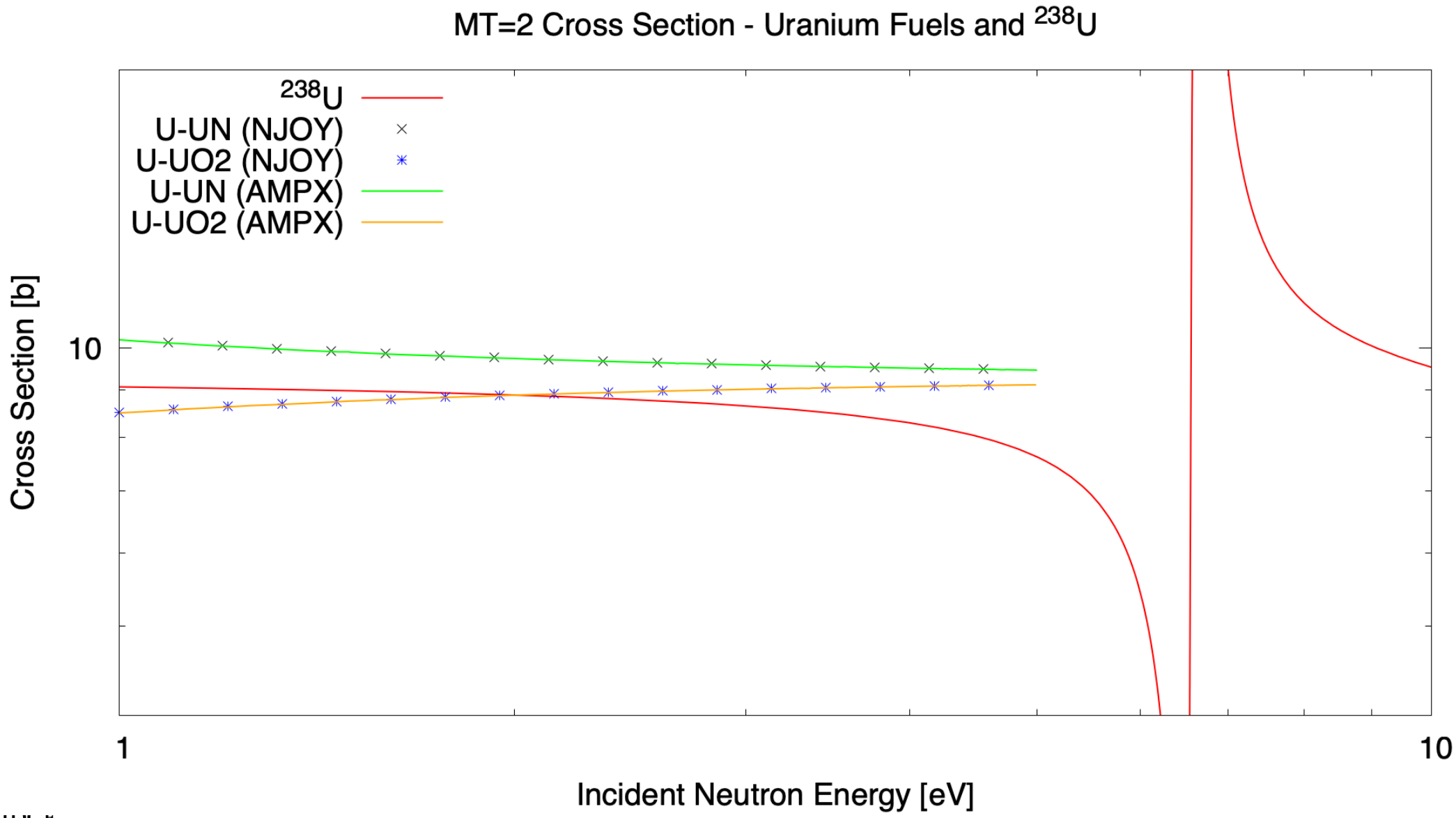
- NJOY & AMPX calculate same MT2 for thermal energies (<10 eV)
- Issue is related to ENDF specification, not processing code

Resonances

- Some isotopes have resonances near (or sometimes IN) the thermal range
- Resonance theory is not currently incorporated into thermal scattering evaluations
- These can have a noticeable effect on the thermal scattering cross section

Isotope	$\frac{\sigma_s}{\sigma_t}$	Resonance Energy [eV]
^{177}Hf	2.42E-4	1.0980
^{239}Pu	7.87E-3	0.2956
^{235}U	5.32E-2	0.2684
^{161}Dy	1.64E-1	2.7100
^{197}Au	5.84E-2	4.8997
^{238}U	8.26E-1	6.6743

Resonances


MT=2 Cross Section - Uranium Fuels and 238U
238U
U-UN (NJOY)
U-UO2 (NJOY)
U-UN (AMPX)
U-UO2 (AMPX)
Cross Section [b]
10
1
10
Incident Neutron Energy [eV]

Discussion

- Should information about the isotopic composition be provided in ENDF TSL files?
- Suggested solutions for incorporating low-lying resonances:
  - Try and match the TSL cross section with the resonance at a specific cutoff energy (tricky, but doable)?
  - Implement resonance theory in thermal scattering evaluations (very difficult)?

Acknowledgements

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References

- [1] https://www.ncnr.nist.gov/resources/n-lengths/