Simultaneous TSL/RRR Evaluation of UO_2 & PuO_2– Theory and Preliminary Results

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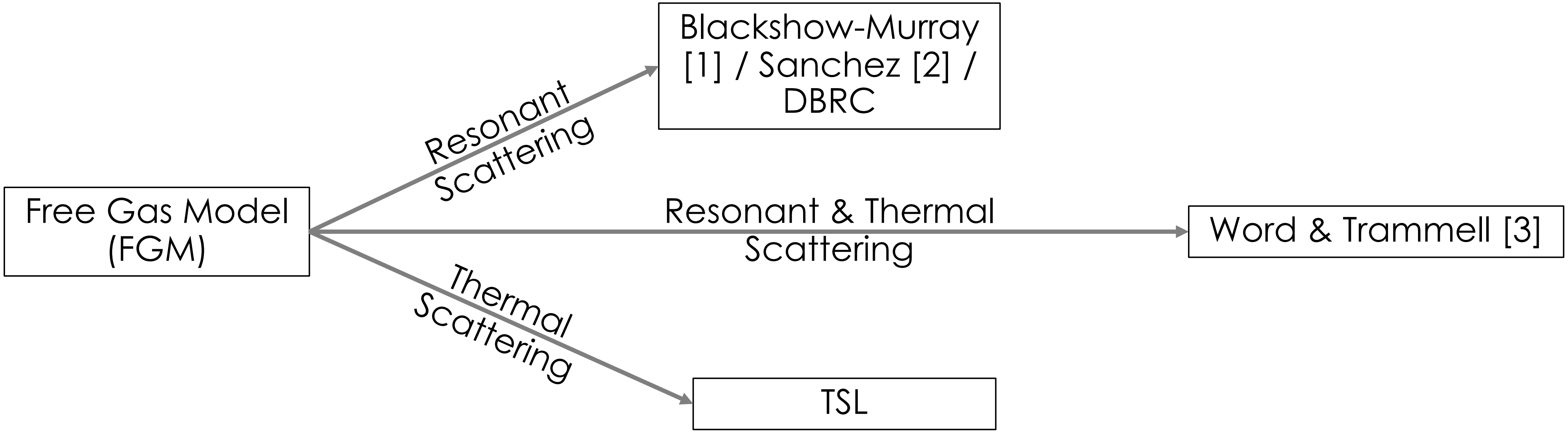
Outline

- Background
- Formalism & Implementation
- Preliminary Results
- Conclusions & Future Work

Background

- Thermal Scattering Law (TSL) and Resolved Resonance Region (RRR): Why we care
  - Scattering is a joint TSL & RRR process near resonances
  - Scattering distribution at resonances
  - Joining at thermal energy
- Historically wasn't an issue, as most thermal scattering materials did not contain isotopes with low-lying resonances

Background: What’s currently done



Formalism & Implementation

- From Word and Trammel [3] based on two assumptions:
  - *s*-wave resonances only
  - Only 1 resonance in thermal range
- The resulting equation is a Fourier-double-Laplace transform of a 4-point correlation function, which is…difficult to solve
- Several different approximations have been made to simplify the equation [4,5], ultimately decided on the formalism by Courcelle & Rowlands (C&R) [5]

Formalism & Implementation: C&R

- Equation implemented in Python script:

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{4\pi}\frac{k_f}{k_i}S(q,E)\left[\sigma_p + \sigma_m\frac{\Gamma_n}{\Gamma}\psi + \sqrt{\sigma_p\sigma_m\frac{\Gamma_n}{\Gamma}}\chi\right]$$

- Input $S(q,E)$ and resonance parameters taken from ENDF/B-VIII.1.beta2 release
- Implementation was:
  - Verified against figures provided in [2] (without TSL contribution) and [5] (with both TSL & RRR contribution)
  - Validated against available total cross section measurements of UO_2

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Formalism & Implementation: C&R

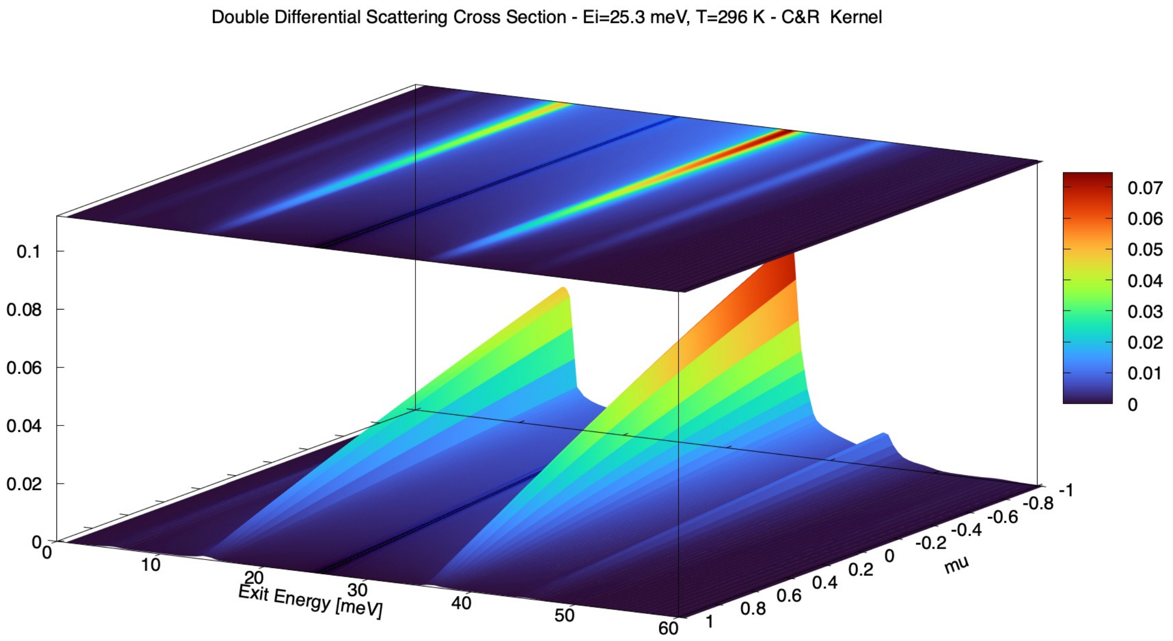
Pros

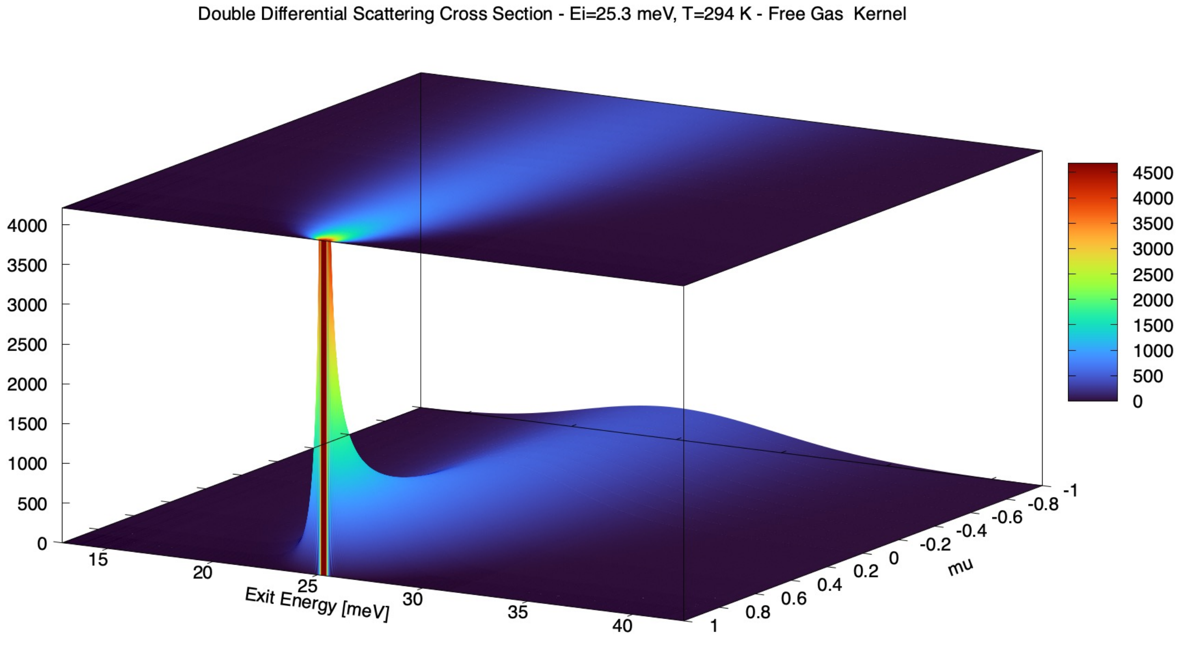
- Accounts for combination of resonant and thermal scattering differential cross sections simultaneously
- Full double differential
  - Most accurate representation
- Temperature broadening accounted for through $S(q, E)$, ψ, and χ

Cons

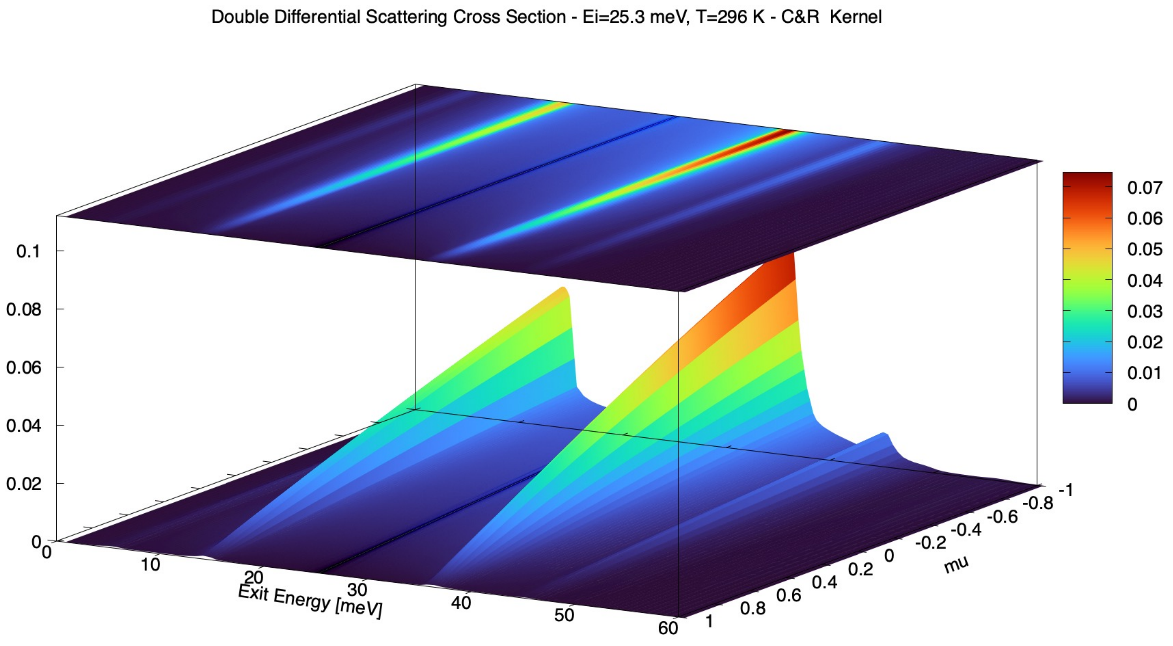
- Full double differential
  - Computationally expensive
- Coherent elastic contribution from thermal neutron scattering not accounted for
- Single-level Breit Wigner, s-wave resonances only

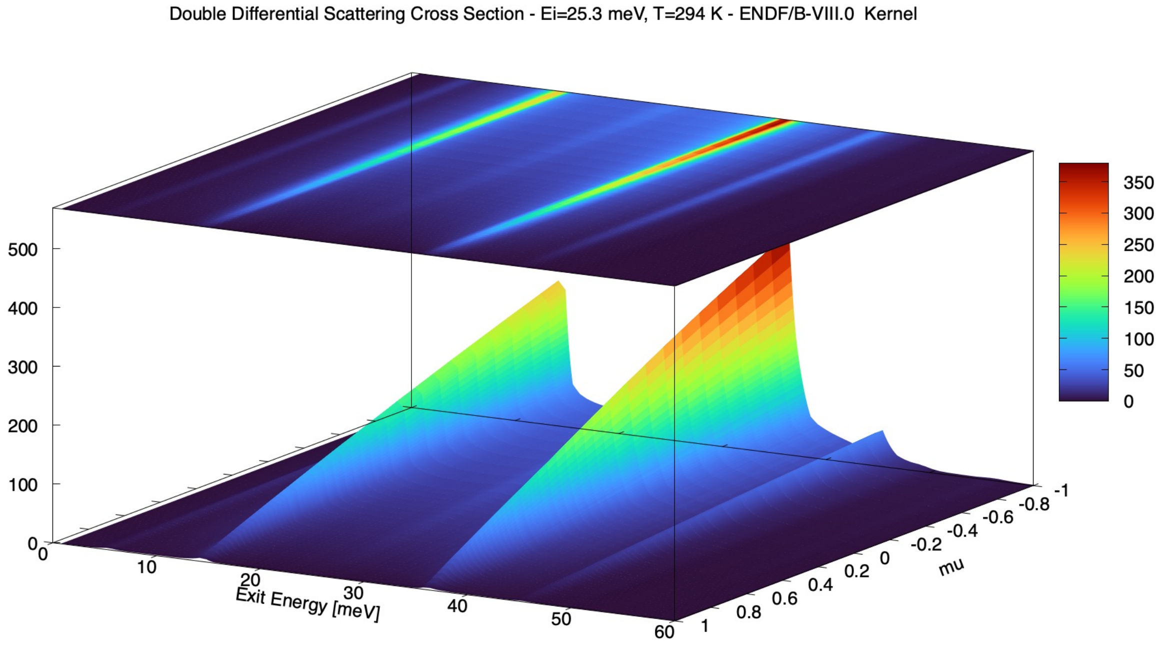
Preliminary Results: UO_2 – C&R vs. Free Gas – 25.3 meV





Preliminary Results: UO_2 – C&R vs. ENDF8.1β2 – 25.3 meV





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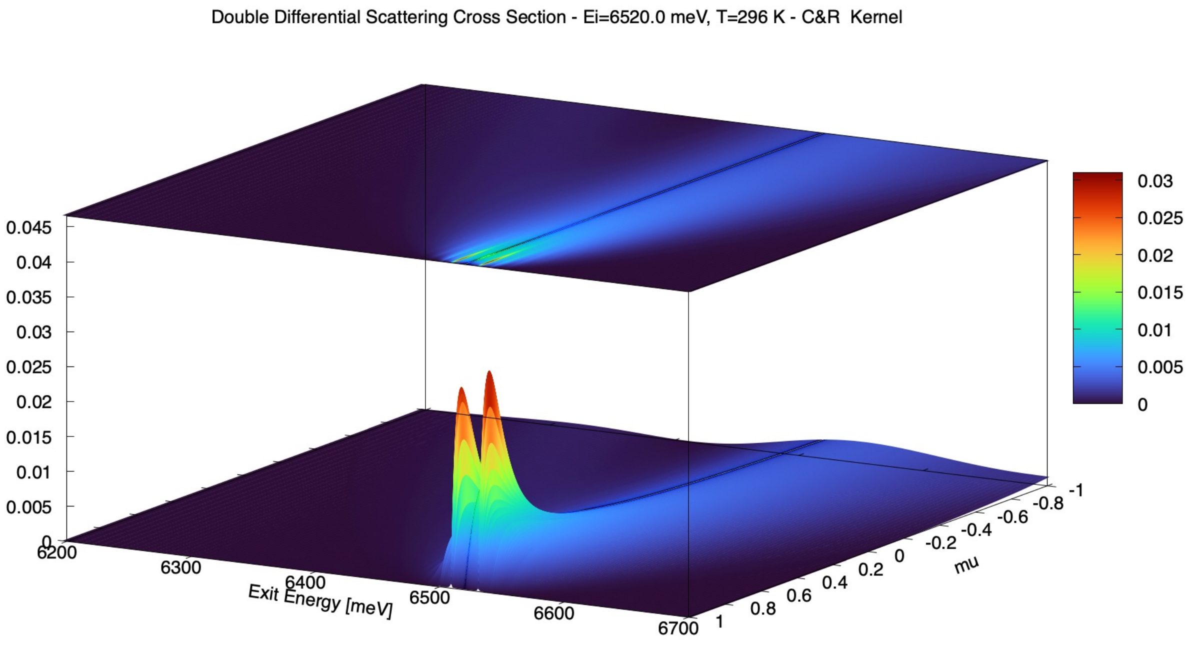
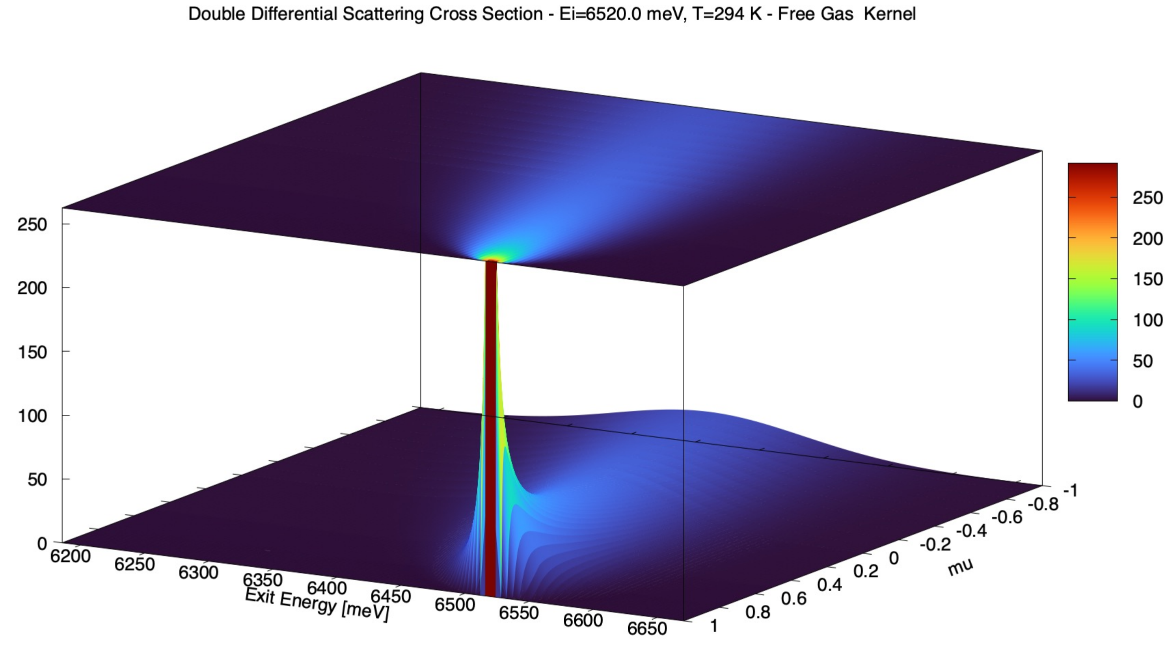
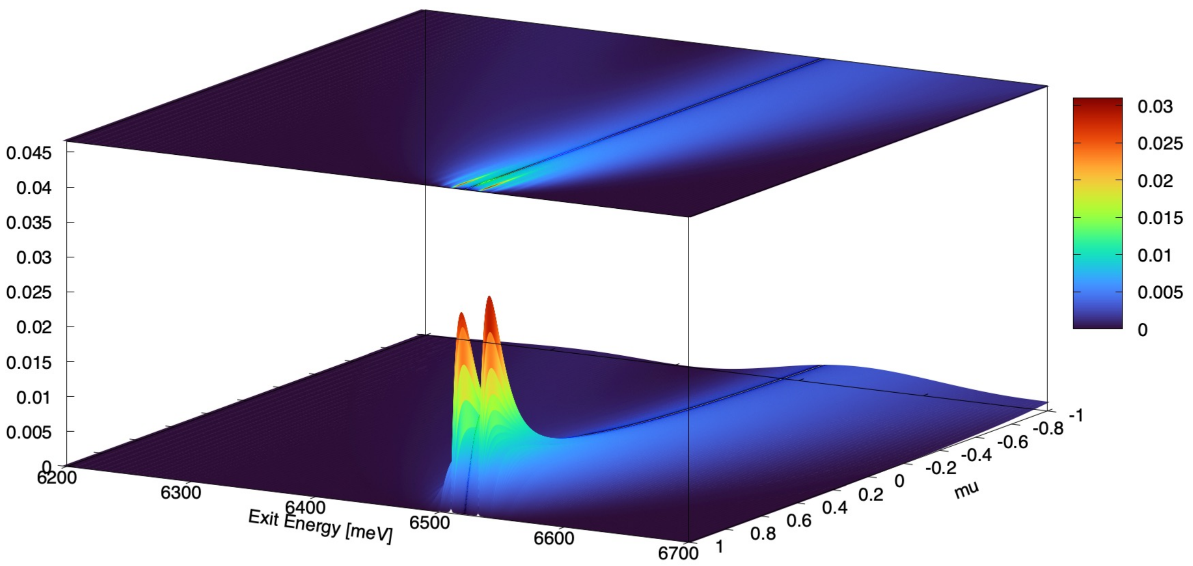
Preliminary Results: UO_2 – C&R vs. Free Gas – 6.52 eV



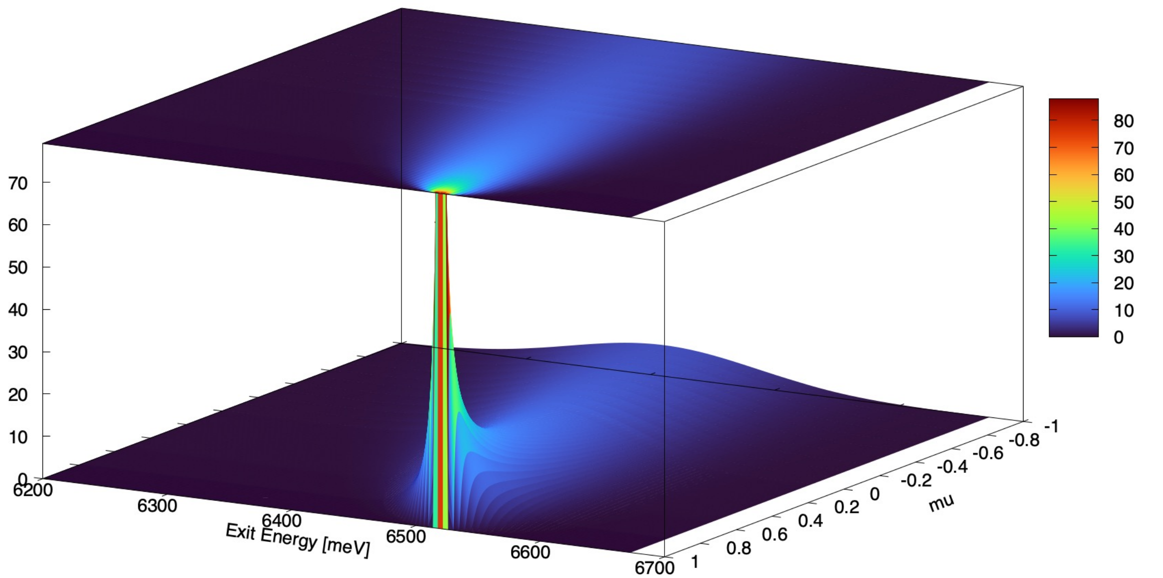


Preliminary Results: UO_2 – C&R vs. ENDF8.1β2 – 6.52 eV

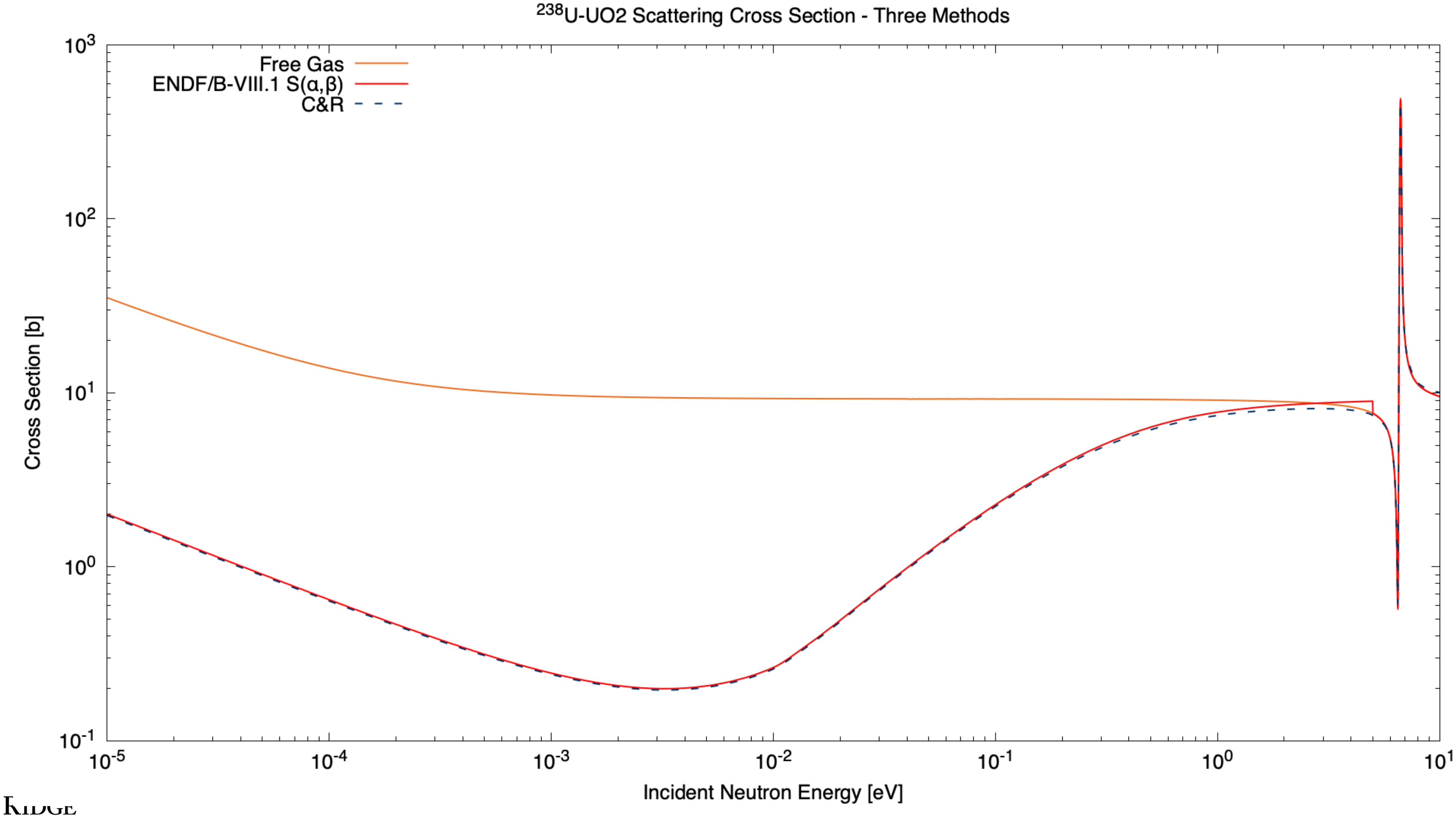
Double Differential Scattering Cross Section - Ei=6520.0 meV, T=296 K - C&R Kernel



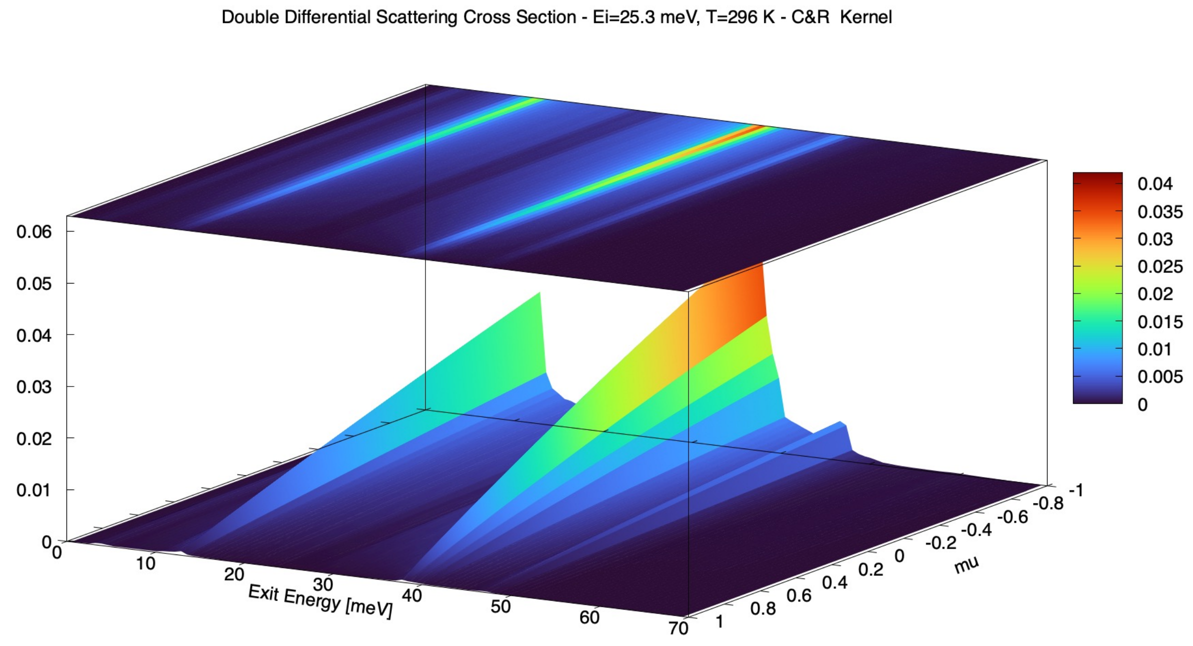
Double Differential Scattering Cross Section - Ei=6520.0 meV, T=294 K - ENDF/B-VIII.0 Kernel

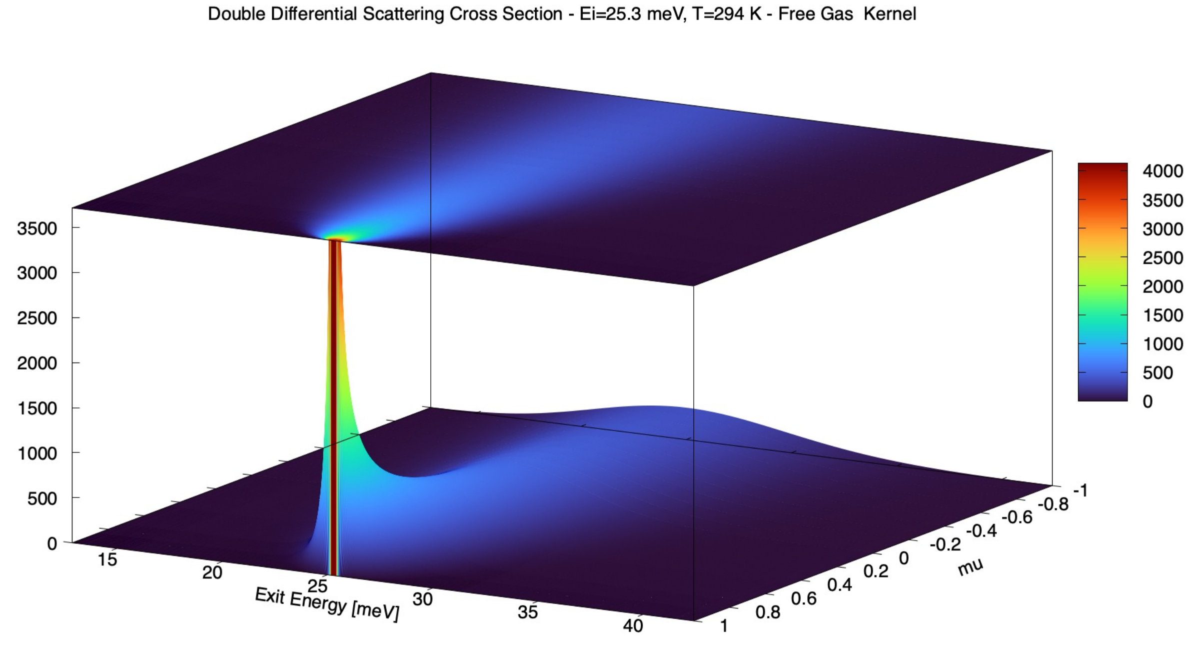


Preliminary Results: UO_2 –Cross Section



Preliminary Results: PuO_2 – C&R vs. Free Gas – 25.3 meV





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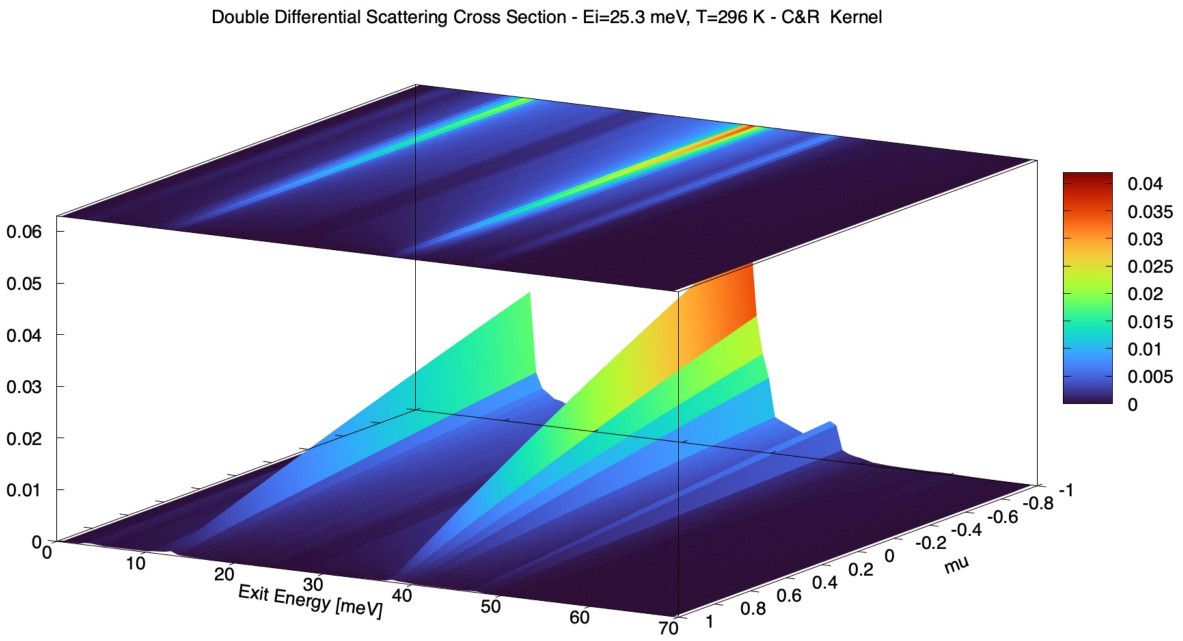
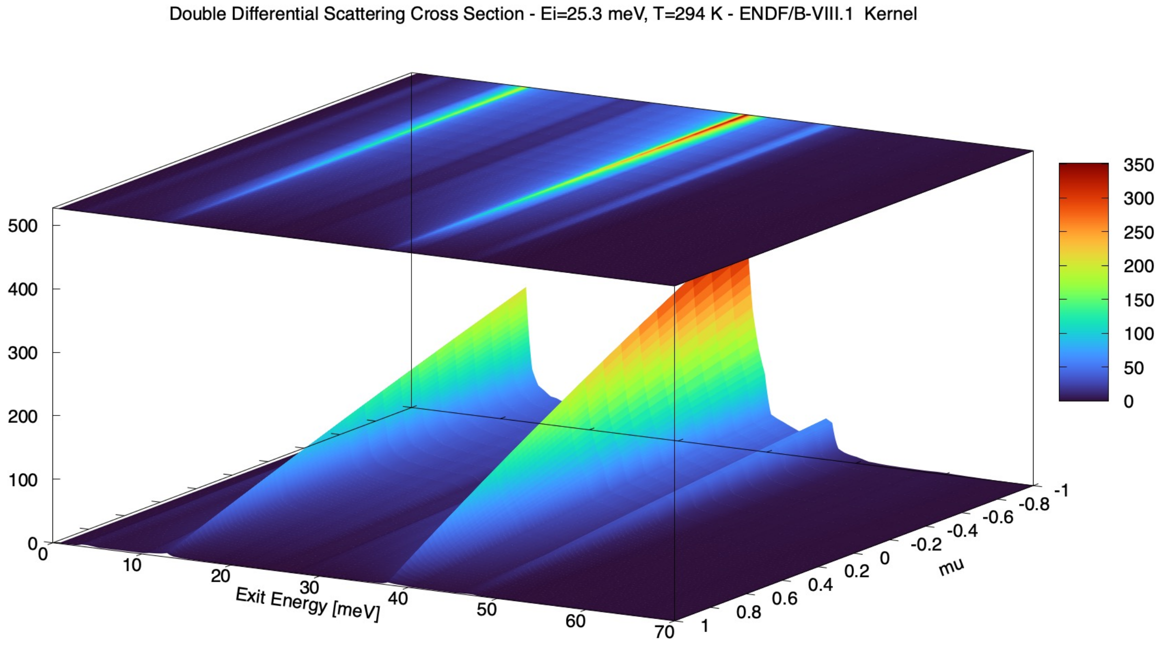
Preliminary Results: PuO_2 – C&R vs. ENDF8.1β2 – 25.3 meV





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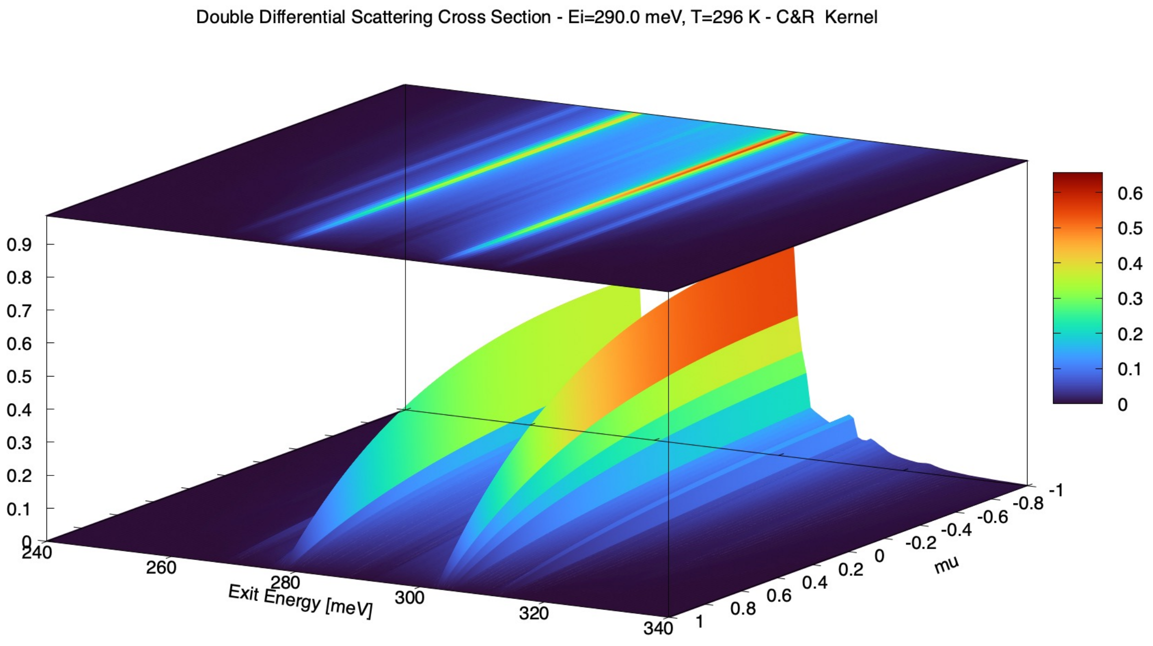
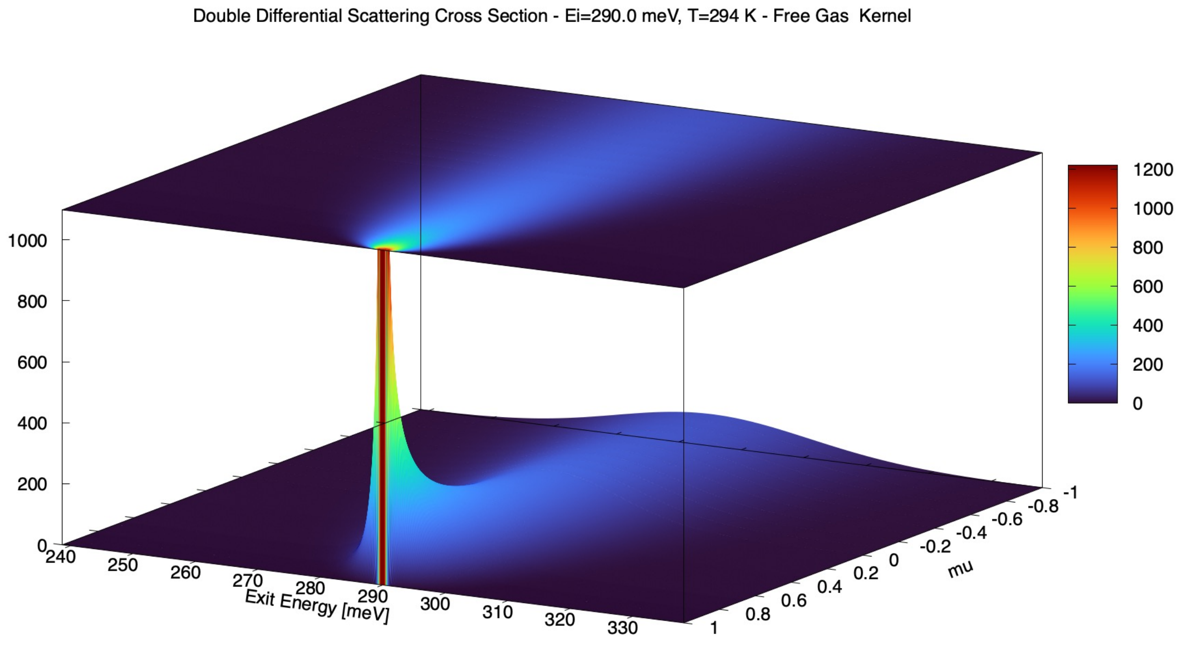
Preliminary Results: PuO_2 – C&R vs. Free Gas – 290 meV





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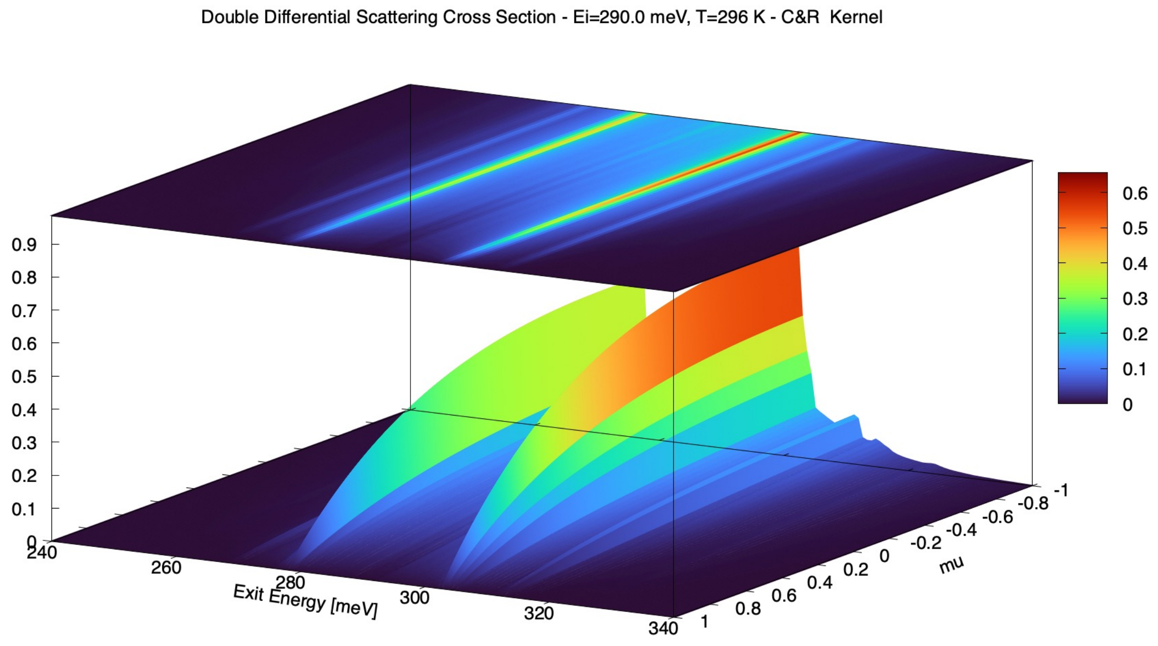
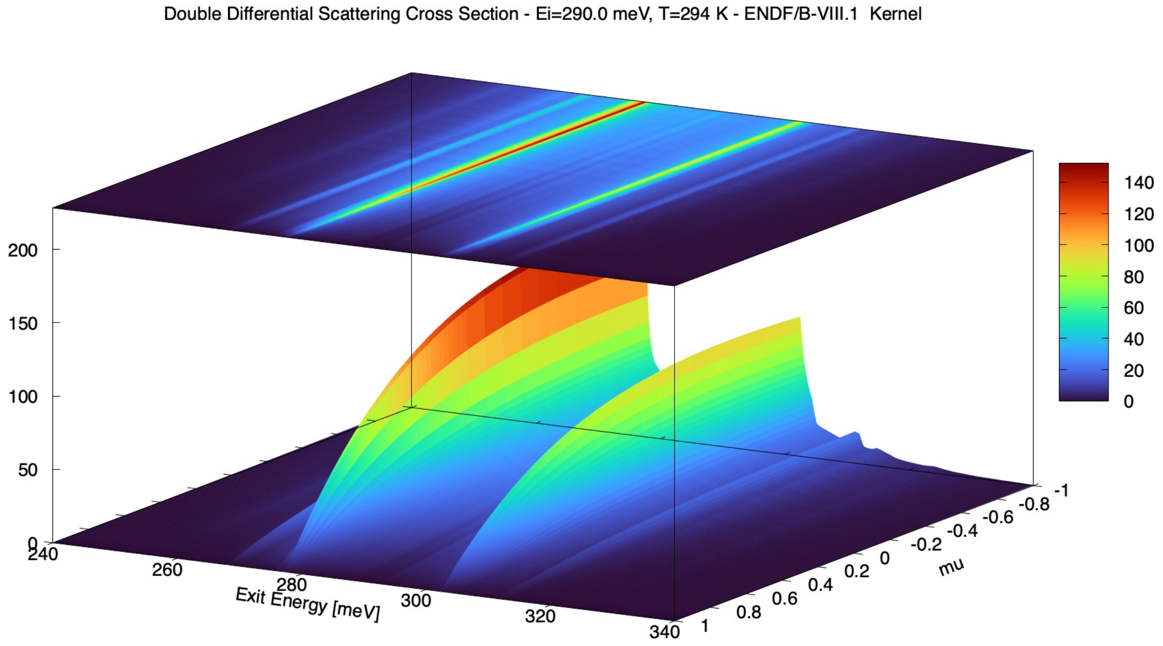
Preliminary Results: PuO_2 – C&R vs. ENDF8.1β2 – 290 meV





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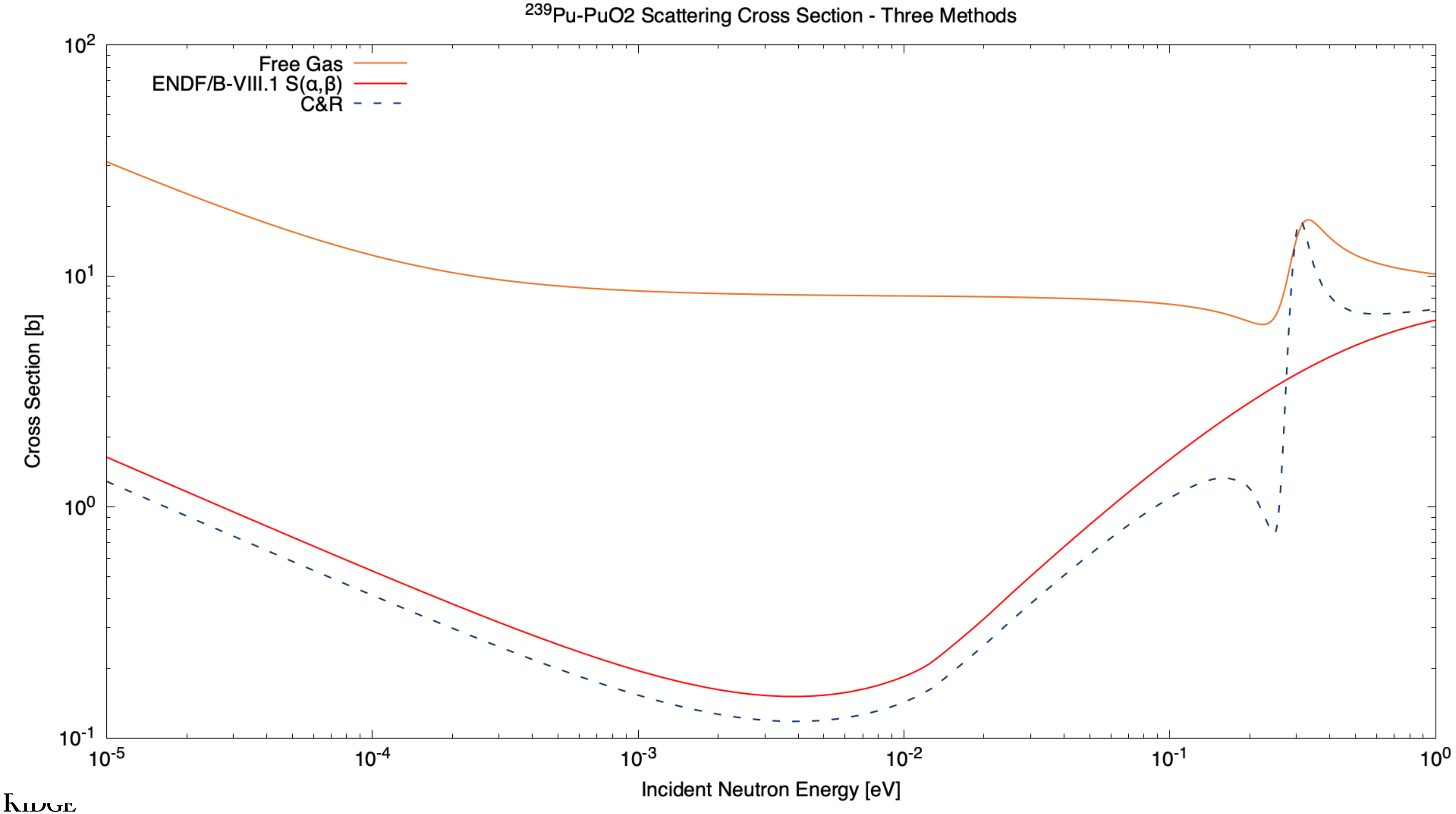
Preliminary Results: PuO_2 – Total Cross Section



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Conclusions

- C&R methodology implemented in Python script
- Differences in epithermal region (UO_2) found to be:
  - Significant compared to free gas
  - Minor compared to TSL
- Differences in thermal region (PuO_2) found to be significant compared to both free gas and TSL

Future Works

- Investigate approximations made within C&R formalism
  - Can single level Breit-Wigner approximation be extended to multi-level? Or full R-matrix?
  - Confirm it works on non-cubic crystals
- Elastic contribution
  - Elastic contribution from resonances included, not from TSL
  - Trammel [6] laid out the underlying framework for accounting for the contribution, but was not included in C&R formalism

Future Works (cont.)

- Temperature effects
  - Ouisloumen [7] suggested that free gas is an appropriate approximation at high temperature / resonance energy
  - Needs to be investigated
- Attempt experimental validation of model
  - Not possible to get high-resolution double differential measurements of U-238 or Pu-239
  - Other isotopes have thermal resonances (e.g., Er-167 or Eu-151) that might be measurable (i.e., not insurmountably large capture cross section)

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Questions?

Extra Slides

Math Bits

- Full DDXS equation

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{2\pi\hbar}\frac{k_f}{k_o} g\left(\frac{\Gamma_n}{2\hbar k_o}\right)^2 \sum_{i,i'} \int_{-\infty}^{\infty} dT \exp\left(-\frac{iET}{\hbar}\right) \int_0^{\infty} dt \exp\left(\frac{i\Delta Et}{\hbar}\right) \int_0^{\infty} dt' \exp\left(\frac{i\Delta E^* t'}{\hbar}\right)$$

$$\left\langle \exp\left[-i\overrightarrow{k_o} \cdot \overrightarrow{r_{i'}}(T)\right] \exp\left[i\overrightarrow{k_f} \cdot \overrightarrow{r_{i'}}(T+t')\right] \exp\left[-i\overrightarrow{k_f} \cdot \overrightarrow{r_i}(t)\right] \exp\left[i\overrightarrow{k_o} \cdot \overrightarrow{r_{i'}}(0)\right] \right\rangle$$

- Equation implemented

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{4\pi}\frac{k_f}{k_i} S(q,E)\left[\sigma_p + \sigma_m \frac{\Gamma_n}{\Gamma}\psi + \sqrt{\sigma_p \sigma_m \frac{\Gamma_n}{\Gamma}}\chi\right]$$