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Title: Oktavian Modeling with MCNP6.3

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Oktavian Modeling with MCNP6.3

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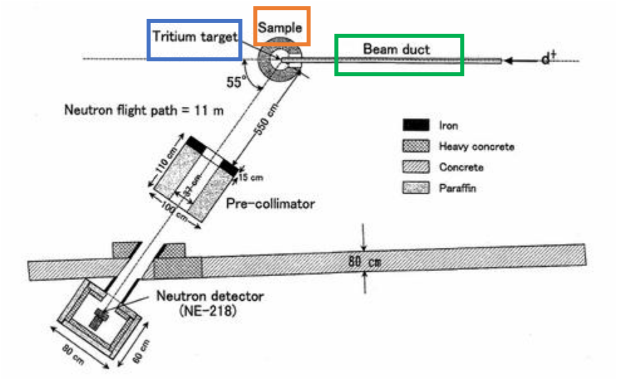
Outline

- Improvements on Oktavian Modeling with MCNP6.3
- Using Oktavian Models to Verify Unstructured Mesh Feature in MCNP 6.3

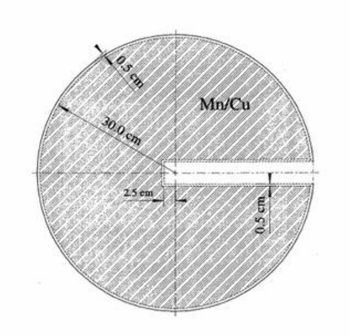
Improvements on Oktavian Modeling

Oktavian Benchmark Experiments

- MCNP5 was used for the design and analysis of the Oktavian experiments in the the Shielding Integral Benchmark Archive and Database (SINBAD). **MCNP5 input files were released with SINBAD**.
- Oktavian experiment setup:
  - A particle accelerator created a deuteron beam that impinged on a titanium – tritium target located at the center of the sample.
  - The spherically shaped samples have an aperture leading to the target at the center. The sample material was packed within a spherical steel shell.
  - The material and shape of the samples was varied in the different experimental trials.



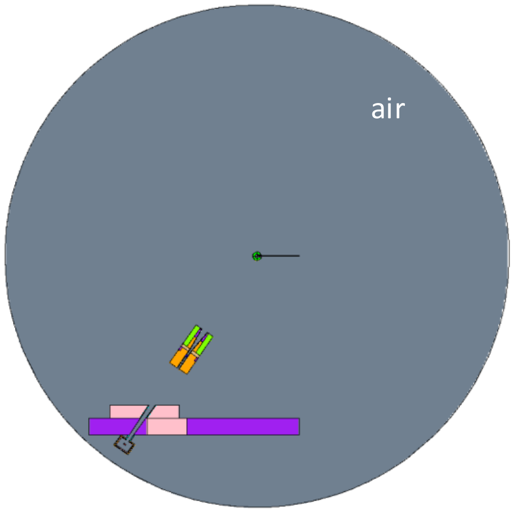
Oktavian experimental configuration [2]



Oktavian target [2]

SINBAD MCNP5 CSG Models

- The geometry models were defined using the constructive solid geometry (CSG) definition.
- Geometry models were large, with a small source and small detector.
- MODE N P E was used to transport neutrons, photons, and electrons.
- Cell importance was applied. However, the statistics results were still poor.



MCNP Geometry Plot

Improvements on Oktavian Modeling with MCNP6.3

- Used ENDF/B-VIII.0 nuclear data.
- Removed the DBCN card.
- Made simple geometry changes to divide the large cell of air.
  - Improvement on applying cell importance
- Added PRDMP to produce MCTAL files.
  - Use MCNPTools to post-process MCTAL files.
- Performed two calculation types:
  - Applied cell importance
  - Applied DXTRAN and weight windows

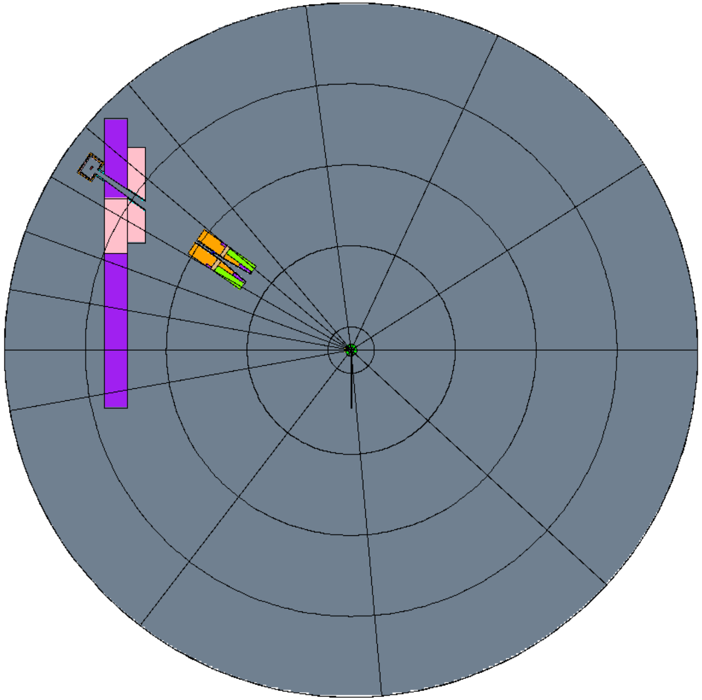
Advanced Variance Reduction Methods Applied to Improve statistics

- Good statistical results were not obtained when applying cell importance, so advanced techniques, DXTRAN and weight windows, were applied
- DXTRAN:
  - A sphere is placed at a region of interest and every collision or starting particle creates a DXTRAN particle, deterministically tracked to the sphere. Weights are adjusted based on mean free paths to the sphere.
  - Non-DXTRAN particles are tracked normally and killed upon attempting to enter the DXTRAN sphere on their next flight.
- Weight Windows:
  - Can be placed on cells or a user defined mesh.
  - Splitting particles above the window bounds and rouletting particles below the bounds, performing weight control.

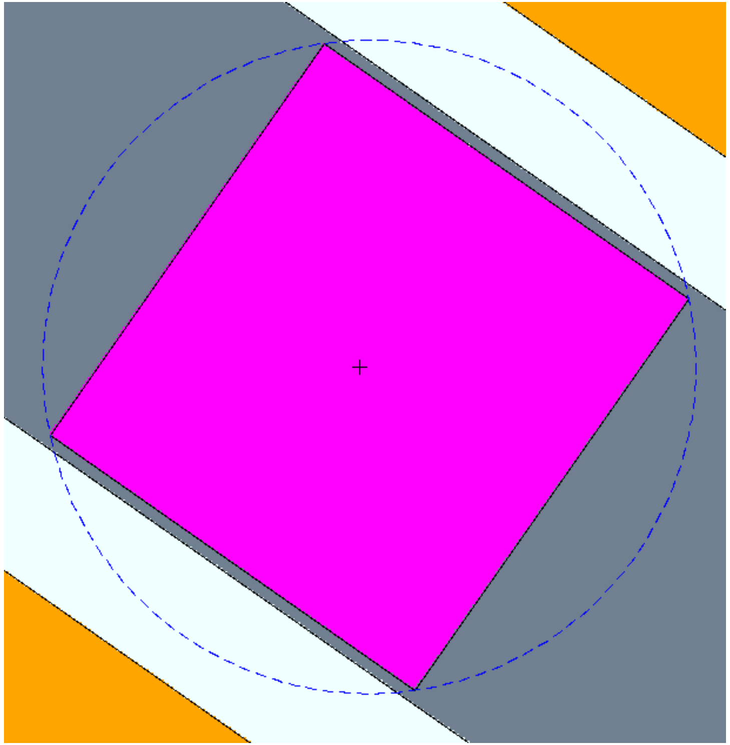
Weight window parameters produced by WWG cards

- To produce MCNP WWG cards:
  - A tally is selected to optimize weight window parameters, and the code stochastically determines which cells or weight window mesh locations are most important to the tally.
  - Lower weight window bounds generated (lower values => more important location)
  - The WWINP output file contains the generated weight window parameters.
- The values in the WWINP file are invoked using the WWP cards.
  - The WWP card is used for many options, including how to set the upper bound, where to check weight windows, and what particle to apply weight windows
  - The WWP card was applied to activate WWs for neutrons, photons, and electrons, **applied at collisions only**.

Variance Reduction Images



Weight Window Mesh



DXTRAN Sphere and Tally Cell

Benchmark Improvement Results

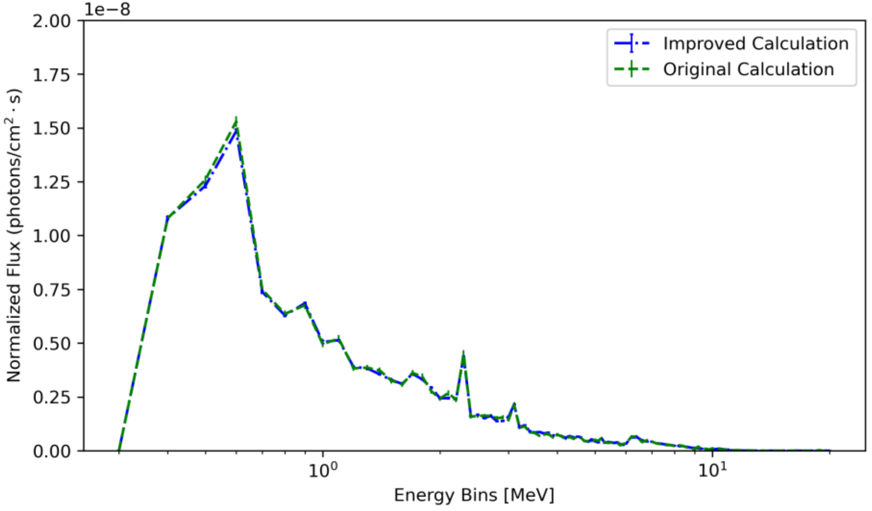
Comparing computational results of applying DXTRAN and weight windows against applying cell importance.

- Error reduced from 16 energy bins with zeros and 48 bins with relative error greater than 10% to 6 energy bins with error greater than 10%.

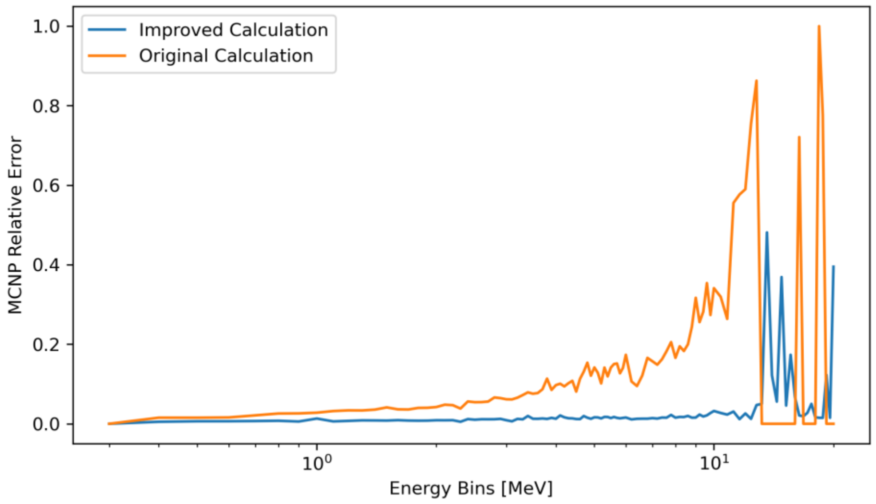
- The FOM, a measure of calculation efficiency, was increased by a factor of 8.4.

Benchmark Improvement Plots

NPS=2E9



CSG F4 Photon Tally Comparison



CSG MCNP Relative Error Comparison

Original Calculation = using cell importance
Improved Calculation = using DXTRAN & weight windows

Unstructured Mesh Verification

Uses of the MCNP Unstructured Mesh (UM) Feature

- In many cases, creating a CSG model for a complex problem can be difficult and very time consuming.

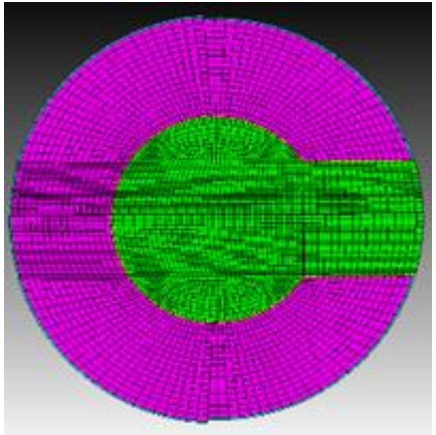
- The UM feature allows a CAD model to be meshed in a software such as CUBIT or Abaqus and used for particle transport in MCNP6, making geometry creation much easier.

- The UM feature also provides the potential for coupled multiphysics calculations
  - Track length estimates such as energy deposition can be performed by MCNP on each individual element and the results can be passed to a finite element analysis (FEA) software such as Abaqus to perform heat transfer.

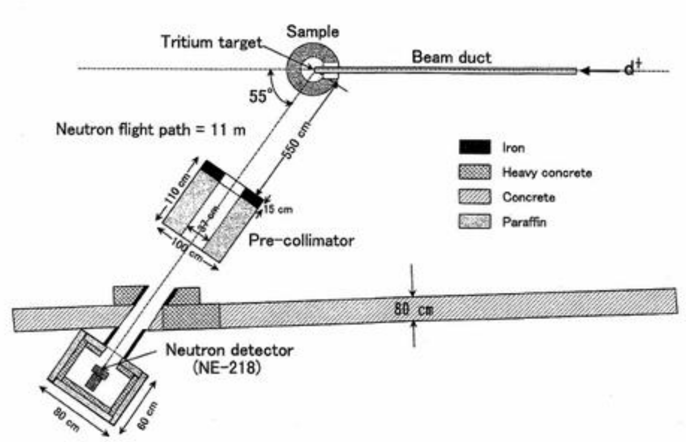
Previous Work to Current Work

- The previous work focused on a simple configuration with a surface tally (F1) placed directly outside the shield and using mode n p to analyze the mesh results in comparison to the CSG results.
  - Due to the simplicity, statistical results were valid, and no variance reduction was required.
  - Aluminum, silicon, molybdenum and copper Oktavian experiments were analyzed, each with slightly different geometry.
- Current efforts have moved to a more complex model including CSG geometry outside the shield with far away tallies and electron transport
  - Focus on aluminum Oktavian
  - Two simplified models with void geometry and a point detector far from the source
  - One complex model including all geometry and a cell tally.

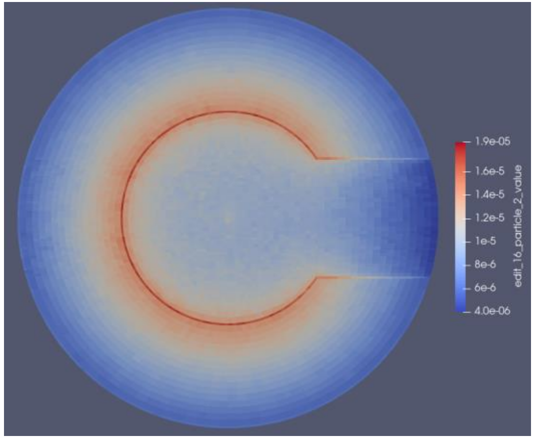
Oktavian UM Calculation



Oktavian Aluminum Hex Meshed Model Created in CUBIT



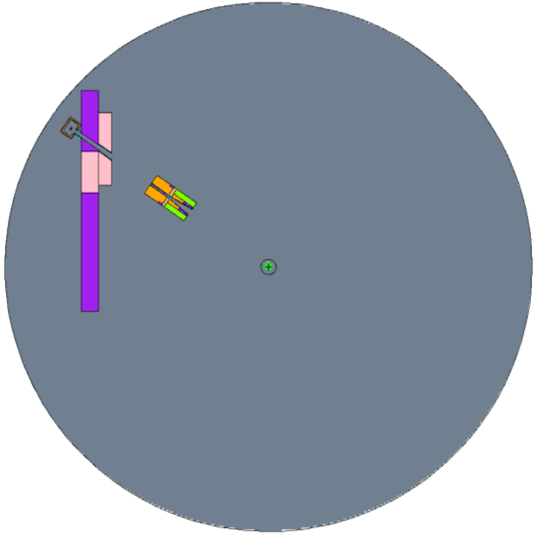
Oktavian Experimental Configuration [2]

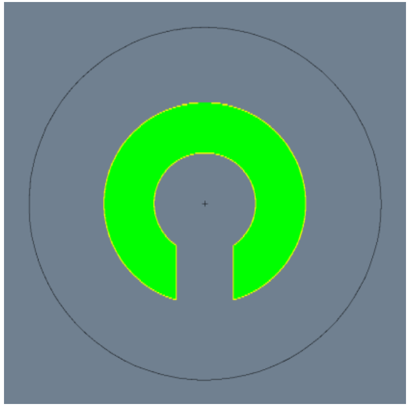


Photon Flux Elemental Edit Output Results From UM Simple Calculation.

UM Model Creation

- The aluminum UM model was embedded in a CSG description of the complex model including collimators and detectors.
- This is accomplished with the universe, fill, and embed cards in MCNP.
  - Pseudo cells are created for the UM geometry, denoted with the null surface, 0.
  - These pseudo cells are assigned a universe number and filled into a CSG cell to insert the UM geometry.
  - The embed card is used to match the pseudo cells to parts in the UM geometry file and designate the material for the background cell.
- For the UM calculation, the beam duct and target were not modelled.





Oktavian experiment geometry (top) with embedded UM (bottom).

Issues with Variance Reduction on UM Geometry

- When DXTRAN was applied to the UM geometry, particles were lost on the boundary of the outermost mesh pseudo cell and the background cell.
  - Only electrons were lost at this interface, and very few in a calculation with 2E9 histories.
  - The issue appeared to result when electrons were reflected by the background cell back into the UM, producing a photon and consequently a DXTRAN particle there.
  - To resolve this issue, the electron importance in the background cell was set to 0, killing particles and removing the potential of scattering back in.
  - This had only minor impacts on the tally results and allowed the calculation to succeed.
- Weight window parameters optimized for the CSG calculation with DXTRAN were ineffective when applied to the UM calculation with DXTRAN.
  - New iterations were performed with the UM model to create effective weight window parameters.

UM Results

- For both the CSG and UM geometry types, three different calculations with different variance reduction techniques were performed.
  - A calculation with only importance mapping.
  - A calculation with no importance changes, only DXTRAN.
  - A calculation with weight windows and DXTRAN, no cell importances.

- The calculation with weight windows and DXTRAN was the best, with the highest FOM and low error across the spectrum, only high above 10 MeV.

UM Results

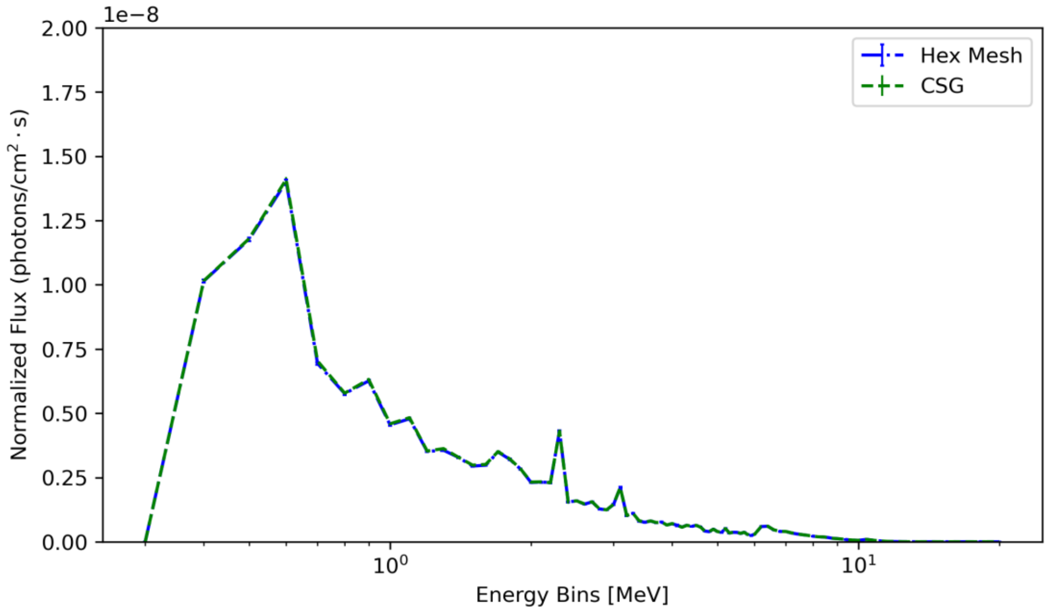
Table 1. Computer times in minutes for variance reduction and varying models.

	Cell Imp	DXTRAN	WW + DXTRAN
Hex	21264.93	26085.51	19341.09
CSG	5966.02	8835.57	4908.32

Table 2. Normalized photon flux (#/cm^2-s) and error for varying techniques and models

	Cell Imp ($\times 10^{-7}$)	DXTRAN ($\times 10^{-7}$)	WW + DXTRAN ($\times 10^{-7}$)
Hex	1.3325±0.0103	1.3455±0.0082	1.3515±0.0059
CSG	1.3382±0.0103	1.3470±0.0082	1.3586±0.0060

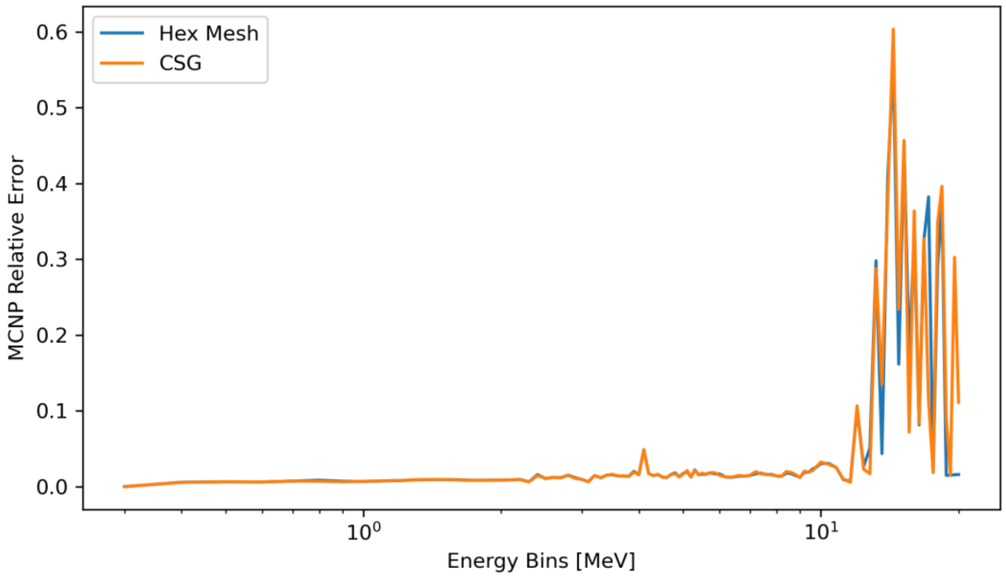
UM Results



UM and CSG Comparison, F4 Photon Tally

- Shows good agreement between the hex mesh and CSG calculations with DXTRAN & weight windows.
- A Kolmogorov Smirnov test, a measure of the closeness of two datasets resulted in a P-value of 1, indicating a close statistical relationship.

UM Results



UM and CSG Comparison, MCNP Relative Error

- Plot showing the comparison of the MCNP relative error for the UM and CSG calculations.
- Generally similar relative error across the spectrum.
- High relative error in the high energy bins due to low likelihood of particle creation at those energies.

Conclusion and Future Work

- Conclusions:
  - The results indicate that in the complex models analyzed, the UM feature performs well in approximating the CSG results.
  - Care should be exercised in using electron transport with the UM feature and DXTRAN.
  - Several of the MCNP5 benchmark input files were significantly improved and modernized for MCNP6.3
- Future work:
  - Can potentially apply other variance reduction techniques to attempt to reduce the relative error at high energies.
  - Further investigate the source of the lost particles.
  - Recreate the source subroutines Fortran file for the D-T source for MCNP6.3.

Question?

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