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Title: Thermal Neutron Scattering Improvements and Fixes for MCNP6.3

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Thermal Neutron Scattering Improvements and Fixes for MCNP6.3

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Thermal Neutron Scattering Laws in MCNP6.3

Outline

- Major error (10,000+ pcm) discovered when using uranium-dioxide or uranium-nitride included in ENDF80SaB2 release.
  - Presented at 2021 NCSP TPR, LA-UR-21-21189
  - Fixed for MCNP6.3, but cannot go back and fix previous versions
  - Not covering this issue today as it has been discussed previously
- Improvement towards preparing the code for ENDF/B-VIII.1 (ACE) format updates (more info in LA-UR-21-30355).
- Minor error (0-10's pcm) discovered while working on new capability development for Lab Directed Research & Development (LDRD) project.

Improvement towards preparing the code for ENDF/B-VIII.1 (ACE) format updates.

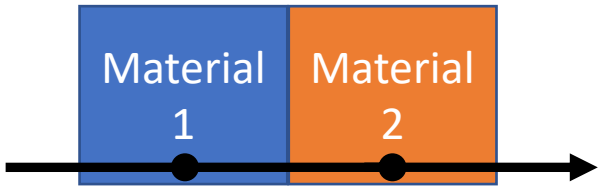
- Previously, only a single coherent or incoherent elastic channel (along with an inelastic channel) was allowed in a thermal neutron scattering evaluation and subsequent processed ACE file.

- Based on what is planned in ENDF/B-VIII.1 release, there will be (a) new thermal scattering evaluation(s) which uses this mixed-mode coherent and incoherent elastic scattering blocks.

- MCNP6.3 has been modified to be able to handle such data in the future. Some reorganization in the cross section calculation (`acetot`, `sabcol`, `colidn`) in the presence of TSL data.

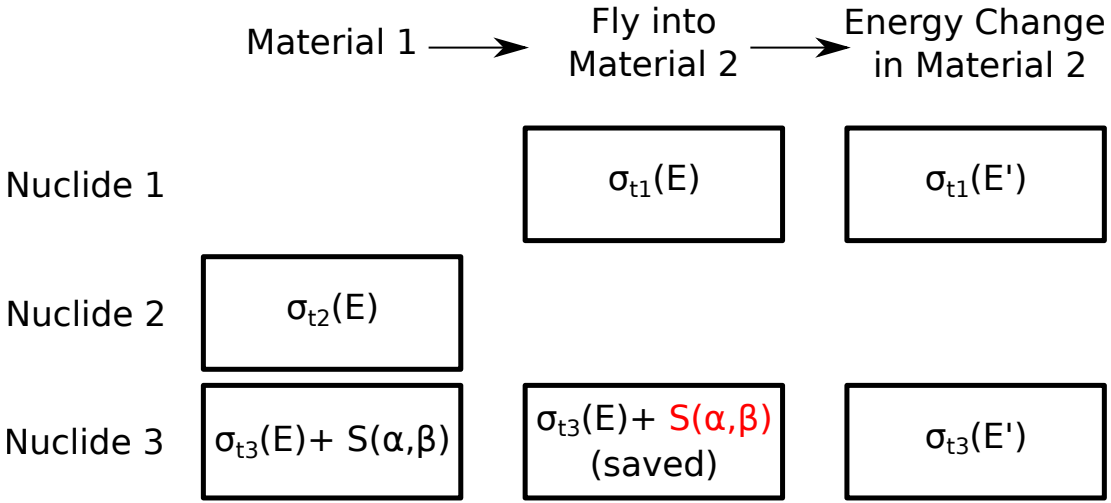
Minor Thermal Neutron Scattering Bug Fix in MCNP6.3

- Minor error (~0-10's pcm) discovered while working on new MCNP capability for LDRD project.
- Under rare circumstances this error may occur due to the MCNP total cross section calculation and caching algorithm.
- When a particle moves through a region, it needs to have the total cross section to do the free-flight distance-to-collision sampling done correctly
  - Upon entering a region (potentially) compute total cross section
  - Upon surviving a collision in a material, compute total cross section for particle at new energy



Minor Thermal Neutron Scattering Bug Fix in MCNP6.3

- The nuclide-specific total cross section (and other partial cross sections) are cached so that in the case that they are needed again at that energy, the cost of retrieving and calculating the cross section is not duplicated.



Material 1 has S(α,β), Material 2 Doesn't

Minor Thermal Neutron Scattering Bug Fix in MCNP6.3

- The problem:
  - The TSL component of the total cross section is simply added to the nuclide-specific total cross section saved in cache and there was no flag indicating if this had been done. Only a change in particle energy would lead to recomputing the cross section.
  - The checking for valid cached cross sections is done per nuclide in the material.
  - Therefore,
    - If Material 1 includes Nuclide A **with** a TSL component, and
    - If the neighboring Material 2 includes Nuclide A **without** a TSL component,
    - Then MCNP6.2 (and all before it) do not invalidate this cache for this nuclide and the particle continues through Material 2 with the wrong cross section with TSL included.
- The impact: rarely seen in practice 1/119 crit_expanded V&V problems have this configuration, and the change in k-effective is hardly measurable (~3 $\pm$ 4 pcm).

Questions?

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