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MCNP6.3 Unstructured Mesh Verification: GodivR and CANDU Models

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Introduction

A geometric cell of the Monte Carlo N-Particle (MCNP)[1] transport code is traditionally created by using Boolean operators on defined surfaces. This constructive solid geometry (CSG) capability has been available in the MCNP code since its beginning. However, a CSG model approach is limited when it comes to constructing a representative geometry for a complex model in its ability to capture a correct model representation. Starting with the version 6.0, the MCNP code has the ability of embedding an unstructured mesh (UM) model into a CSG cell to create a hybrid geometry [1]. The MCNP UM feature provides the flexibility of defining very complex geometries because computer aided design (CAD) and mesh generation software packages can be utilized to construct UM models for MCNP simulations.

The objective of this work is to verify the MCNP UM feature by comparing the UM and CSG results. An analysis of the results provided by the MCNP UM simulations is required to verify that the UM results are comparable to the CSG results. This would result in the MCNP UM capability being trusted for applications involving complex geometries. The MCNP CSG feature has been well verified and validated for multiple areas of applications and one particular area of focus is criticality (i.e., KCODE) calculations for fissile systems. We verify two MCNP criticality application problems in this report. The first test problem is a model of the simple Godiva sphere reflected by water. This model is a benchmark model in the International Handbook of Evaluation Criticality Safety Benchmark Experiments and referred to as the GodivR in this report. The second test problem is a model of the Canadian Deuterium Uranium (CANDU) reactor's fuel bundle. All calculations in this report were run on an Intel(R) Xeon(R) W-10855M CPU @ 2.80GHz 2.81 GHz with 128 GB of RAM and using 6 threads on a single processor.

MCNP Unstructured Mesh Simulations

A UM geometry model is a representation of a solid geometry model decomposed into small pieces call finite elements or elements. An element is defined by nodal data (i.e., node ids and locations) where a number of nodes formed an element and nodal locations define an element type. The MCNP code can process UM model consisting of several element types including linear tetrahedra (tet) and hexahedra (hex) elements. A linear tet element has 4 faces and 4 nodes at vertices while a linear hex element has 6 faces and 8 nodes at vertices.

A UM calculation requires an MCNP input file and an accompanying UM geometry input file. The MCNP code version 6.3 can process Abaqus or Hierarchical Data Format version 5 (HDF5) mesh input files and produce ASCII or HDF5 elemental edit output (EEOUT) files [1]. The MCNP results written into HDF5 EEOUT files can be analyzed and visualized by a modern visualization software such as ParaView (https://www.paraview.org). The EEOUT results can be requested by the use of EMBED and EMBEE cards in an MCNP input file. The EMBEE card can be used to tally the flux (type 4 edit) and energy deposition (type 6 edit) at each element in the UM model. The type 4 and 6 edits generated the MCNP code are analogous to the standard F4 and F6 tallies as they represent flux [particles/cm^2] and energy deposition [MeV/g], respectively.

An Abaqus UM model is typically created by using a computer aided design (CAD) and mesh generation software packages, where a solid model constructed by CAD is imported into a mesh generation software to create a UM model. Some meshing generation tools also have the ability to create solid geometries and thus a CAD model is not needed. Cubit, Sandia National Laboratory's automated mesh generation toolkit [2], can be used to create solid geometries and generate UM models. Since the UM models generated by Cubit can be exported as Abaqus format files, we used Cubit to generate solid geometries and construct UM models for MCNP UM calculations.

Cubit has the ability to generate a mesh from a solid model and export a mesh model as an Abaqus input file. An Abaqus input file is an ASCII file that contains a series of lines representing a UM model. This file must satisfy the Abaqus syntax and the additional restrictions required by the MCNP code. Since the MCNP code requires that an Abaqus model must have a material and tally element set block (i.e., elset) in each part, the Abaqus file generated from Cubit cannot be directly used. A Python code has been developed to convert an Abaqus file exported from Cubit into an Abaqus file that the MCNP can process [3]. Creating an MCNP UM input file is tedious and error-prone. Thus, another Python script has been developed to extract the information from an Abaqus input file to create an MCNP UM input [4].

GodivR Modeling and Results

The GodivR model consists of a solid, homogeneous sphere of Highly Enriched Uranium (HEU) with a radius of 6.5537 cm and an enrichment of 97.67 wt.% reflected by a sphere of water that has a radius of 33.4717 cm surrounding it. The mass density of the HEU sphere and the water are respectively 18.74 g-cm^{-3} and 0.9998207 g-cm^{-3}, and these density values are used for both the MCNP CSG and UM simulations. The KCODE calculations of the GodivR CSG and UM geometries using 10,000 neutron histories per cycle and discarding the first 50, for a total of 250 cycles.

The CSG k-eigenvalue value is within one standard of the experimental benchmark value shown in Table I.

TABLE I. GodivR Reference k-eigenvalue

	CSG	Benchmark
k_{eff}	0.9998	0.9985
σ	0.0006	0.0011

Reconstruction of the model as a UM through Cubit details a sphere of radius 6.5537 cm within another sphere of radius 33.4717 cm which represents the HEU surrounded in water. This solid geometry is then prepared to be meshed by splitting it up into individual subsections which can be imprinted and merged to each other. The HEU interior sphere was more important, with respect to the geometry since it is the fissile material. The focus for this model was on generating a UM model where the overall volume of the HEU part was captured to an accuracy of a high degree in comparison with the solid geometry volume. This resulted in a volume of 157,080.152 cm^3 with 99.9% of the HEU and 99.8% of the water volume being represented. Since the most important component of this model is the highly enriched uranium, more elements were devoted to accurately represent its geometry while fewer elements were used to represent the water. This resulted in a total of 253,616 linear hexahedral elements where 127,688 compose the smaller interior HEU sphere and the remaining 125,928 represent the surrounding water sphere. The average meshing quality on a scaled Jacobian comparison is 0.9443, which means that the components are not over compensating for any volume and the geometry is representative of the solid model. Alternatively, a linear tetrahedral element geometrical meshing scheme may be used. The number of elements is significantly increased when creating a Tet model that has a comparable quality as a hex model. A linear Tet GodivR model was created that had 3,675,758 elements in order to

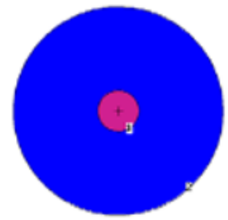


Fig. 1. CSG GodivR

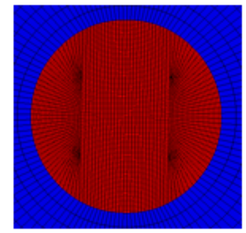


Fig. 2. UM GodivR zoomed in

capture 99.95% of the solid volume. This Tet version of the input file was not used in the MCNP calculation since the mesh element is too big for the MCNP code to handle. A different approach to meshing geometry can be taken which would result in a reduced number of elements and computational time, but meshing volume accuracy may be sacrificed. Generating UM models that have good mesh qualities is problem-dependent and resource dependent. Ultimately it is dependent on the knowledge of the user with respect to the model and the desired accuracy of results, as well as a computing resource available for perform simulations. It is computationally expensive to use a UM model with a large number of elements.

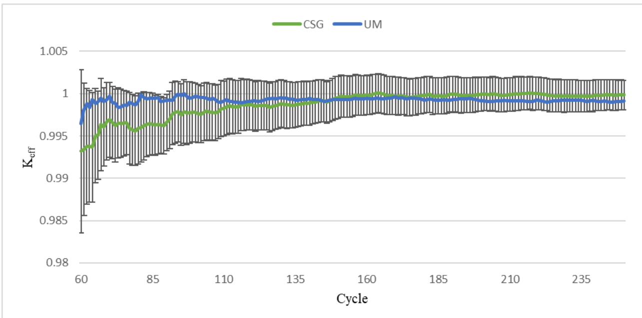
After the hexahedral element model is made in Cubit, blocks are made for the HEU and water sections to assign the material names and densities. The final step in Cubit is to export the UM model as an Abaqus file. This Abaqus file is then processed with the Python script producing the new Abaqus file satisfying the MCNP requirements. Another Python script is then used to extract the data from this new Abaqus input file to create a file containing the MCNP input cards representing the UM geometry. More MCNP cards are then added into the MCNP UM input file to reflect the material compositions in the data card using the ENDF/B-VIII.0 nuclear data library and a KCODE calculation. The CSG and UM models are shown in Fig. 1 and 2. The UM model was run by using the same KCODE setup used by the CSG run. It was found that the computing times of the CSG and UM model are 12.42 and 55.46 minutes, respectively.

TABLE II. GodivR CSG & UM k-eigenvalue

	68% confidence	95% confidence
CSG	0.99924 to 1.00042	0.99866 to 1.00101
UM	0.99860 to 0.99965	0.99808 to 1.00017

The resulting k-eigenvalue for this UM input file following the same parameters and material compositions is found to be 0.99913 ± 0.00053 which lines up with both the CSG result and the benchmark experimental result within one standard deviation. The comparison of confidence interval results is shown in Table II. Further analysis into cycle results is shown in Graph I.

Graph I. GodivR K_{eff} cycles with 99% confidence.



In addition to having comparable k eigenvalues, UM and CSG results can be visualized and analyzed in high fidelity using ParaView as shown in Fig 3 and 4.

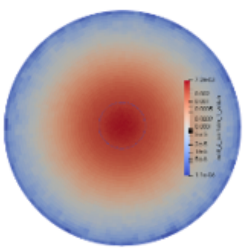


Fig. 3. GodivR Neutron Flux

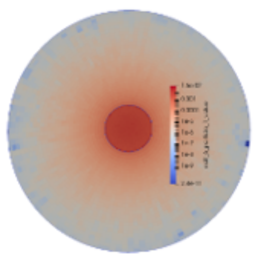


Fig. 4. GodivR Energy Deposition

CANDU Modeling and Results

For a comparison of a more complex geometrical model both the UM and CSG version of the CANDU fuel bundle are analyzed. This includes using heavy water thermal neutron (S(a,B)) treatment of the deuterium in the coolant and moderator. The bundle is inside cells comprising the moderator for both the CSG and UM models and is reflected infinitely in every direction (x, y, and z). The MCNP input files are generated again using the ENDF/B-VIII.0 nuclear data library. The UM model was created to be contained within ordinary CSG cells which then could be reflected to represent the full core of the reactor and obtain a representative k-eigenvalue. The bundle was then enclosed within a moderator box with dimensions that represent the pitch of adjacent bundles throughout the core. However, it should be noted that this is a simple approximation of the full core as the interest for this comparison is of a single bundle. This analysis will focus only on a bundle that has adjacent bundles, i.e bundles that are not at the core's periphery. A full representation of the CANDU core would consist of 12 bundles in a channel with 280 channels.

This representation of 37 fuel elements surrounded in coolant flowing through the bundle was then created in both CSG and UM geometry (Fig. 5). This complex model consists of fuel pins which are encased in cladding with a gap of air surrounding it. Then the coolant flows around the fuel pins which are enclosed in a pressure tube. The pressure tube is surrounded by an annulus gas (CO2). The annulus gas is enclosed by another material that is the Calandria tube.

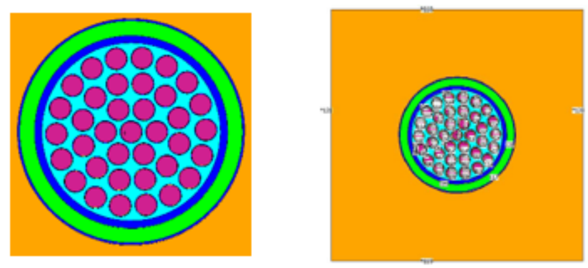


Fig. 5. CANDU CSG
left: Zoomed in Bundle right: Bundle in moderator

The meshed version results in 100.08% of the UM volume compared with the solid mesh. The additional 0.08% volume is due to the complexity of the coolant's geometry that is actively flowing through the bundle and has little impact on the resulting neutron flux and energy deposition so it can be omitted in the post-processing step. Totaling in 1,086,339 linear hexahedral elements, this model is comparable while being in line with the available computational resources. Each individual fuel pin of natural uranium, which is the material of most importance, results in being 98.86% meshed.

TABLE III. CANDU CSG & UM k-eigenvalue

	68% confidence	95% confidence
CSG	1.15519 - 1.15575	1.15491 - 1.15602
UM	1.15552 - 1.15608	1.15524 - 1.15636

Running 10,000 neutrons per cycle for 250 cycles while skipping the first 50. The function KCODE is used and results in computational run time for the UM being 1516.84 minutes in comparison to the 16.6 minutes for the CSG. K-eigenvalue

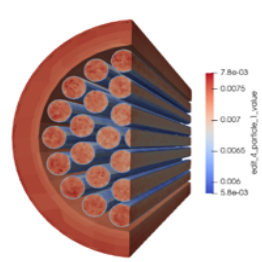


Fig. 6. CANDU Neutron Flux

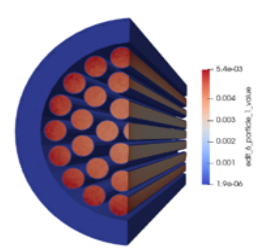
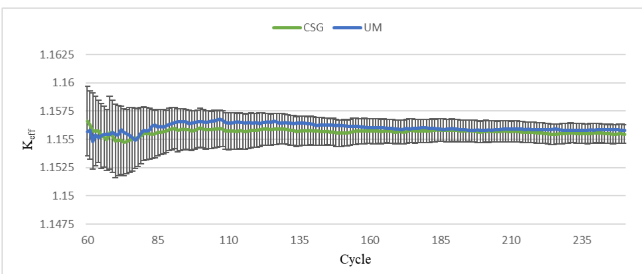


Fig. 7. CANDU Energy Deposition

values are found to be within one standard deviation of each other for both models, shown in Table III.

For the post processing of the HDF5 file in ParaView, the coolant is omitted in the visualizer. A further look is taken into the individual fuel pins within the bundle in regards to their neutron flux and energy deposition shown in Figures 6 and 7. As shown in the visualizer, it is expected that the neutron flux and the energy deposition concentrate both towards the outer areas of the fuel pins within the bundle. This is because of the moderator surrounding the fuel bundles being infinitely reflected with a lattice pitch of 28.575 cm in the X and Y direction. Representing adjacent bundles which are also undergoing fission. It is to be noted that the interior fuel portion of the bundle is treated as a single continuing fuel pellet extending the full length of the bundle. Further analysis into these results show the difference in volume in fissile material which leads to an initial higher K_{eff} through the first cycles until it eventually begins to converge into a comparable result pictured in Graph II.

Graph II. CANDU fuel bundle K_{eff} with 99% confidence.



Conclusions and Future Work

Cubit was used to create the UM models for the GodivR and CANDU fuel bundle where both UM models consist of linear hexahedral elements. The UM models were then imported into the MCNP code for the KCODE calculations. Both MCNP CSG and UM problems were run by using the same parameters. It was found that the results are comparable for both the CSG and UM versions of the GodivR and CANDU geometric models. This verifies that the MCNP6.3 UM feature is reliable for an analysis of the k-eigenvalue results for these test problems.

Future work for this analysis involves a comparison of the standard CSG, F4 and F6, tallies with specific material properties to the UM, edit 4 and edit 6, tallies. Additional work on the modeling of the CANDU fuel bundle must be performed to create a more representative distribution of the neutron flux and energy deposition. This involves creating a complex geometrical model of a larger fraction of the full reactor core with its boundaries. Further analysis using the BURN depletion/burnup card for this KCODE problem is to be done as well in order to obtain further details on the specific elemental sections which have higher neutron flux profiles.

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