LA-UR-24-25512

Title: Implementation and Verification of Element-Wise Density and Temperature Specifications in MCNP6 Unstructured Mesh Simulations

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Intended for: American Nuclear Society (ANS) Annual Meeting, 2024-06-17/2024-06-20 (Las Vegas, Nevada, United States)

Issued: 2024-07-15 (rev.1)

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Implementation and Verification of Element-Wise Density and Temperature Specifications in MCNP6 Unstructured Mesh Simulations

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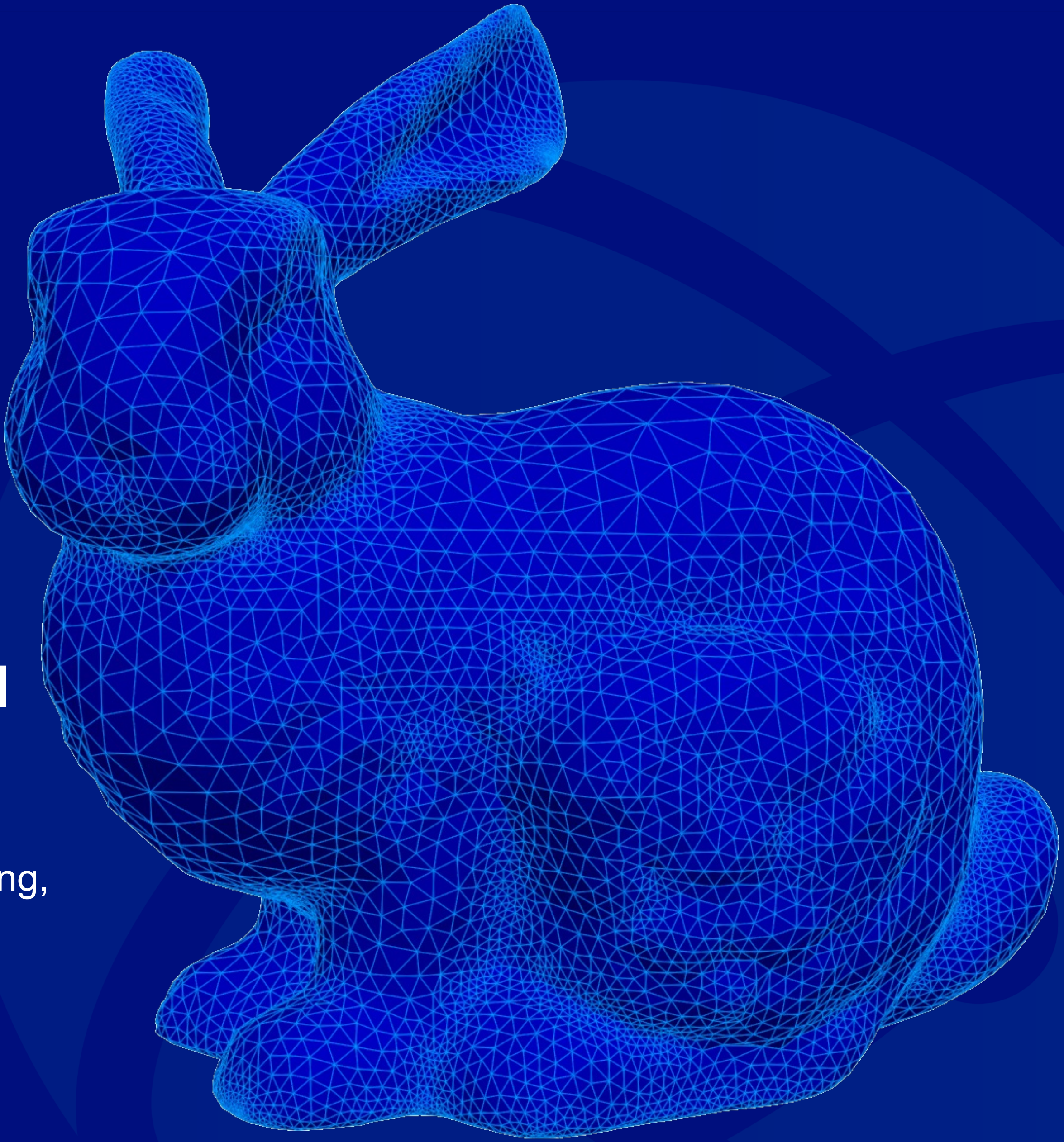
June 19, 2024



"The Stanford 3D Scanning Repository". graphics.stanford.edu. Retrieved June 2024.
Converted into an unstructured mesh.

Errors related to spatial resolution are often overlooked in nuclear simulations

- Even if the geometry is modeled with a high spatial resolution, material properties are often modeled at a much coarser spatial resolution and this error is sometimes neglected
  - This work is intended to reduce this error in MCNP simulations

The motivation for this work is to generate higher-fidelity multi-physics MCNP simulations

- The ability to specify element-wise material densities and temperatures in MCNP unstructured mesh simulations was recently added (and will supported in MCNP6.4)
  - “Element” refers to an individual tetrahedron, pentahedron or hexahedron in an unstructured mesh
  - MCNP users will no longer need to average densities and temperatures on a much coarser spatial resolution for multi-physics simulations

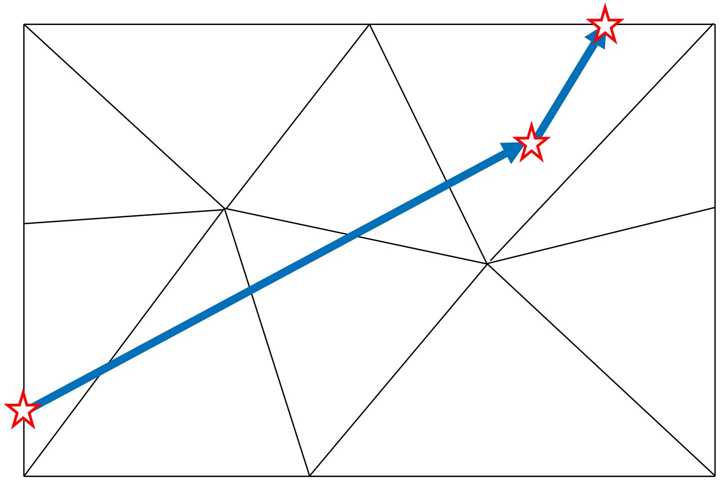
The MCNP UM HDF5 file was modified to include element-wise densities and temperatures

- The material group in the new MCNP UM HDF5 file must now contain the following attributes and datasets
  - **material_id**: a 1D dataset composed of a single integer
  - **density_by**: an ASCII string (either “element” or “pseudocell”)
  - **density**: a 1D dataset of non-negative real numbers
  - **temperature_by**: an ASCII string (either “element” or “pseudocell”)
  - **temperature**: a 1D dataset of non-negative real numbers

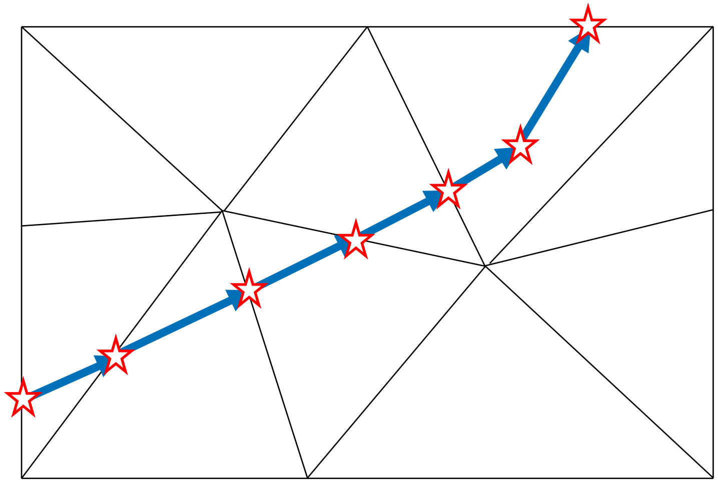
☆ *The MCNP UM HDF5 format in this presentation is more recent than the format described in the ANS summary and is likely the format that will be required in MCNP6.4*

If there are element-wise differences in material properties, particle tracking behavior is modified

If there **are no** element-wise differences



If there **are** element-wise differences



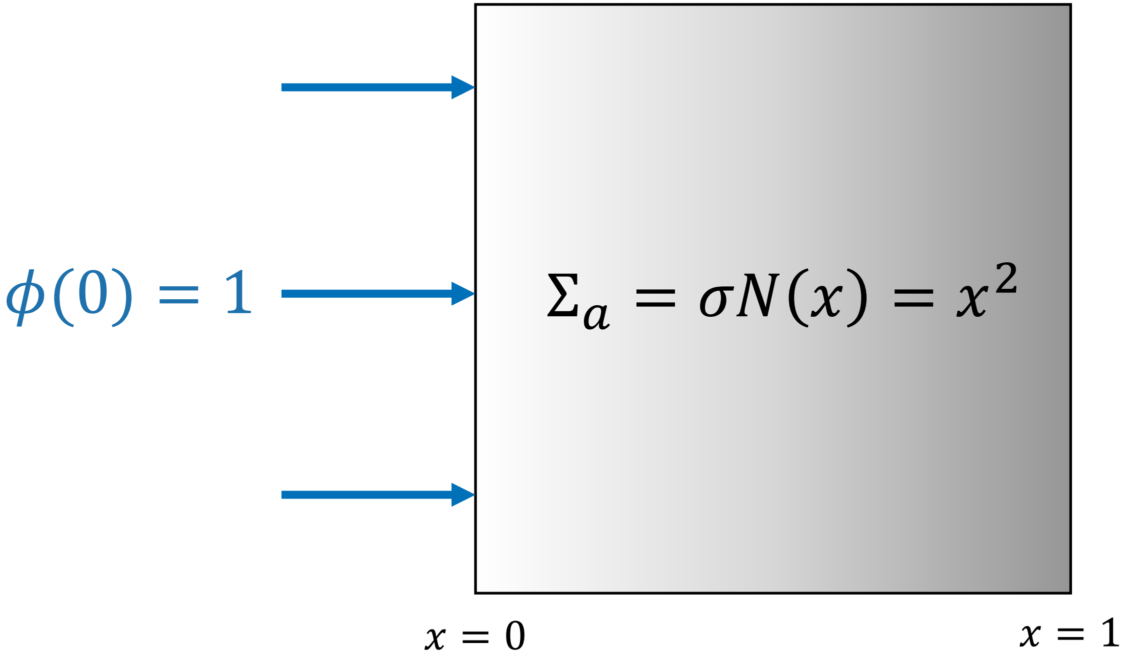
→ represents particle tracks

☆ represents material property look-ups & resampling of distance-to-collision

Element-wise material specification was verified using three test problems

- Implementation was verified using:
  - two analytical test problems
  - one code-to-code verification

Analytical test problem 1: A cube (1 cm^3) with density varying in the x-dimension



$\phi(0) = 1$

$\Sigma_a = \sigma N(x) = x^2$

$x = 0$

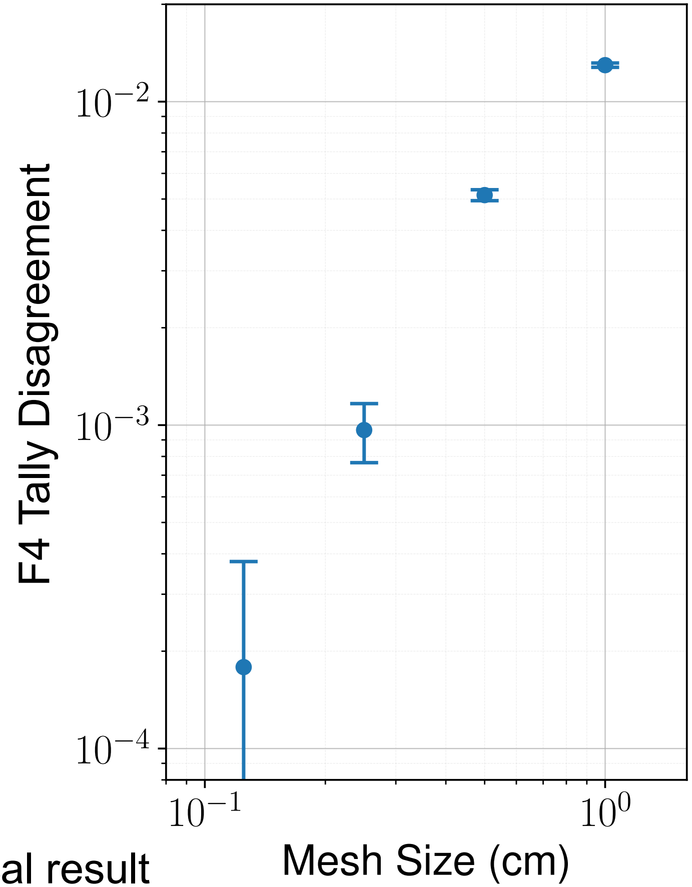
$x = 1$

Analytical result for volume-averaged flux (F4) for the cube:

$$\overline{\phi} = \int_0^1 dx \exp\left(- \int_0^x dx' \, \Sigma_a(x') \right) \approx 0.924023$$

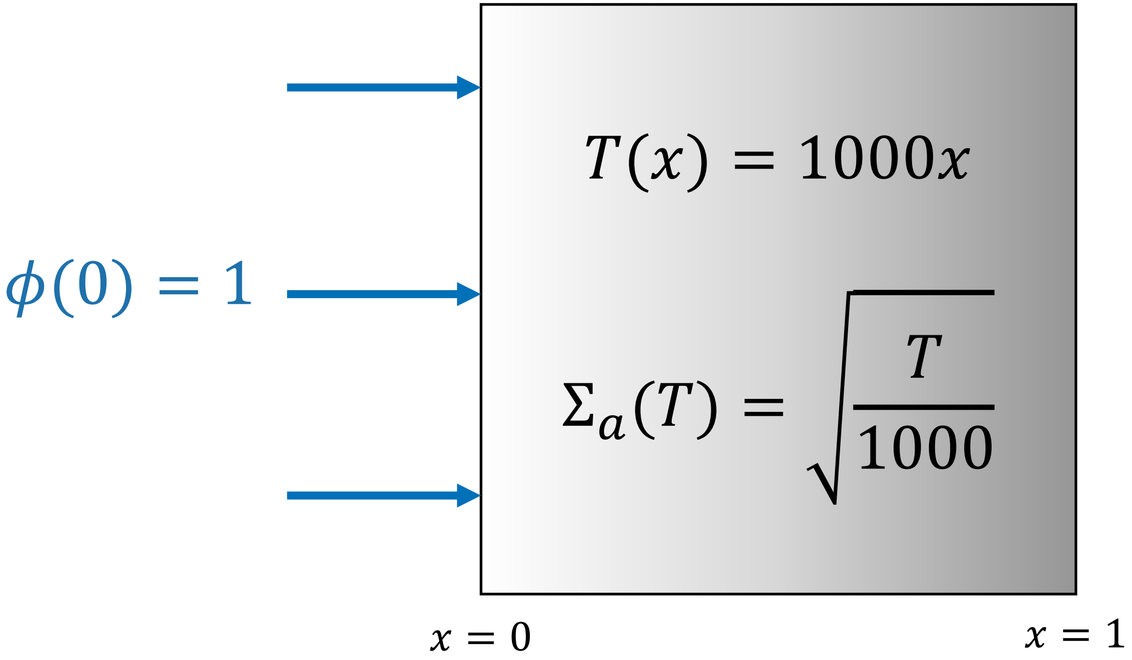
Analytical test problem 1 convergence study: simulation error as function of mesh resolution

Mesh Size (cm)	Number of Tetrahedra	Disagreement ± Noise
1	12	$1.3\times10^{-2} \pm 2\times10^{-4}$
0.5	49	$5.1\times10^{-3} \pm 2\times10^{-4}$
0.25	430	$9.7\times10^{-4} \pm 2\times10^{-4}$
0.125	4051	$1.8\times10^{-4} \pm 2\times10^{-4}$



- **Disagreement:** relative error between MCNP and analytical result
- **Noise:** one standard deviation of statistical uncertainty in MCNP

Analytical test problem 2: A cube (1 cm^3) with temperature varying in the x-dimension



$\phi(0) = 1$

$$T(x) = 1000x$$

$$\Sigma_a(T) = \sqrt{\frac{T}{1000}}$$

$x = 0$

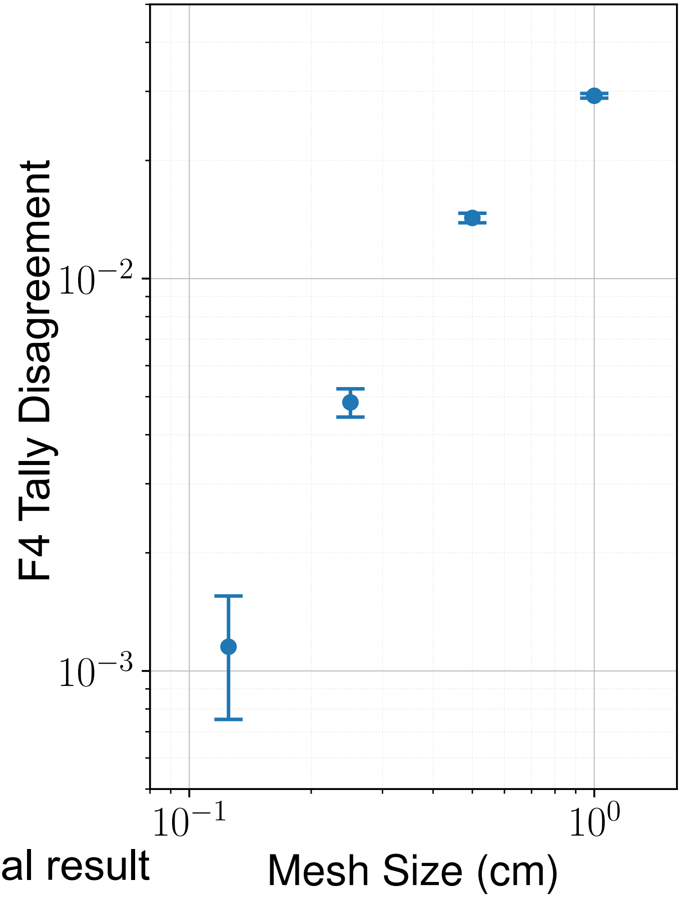
$x = 1$

Analytical result for volume-averaged flux (F4) for the cube:

$$\overline{\phi} = \int_0^1 dx \exp\left(-\int_0^x dx' \, \Sigma_a(x')\right) \approx 0.780968$$

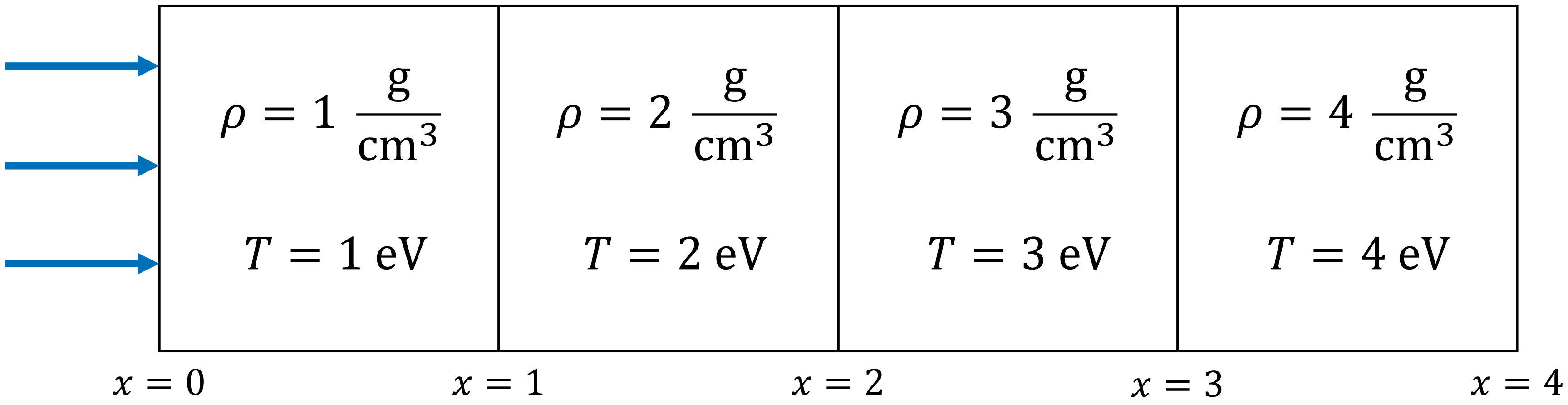
Analytical test problem 2 convergence study: simulation error as function of mesh resolution

Mesh Size (cm)	Number of Tetrahedra	Disagreement ± Noise
1	12	$2.9\times10^{-2} \pm 4\times10^{-4}$
0.5	49	$1.4\times10^{-2} \pm 4\times10^{-4}$
0.25	430	$4.8\times10^{-3} \pm 4\times10^{-4}$
0.125	4051	$1.2\times10^{-3} \pm 4\times10^{-4}$



- **Disagreement:** relative error between MCNP and analytical result
- **Noise:** one standard deviation of statistical uncertainty in MCNP

Code-to-code verification problem: UM implementation versus equivalent CSG



$\rho = 1\ \frac{\mathrm{g}}{\mathrm{cm}^3}$ $T = 1\ \mathrm{eV}$

$\rho = 2\ \frac{\mathrm{g}}{\mathrm{cm}^3}$ $T = 2\ \mathrm{eV}$

$\rho = 3\ \frac{\mathrm{g}}{\mathrm{cm}^3}$ $T = 3\ \mathrm{eV}$

$\rho = 4\ \frac{\mathrm{g}}{\mathrm{cm}^3}$ $T = 4\ \mathrm{eV}$

$x = 0$ $x = 1$ $x = 2$ $x = 3$ $x = 4$

- 26056.00c ACE file used as room-temperature cross-section data
- Four MCNP tallies are used:
  - F1: a surface current tally on the right boundary, x=4
  - F2: a surface flux tally on the right boundary, x=4
  - F4: a volume-averaged flux tally for all four cubes
  - F6: an energy deposition tally for all four cubes
- Only 1000 particle histories for each simulation

Code-to-code verification problem results: UM and CSG simulations were identical

Tally	Geometry	Mean ± One Standard Deviation
F1	CSG	$2.5867\times10^{-1} \pm 1.3839\times10^{-2}$
	UM	$2.5867\times10^{-1} \pm 1.3839\times10^{-2}$
F2	CSG	$2.5867\times10^{-1} \pm 1.3839\times10^{-2}$
	UM	$2.5867\times10^{-1} \pm 1.3839\times10^{-2}$
F4	CSG	$7.6052\times10^{-1} \pm 9.2023\times10^{-3}$
	UM	$7.6052\times10^{-1} \pm 9.2023\times10^{-3}$
F6	CSG	$5.6952\times10^{-7} \pm 9.9096\times10^{-9}$
	UM	$5.6952\times10^{-7} \pm 9.9096\times10^{-9}$

Implementation of element-wise material properties was also tested using the MCNP test suite

- The MCNP test suite verified that new feature is compatible with other existing code features
- A few new tests related to element-wise material properties were added to the test suite

Conclusions

- Element-wise density and temperature specification were successfully implemented in the MCNP code
  - In MCNP6.4, a user will be able to specify element-wise densities and temperatures in the MCNP UM HDF5 file
  - Two analytical verification problems demonstrated mesh convergence for MCNP simulations with element-wise densities and temperatures
  - A code-to-code comparison verified that MCNP particle-tracking and tallying are agnostic to the geometry system (CSG/UM)
  - The code implementation was also verified by the MCNP test suite

Future Work

- Investigating MCNP computational performance and memory use for simulations with element-wise densities and temperatures
- Testing element-wise densities and temperatures with more complicated geometries, including problems with mixed element types
- Extending the MCNP code's UM capability to also enable element-wise isotopic compositions

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