Simultaneous TSL/RRR Evaluation of UO_2 & PuO_2 – Expanded Theory & Simulations

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Outline

- Theoretical improvements
- Attempts at experimental validation
- Conclusions & Future Work

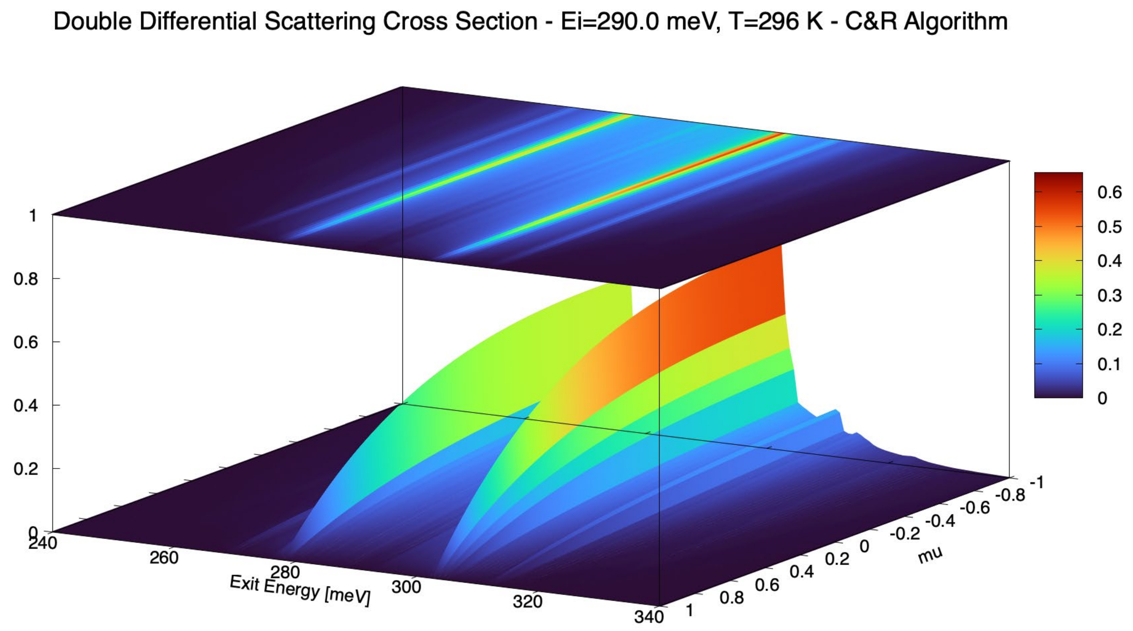
Previous FY

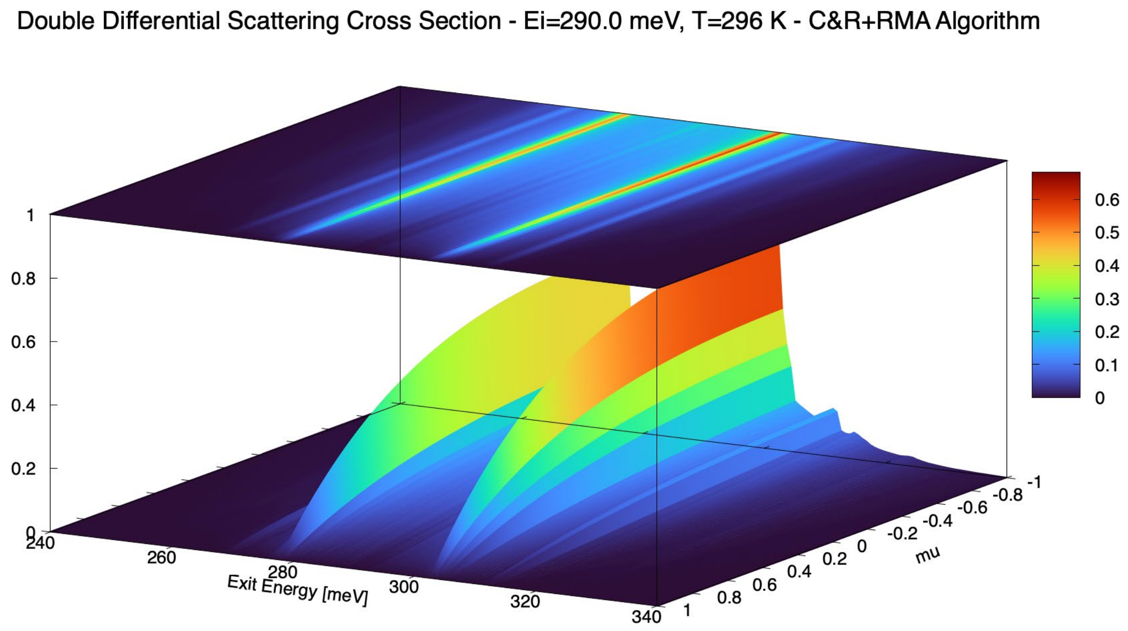
- Formalism was coded up from the writeup by Courcelle & Rowlands (C&R) [1]
- Some limitations were identified:
  - Theoretical limitations (SLBW, *s*-wave only)
  - Experimental validation
  - Elastic contribution
  - Temperature effects
- Focus last FY was spent on the first 2 points

Theoretical Improvements

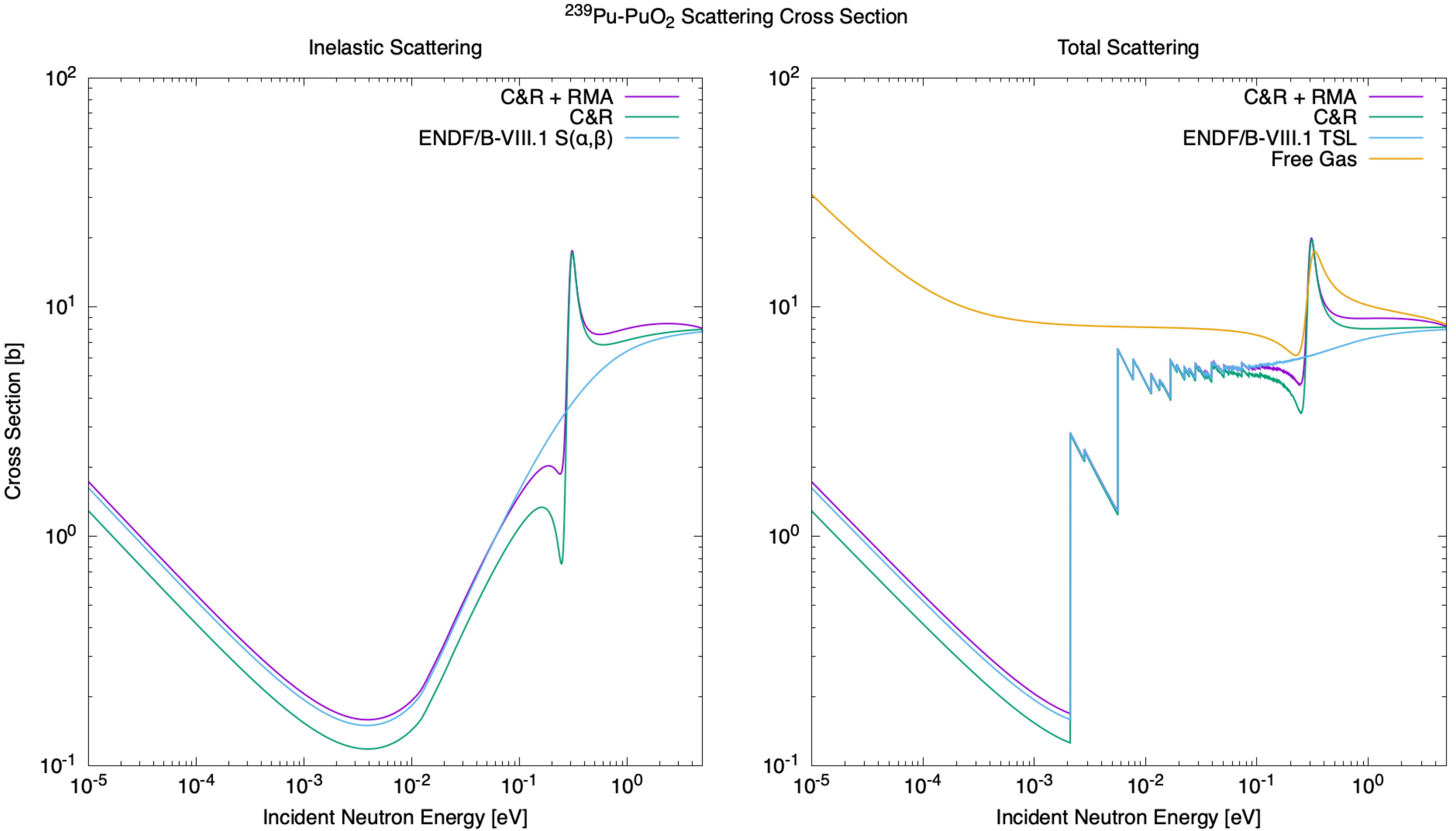
- This work expands on the work of C&R:
  - Removing the restriction of SLBW by re-casting the derivation in the Reich-Moore approximation (C&R+RMA)
  - Allowing for arbitrary number of resonances & spin groups
- Can treat arbitrary levels as either ‘resonant’ or ‘background’ contribution
- Can be extended to other reaction channels besides scattering (to be implemented later)

Simulation Results – PuO_2 – DDXS – C&R vs. C&R+RMA





Simulation Results – PuO_2 – 1D Cross Section



Experimental Validation

- Need a material that:
  - Has a resonance in the low-eV or meV range,
  - Has an acceptable scatter-to-capture ratio,
  - Has a not-complicated phonon density of states,
  - Doesn't have hydrogen
  - Is stable (or has a long half-life)
- There are a few options, we landed on metallic erbium
  - Er-167 has 2 low-lying resonances at 460 and 584 meV
  - Samples were available on hand

Experimental Validation – Results

- Metallic sample contained hydrogen
- Attempts to ‘burn out’ the hydrogen were unsuccessful
- Forced to pivot to erbium oxide (Er_2O_3)
- Results were difficult to parse due to complicated phonon DOS of Er_2O_3

Conclusions

- Novel simultaneous TSL/RRR theory implemented in Python script
- Differences between previous formalism found to be small, but non-negligible

Future Work

- Continue attempts of experimental validation
- Implement formalism in AMPX/SAMMY for validation in SCALE

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References

[1] Courcelle, A., Rowlands, J., 2007. “Approximate model of neutron resonant scattering in a crystal”, arXiv:0709.2767, https://doi.org/10.48550/arXiv.0709.2767

Questions?