LA-UR-22-30541

Approved for public release; distribution is unlimited.

Title: Cubit for MCNP Unstructured Mesh Analysis of Oktavian Benchmarks

Author(s): Dzur, Micky Ray
Armstrong, Jerawan Chudoung
D'Angelo, Chelsea Ann

Intended for: 2022 MCNP User Symposium, 2022-10-17/2022-10-21 (Los Alamos, New Mexico, United States)

Issued: 2022-10-10

Los Alamos NATIONAL LABORATORY

Cubit for MCNP Unstructured Mesh Analysis of Oktavian Benchmarks

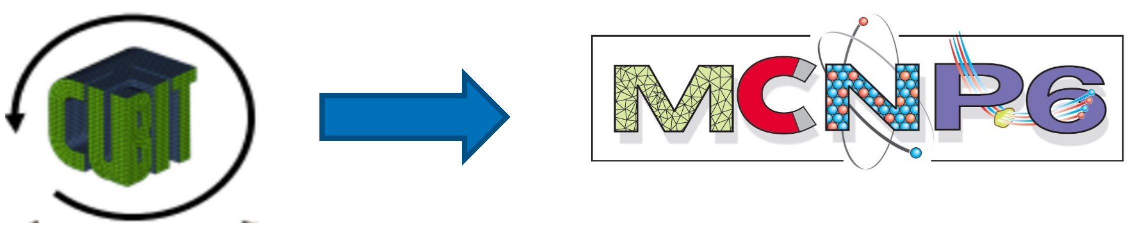
Micky Dzur
Jerawan Armstrong
Chelsea D' Angelo

2022 MCNP User Symposium
October 17-21, 2022

MCNP Unstructured Mesh (UM) Feature

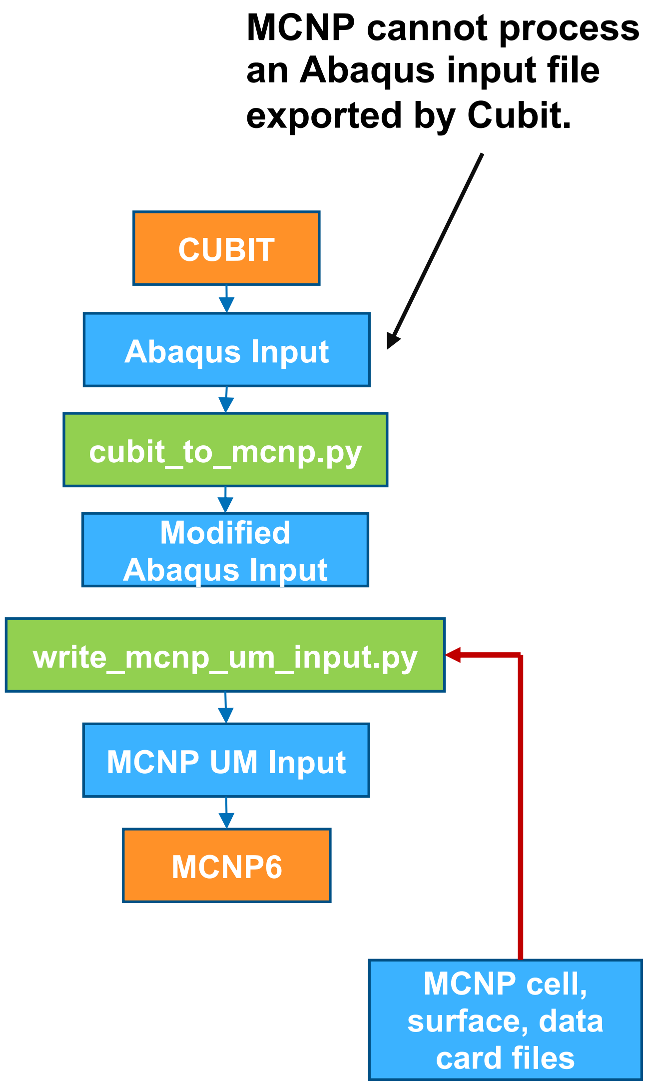
- The UM feature was implemented to allow the MCNP code to read in an Abaqus mesh geometry file created by an external software such as Abaqus or CUBIT.
  - Abaqus is a commercial finite element analysis (FEA) software suite.
  - CUBIT is a mesh generation software developed by Sandia National Laboratories.
- UM models are useful for defining complex geometries that would be otherwise very difficult or impossible to create using the constructive solid geometry (CSG) approach.
  - CSG models are constructed by using Boolean operations on defined surfaces to create 3D regions known as cells.
- The use of an MCNP UM feature allows for Multiphysics simulations such as coupling MCNP with Abaqus.
  - MCNP is used to perform neutronics analysis. Other FEA analysis such as heat transfer can be performed with Abaqus.

– We used CUBIT to create UM models in this work.



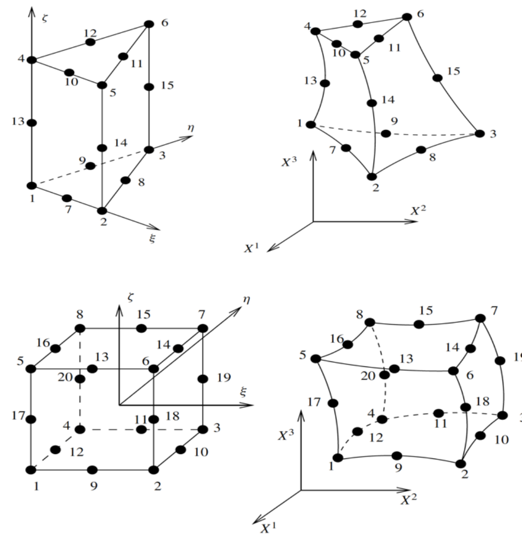
MCNP UM Process with CUBIT

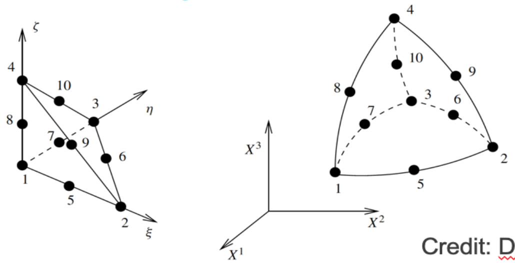
- Most CUBIT commands entered during a session are written into an ASCII file called a journal file that can later be edited and executed. A Python script, that leverages the CUBIT Python interface, was developed to generate an Abaqus-formatted mesh geometry by reading and executing a journal file.
- The Python script **CUBIT_TO_MCNP** is used to convert an Abaqus input file created by CUBIT to an Abaqus input file that MCNP can process.
- **WRITE_MCNP_UM_INPUT** is another Python script that uses the mesh information from the Abaqus file along with any user supplied data cards to write an MCNP UM input file.



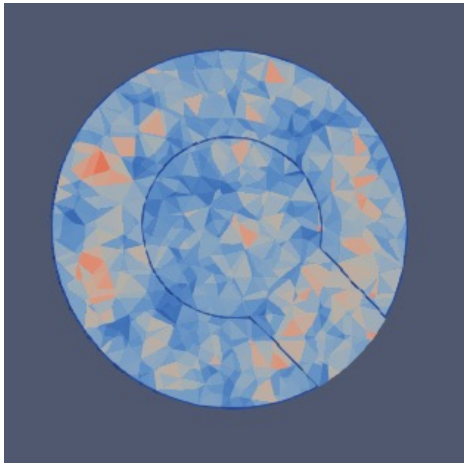
Element Types

- A computer program is used to decompose a solid geometry model into elementary pieces called finite elements or elements.
- A number and position of nodes in each element defines an element type:
  - tetrahedron (4 faces), pentahedron (5 faces), hexahedron (6 faces)
  - 1st order: vertex nodes only; 2nd order: vertex + edge nodes





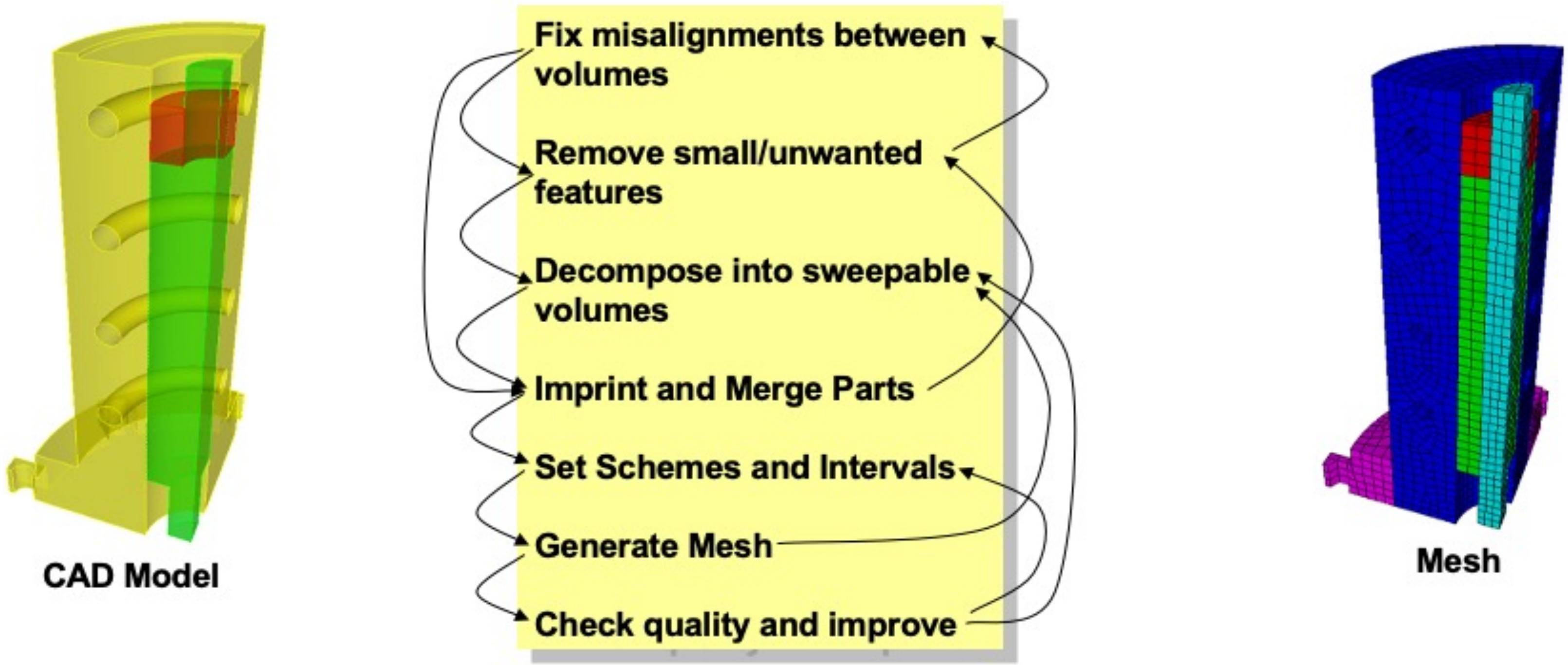
Credit: Dhondt, FEM for 3D Thermomechanical Applications, 2004



UM models with linear tet, hex, and/or mixed hex/pent elements are typically used in MCNP UM calculations.

Geometry Creation and Meshing

- The geometry creation and meshing process can be complicated.



The CAD to mesh process can be a complex series of iterative steps requiring in-depth understanding of the model and its flaws, expertise in using the software, and creativity to infer and apply solutions.

Credit: SNL Cubit100 Tutorial

Oktavian Benchmark Calculations

- The Oktavian experiments are contained in the SINBAD database.
- The Oktavian benchmark specifications can be found at the IAEA website: https://www-nds.iaea.org/fendl2/validation/benchmarks/jaerim94014/oktavian/n-leak
- Okatavian Benchmark calculations were performed for three nuclear data libraries using MCNP6 with CSG geometries [S. C. van der Marck, Benchmarking ENDF/B-VII.1, JENDL-4.0 and JEFF-3.1.1 with MCNP6, Nuclear Data Sheets 113 (2012) 2935-3005]
  - Four geometry types and eleven materials are used.
  - The results for the Oktavian benchmark calculations were compared with the experimental results and they were generally agreed.
  - Eleven MCNP CSG input files of Oktavian benchmark calculations were released with the MCNP source code [MCNP6/Testing/VERIFICATION_SHLD_SVDM]. The MCNP team does not have the experiment data shown in the Nuclear Data Sheets.

Oktavian Geometries & Materials

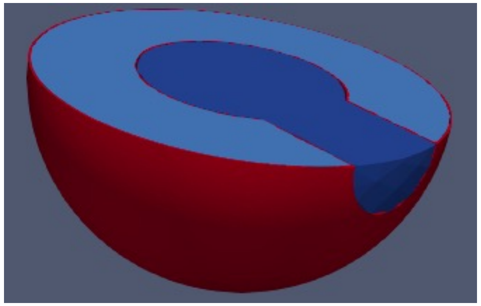
Four Geometries:

- aluminum, cobalt, chromium, titanium, tungsten
- cupper, lithium fluoride, manganese, zirconium
- Silicon
- molybdenum

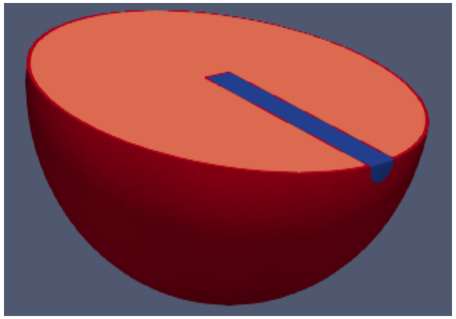
A 14 MeV D-T neutron source was in a center.

Measured Quantity:
The leakage current spectrum from the outer surface of a spherical pile of a material.

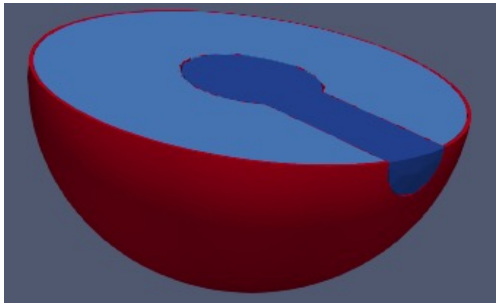
Al, Co, Cr, Ti, W



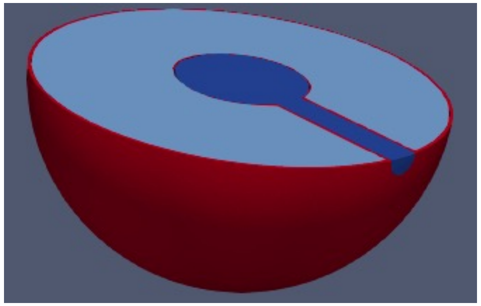
Cu, LiF, Mn, Zr



Si

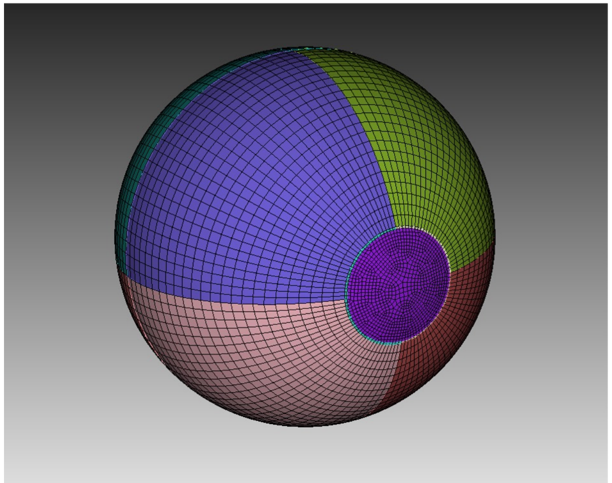


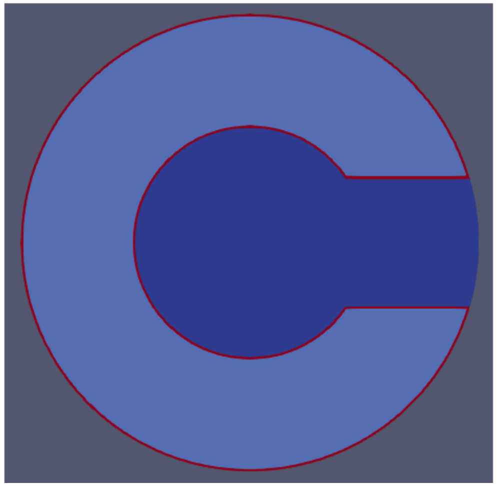
Mo



Linear Hexahedral (Hex) Meshing

- In general, hex meshing can be difficult, requiring a geometry to be split into simpler components in order to be meshed.
- CUBIT was used to create linear hex Oktavian models.
  - A model must be split into pieces that can be "swept" (i.e., a meshing algorithm that CUBIT employs).
- The meshing method used for the Oktavians was to cut a core out of the center using the cylindrical aperture as a guide so that the remaining spherical components could then be cut into eighths and the entire model then meshed.

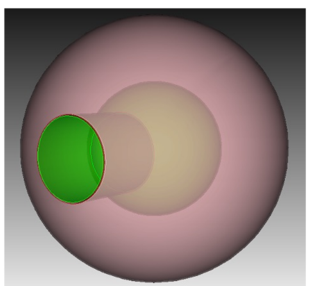




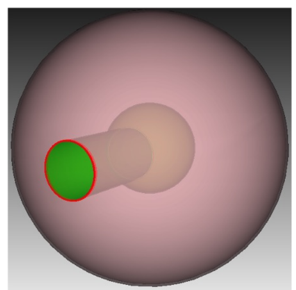
Oktavian geometry cross section, red borders are steel, interior dark blue is air and light blue ring composed of aluminum powder

Verify Linear Hex Oktavian Models

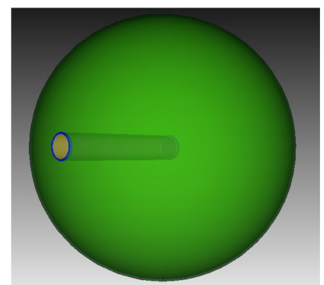
- Use CUBIT to mesh four linear tet and hex Oktavian models.
  - It is easier to mesh linear tet models, but these models are computationally more expensive.
- Run MCNP6.3 to compare the tally results from linear tet/hex and CSG models.



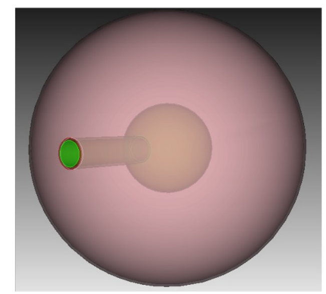
Aluminum



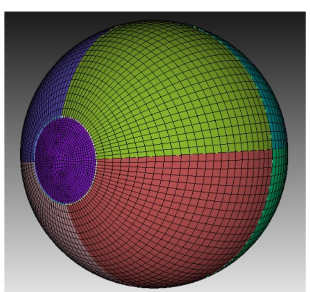
Silicon

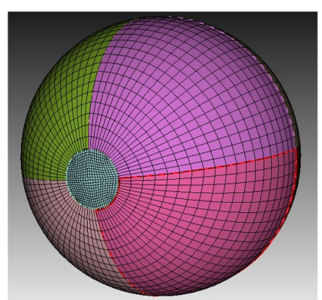


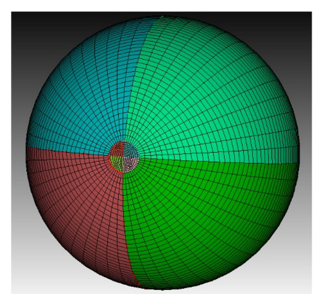
Copper

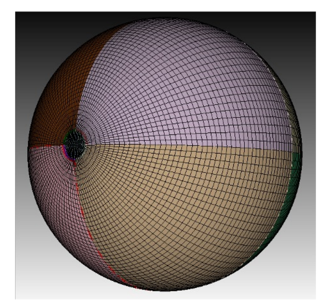


Molybdenum



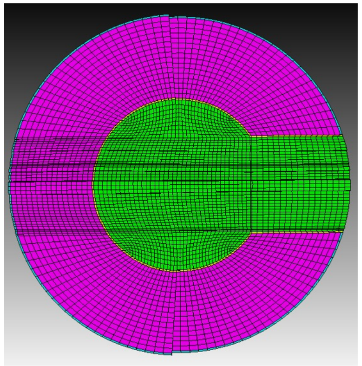


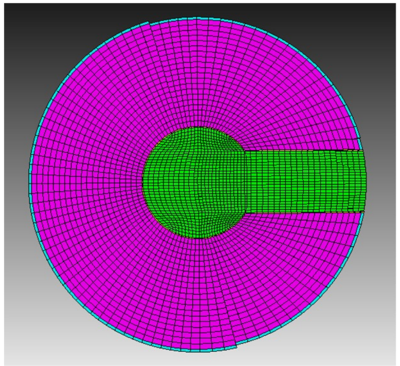


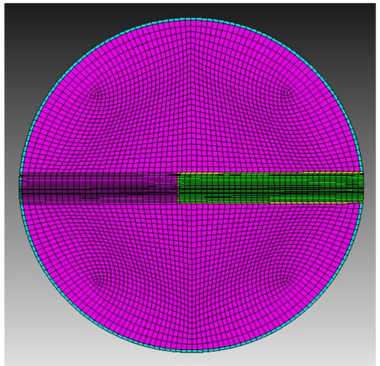


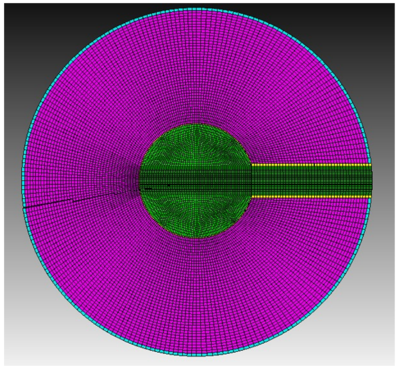
Oktavian UM Models

	Al	Si	Cu	Mo
Volume Difference (%)	0.13	0.21	0.27	0.07
Number of Elements	195848	111200	93788	702800
Average Quality	0.85	0.84	0.70	0.80


Aluminum


Silicon

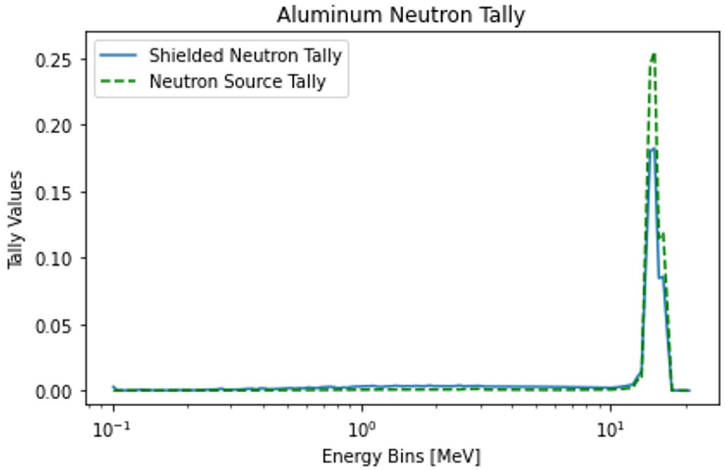

Copper


Molybdenum

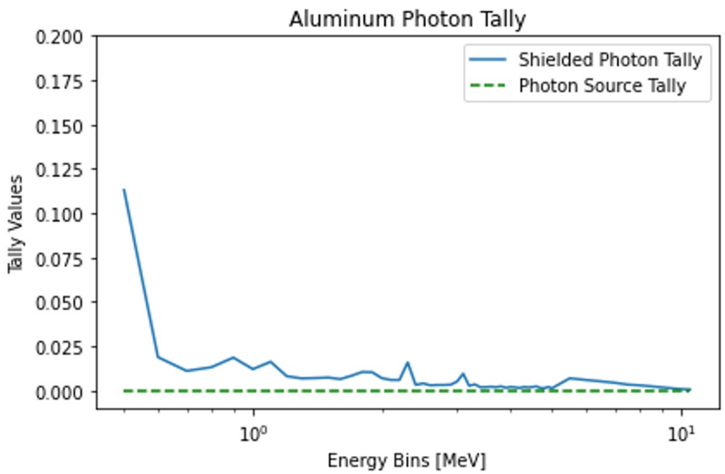
Los Alamos NATIONAL LABORATORY

Aluminum Oktavian Tally Results

Number of histories (NPS): 1E8



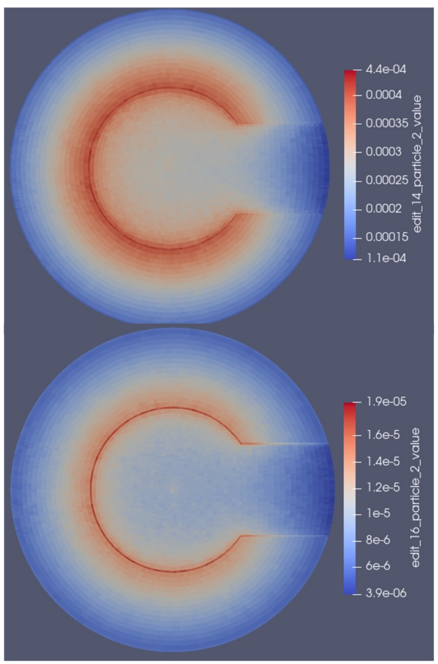
F1 neutron tally results compared to source neutrons. Tally on surface just outside the Oktavian.



F1 photon tally results. Photons generated from neutron inelastic scattering.

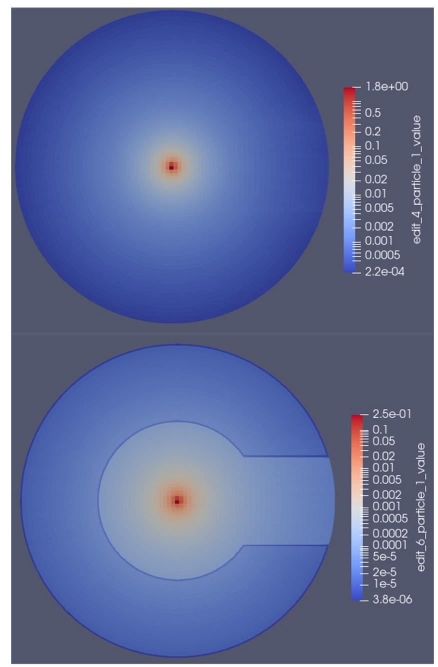
Aluminum Oktavian MCNP Results

- Mesh geometries allow the calculations of elemental edits on elements, functioning similarly to tally over cells.
- HDF5 elemental edit output (eeout) files created by MCNP 6.3 allow results to be viewed using a 3D visualization program such as ParaView.



Photon Flux

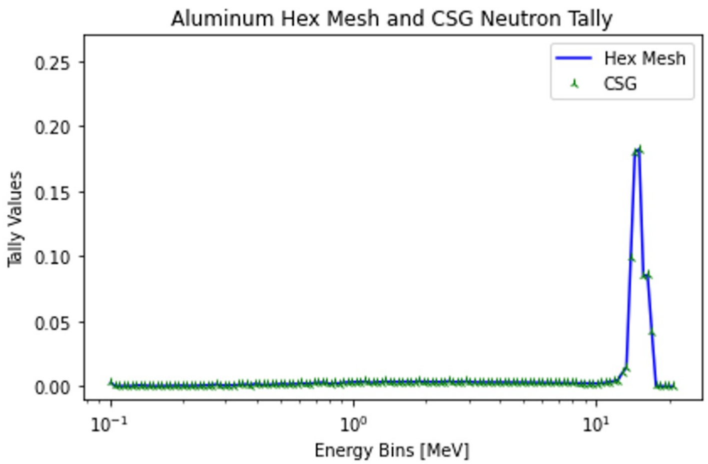
Photon Energy Deposition

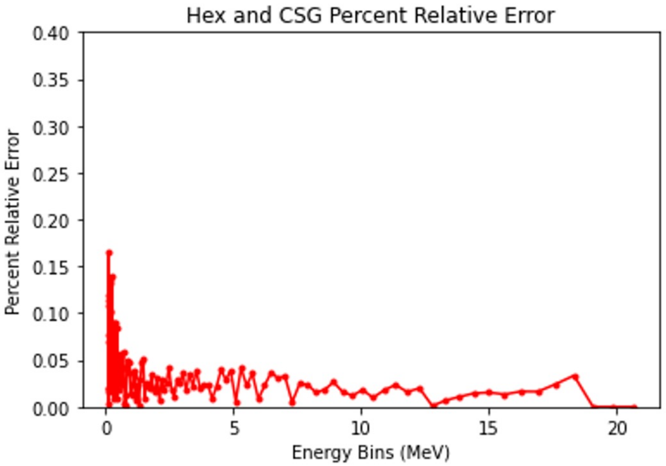


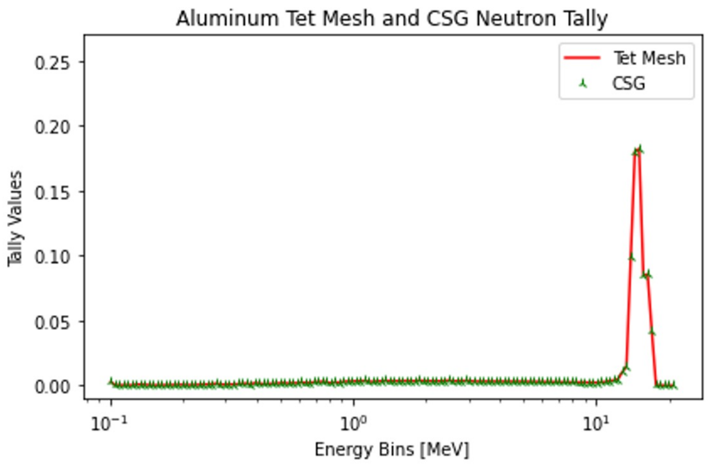
Neutron Flux

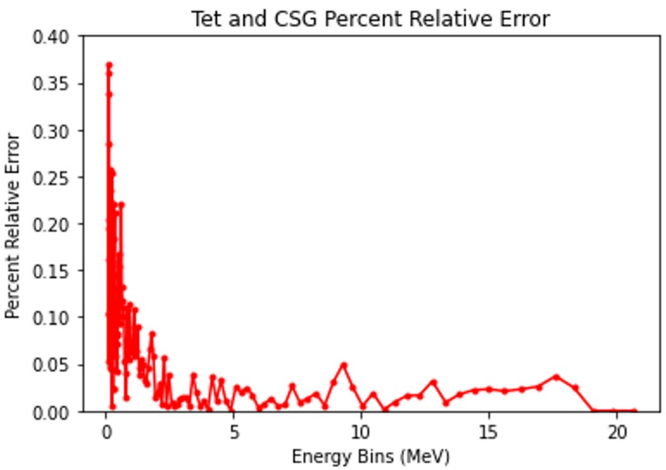
Neutron Energy Deposition

Aluminum Oktavian Comparison F1 Results

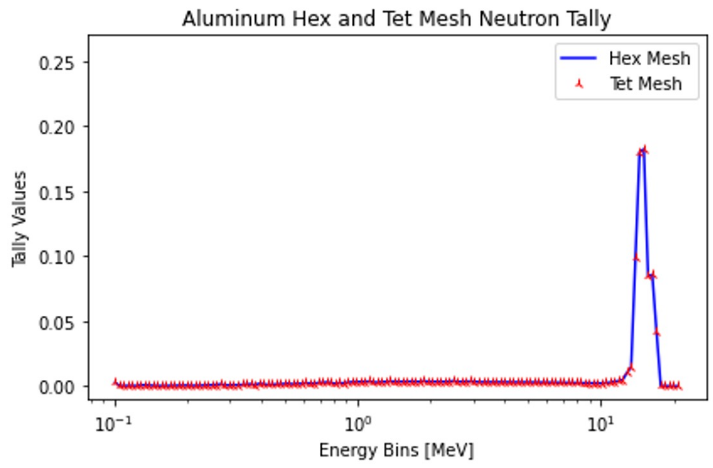


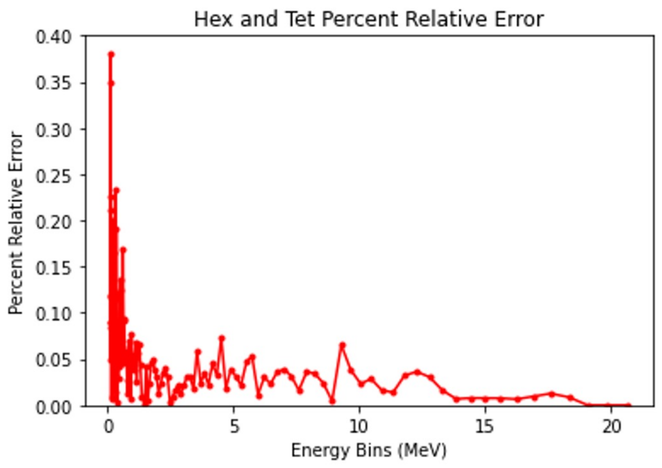






Aluminum Oktavian Comparison F1 Results





- MCNP Results and Information
  - Larger error in tet mesh could be due to coarse mesh size in air region of least importance for faster computation. Despite this, tet mesh still has 31% more elements.
  - Computer times:
    - CSG: 42.08 minutes
    - Hex mesh: 818.28 minutes
    - Tet mesh: 1420.7
  - Used 48 processors with MPI on ORGA.

Los Alamos NATIONAL LABORATORY

Cu, Mo, Si Oktavian Results

LA-UR-22-29621
Approved for public release; distribution is unlimited.

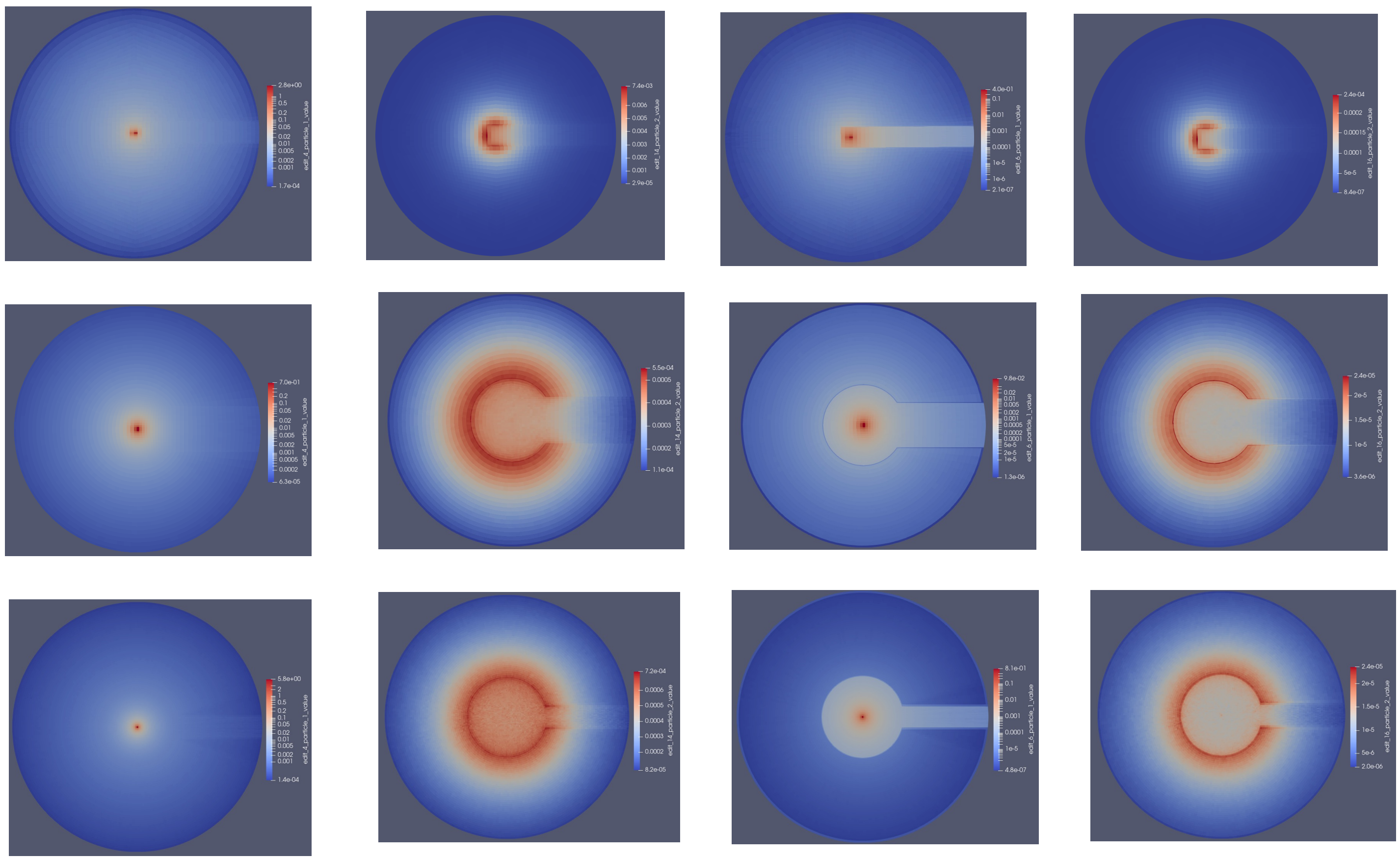
Title: Cubit for MCNP Unstructured Mesh Analysis of Oktavian Benchmarks

Author(s): Dzur, Micky Ray
Armstrong, Jerawan Chudoung
D'Angelo, Chelsea Ann

Intended for: Report

Issued: 2022-09-16

- Good agreement between the results of CSG models and hex and tet UM models. The results of these models are in the LA-UR-22-29621 report



Cu

Si

Mo

Neutron flux | Photon flux | Neutron energy deposition | Photon energy deposition

Conclusion and Future Work

- **Procedure**
  - Use Cubit to create UM models, run CSG and UM models, and compare the results.
- **Results**
  - The UM hex results show rather low difference when compared to CSG or tetrahedral results.
  - The hex mesh models provide more accurate than the tet mesh models when comparing with CSG results.
  - The hex mesh models run faster than the tet mesh models.
  - The UM feature allows analysis and display of otherwise unavailable high-fidelity results. HDF5/XDMF EEOUT files created by MCNP6.3 can be visualized by ParaView.
- **Future Work**
  - Embed mesh geometry in CSG universe defining collimators and detector setup reflecting actual experiment.
    - Potential for comparison to experimental results to perform validation.
  - Verify variance reduction methods using within MCNP UM calculations.