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Title: Big Ten MCNP6 Unstructured Mesh Benchmark

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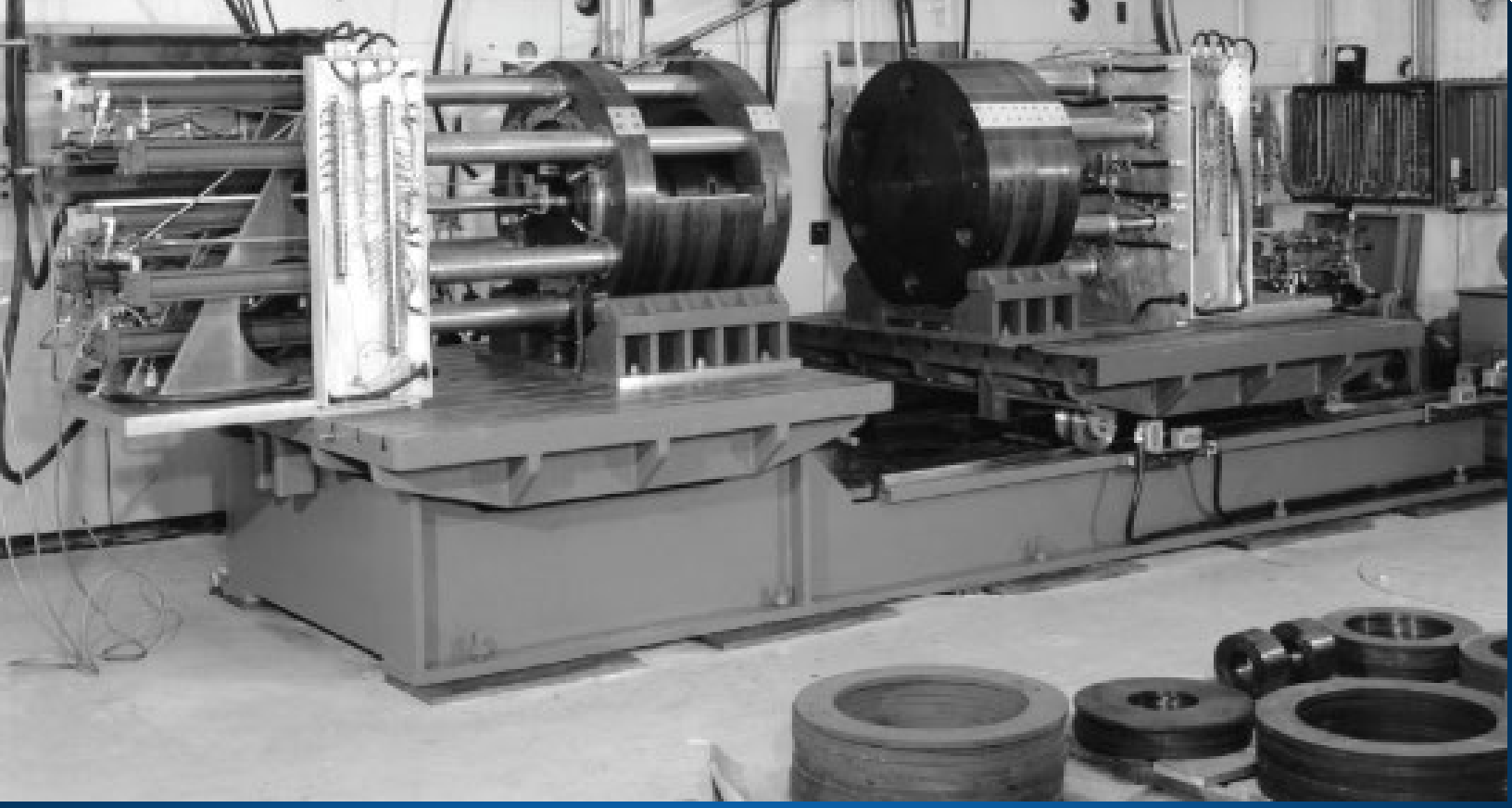

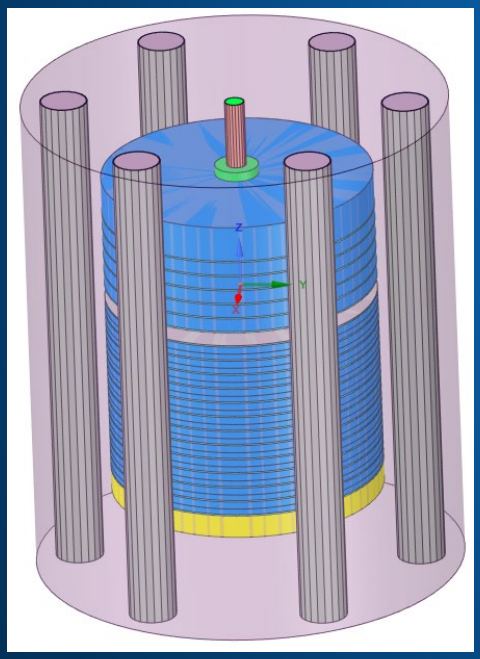

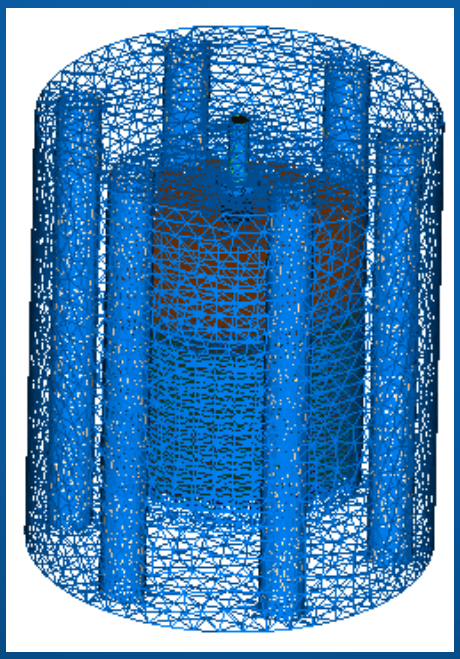

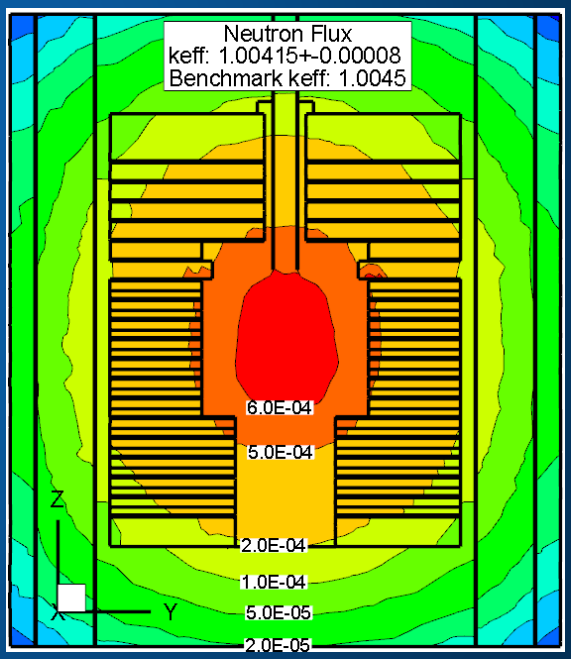

Big 10 MCNP Unstructured Mesh Benchmark

Joshua B. Spencer
Jennifer L. Alwin

20 June 2019

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Big Ten MCNP6 Unstructured Mesh Benchmark

J.B. Spencer, J.L. Alwin
Monte Carlo Methods, Codes, and Applications
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Los Alamos National Laboratory

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1. Purpose

The purpose of this report is to document a benchmarking effort for the MCNP6 Unstructured Mesh (UM) geometry description method applied to a large and fairly complex critical assembly, Big Ten. A secondary goal of this effort is to provide a set of best practices for modeling a critical assembly with the MCNP UM method. Specification of geometry using UM requires creating a mesh from a solid geometry model and there are some important considerations when using this method for criticality problems. These considerations will be discussed along with suggested practices for correctly modeling these types of problems.

2. Background

The Big Ten critical experiment, conducted at the Los Alamos Critical Experiment Facility (LACEF), is so named for two reasons; first because it is made almost entirely of metallic uranium with an average ^{235}U enrichment of 10% and, second because the total uranium mass is approximately 10 metric tons. A schematic drawing of the Big Ten experiment is shown in Figure 1.

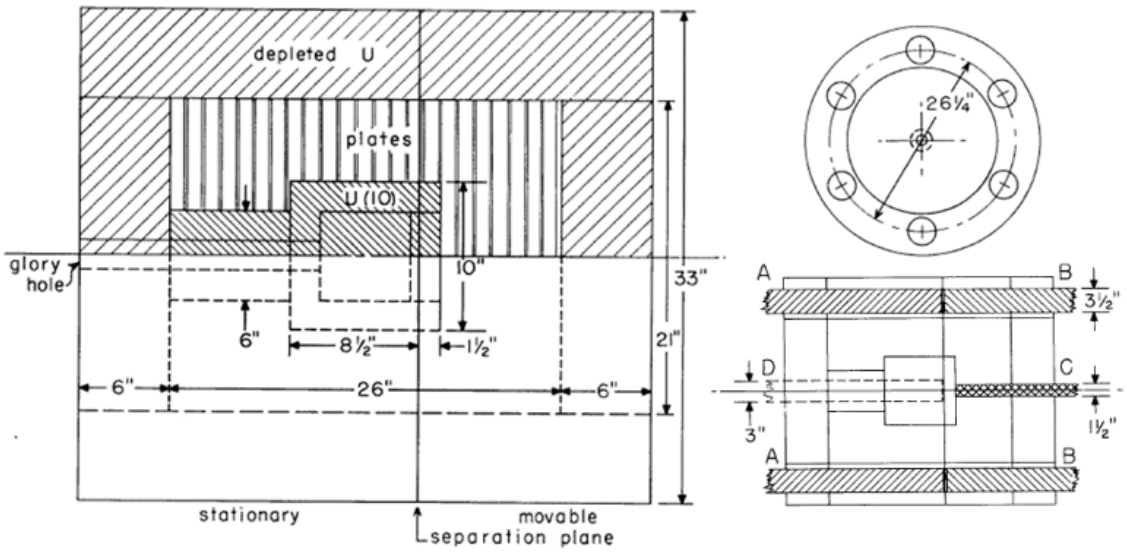

Figure 1 - Cross Section Illustration of the Big Ten Critical Assembly, Reference (1)

The primary purpose of the Big Ten assembly was to evaluate effective cross sections with a neutron spectrum that would resemble that of a liquid-metal fast breeder reactor. This was achieved with a cylindrical core with a radius of approximately 21 inches surrounded by 6 inches of depleted uranium that served as a reflector, Reference (2) (3) (1).

The Big Ten assembly is considered a benchmark experiment in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP), Volume 3 IEU-MET-FAST-007, Reference (4). The MCNP6 example input file for specifying the geometry in the ICSBEP manual includes the geometry shown below in Figure 2, which is represented in Combinatorial Solid Geometry (CSG) format. The primary model discussed in this report is intended to duplicate the level of detail contained CSG model shown in Figure 2 as closely as possible with an UM geometry. A simpler version of this model was also created where the thin cylindrical fuel and reflector plates were homogenized and gave similar results with substantially better computational performance.

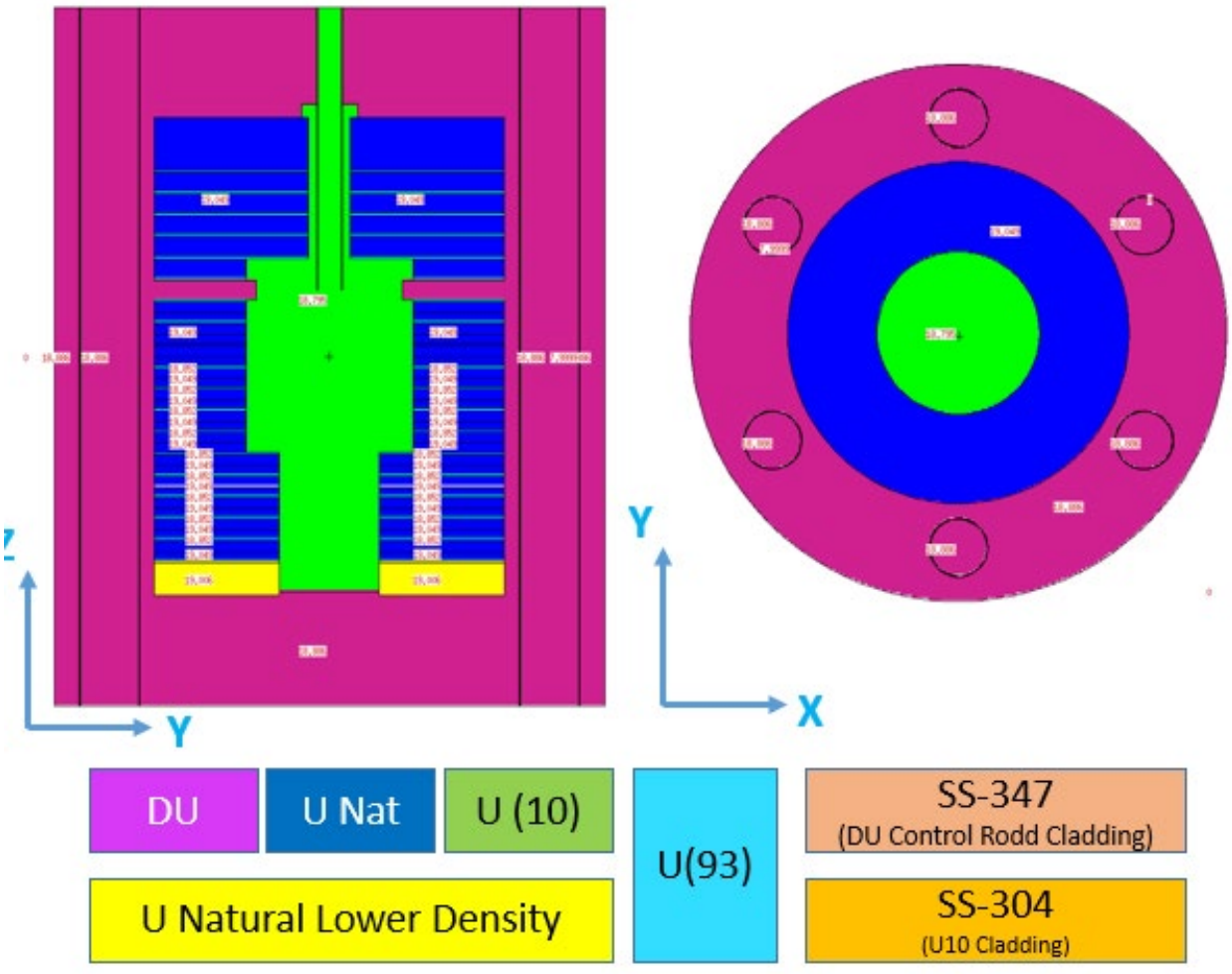

Figure 2 – Cross Section Illustration of IEU-MET-FAST-007 CSG Model with MCNP6.2

The following workflow was used to set up the MCNP6 UM model. First, a Computer Aided Design (CAD) model based on the CSG geometry was constructed in SpaceClaim as shown in Figure 3. Second, this CAD model was then exported in ParaSolid format and the solid geometry imported into Attila4MC, version 10.0. The Attila4MC mesh generation function was used to produce a UM representation of the geometry using first order tetrahedral elements. Attila4MC was also used to read in the exact materials specifications included in the ICSBEP benchmark model description, map those material to the meshed geometry and then write out the MCNP6 input deck to make use of the UM geometry and material mapping. The input file and accompanying mesh model are then ready for use with MCNP6 in fixed source or kcode calculations.

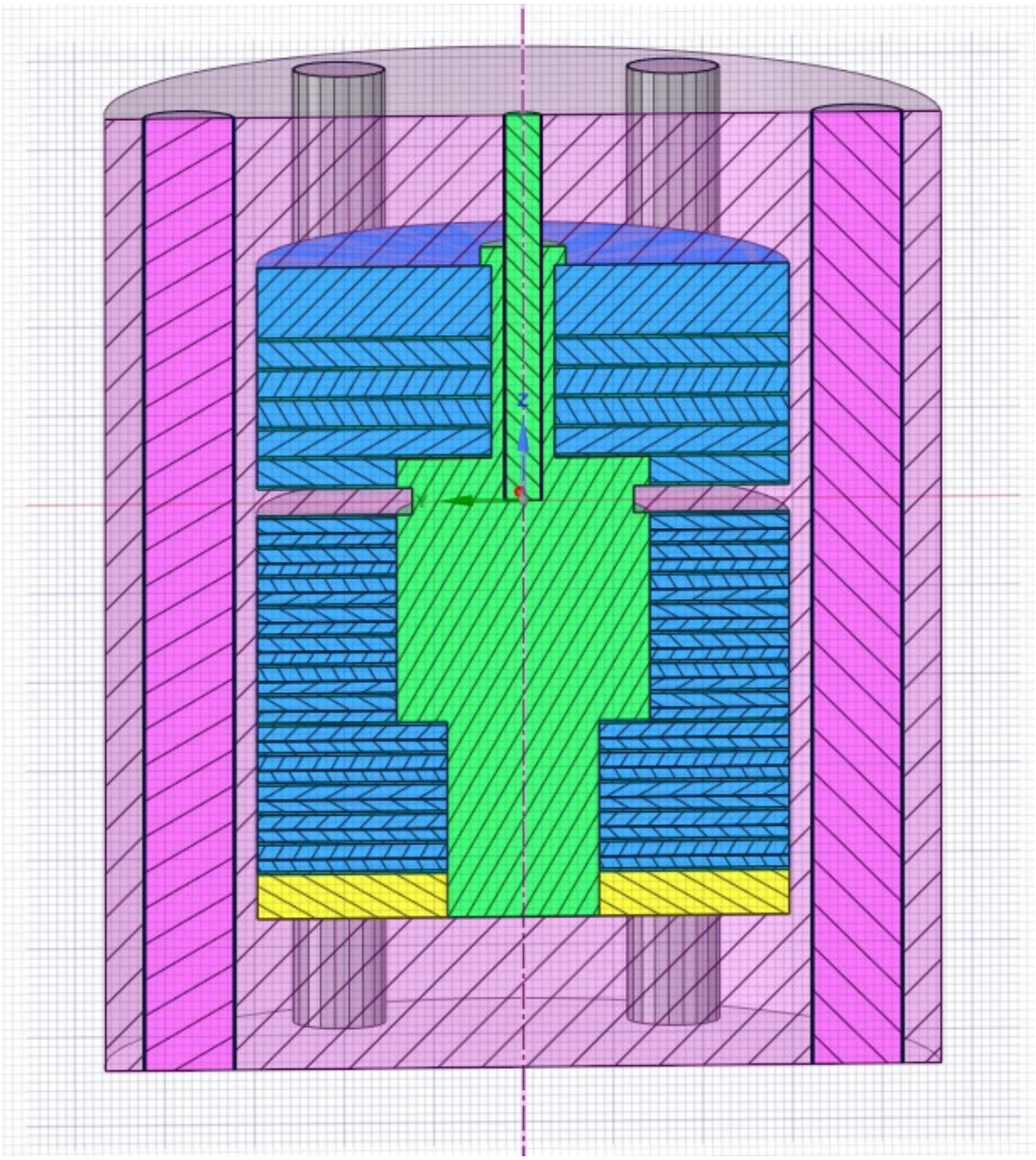

Figure 3 – Cross Sectional Illustration of IEU-MET-FAST-007 10 CAD Model in SpaceClaim

3. Results

The steps described in the previous section to create a UM file for use with MCNP6 with the accompanying mesh geometry were followed for Big Ten. MCNP6 results of the kcode calculation yield a k-effective value of 1.0041±0.00008. This result is in good agreement with the benchmark experiment k-effective value of 1.0046±0.0002. For comparison the equivalent CSG model MCNP6 k-effective result value is 1.00432±0.00007. The simplified homogenized version of this model produced a k-effective value of 1.00025±0.00007, which confirms the system is just critical with a 55% smaller mesh. Because all of the MCNP calculations were produced with Attila4MC, it was a trivial task to set-up independent check calculations to by running the Attila discrete ordinance solver in Eigen value mode. This was done with the Radion15 multi-group cross section set, which has 22 neutron groups and is based on ENDF/B-VI era data. The Attila solver gave a k-effective values of 1.02 which is a little higher than the MCNP6 predictions but also in the just critical regime.

An additional comparison study was done using WHISPER-1.1 Reference (5), which is a statistical sensitivity/uncertainty tool used to support criticality safety validation. Whisper contains a library of 1101 criticality safety benchmarks with pre-computed MCNP6 sensitivity profiles which can be compared with the application being studied to determine neutronic similarity to each of the benchmarks. The Whisper results for the UM model verify that UM version of this model was neutronically similar to the CSG equivalent. The remaining sections of this report provide additional detail into the results of the UM benchmark calculations as well as a discussion of how the model was constructed.

While the use of UM geometry in MCNP6 is a relatively new feature, it has primarily been employed in practical applications for doing shielding and dose calculations, i.e. fixed source types of problems. The preservation of mass and volume when moving from CSG to UM geometry is an essential concern and the importance of this cannot be overstated when employing UM for criticality problems. It is possible to generate a mesh which does not properly preserve mass/volume and can lead to incorrect results. This is especially important because in criticality problems even a slight increase or decrease in fissile/fissionable mass can lead to significant differences in k-effective results. For this reason the practitioner must always check to see that mass and volume are within acceptable tolerances when modeling geometries with UM for criticality problems in MCNP6. The next section discusses details of creating meshes for use with UM in MCNP6 and gives guidance learned by those with experience using UM with MCNP6. This report, with future similar studies, is an effort to begin considering validation using criticality safety benchmark experiments with geometry complexities. It cannot replace site-wide validation guidance, which must be considered by the criticality safety practitioner in the context of the process analysis. The method of analysis in a criticality safety evaluation must be the same method covered by validation for a criticality safety program. It would therefore be inappropriate to use a collection of CSG benchmarks to determine validation for UM cases and vice-versa.

One of the benefits of using the UM geometry type in MCNP is that it facilitates state-of-the-art visualization of both the model and its results which improves an engineer's ability gain insight from the simulation while at the same time reducing risks associated with geometry errors. MCNP6 has implemented the UM geometry such that as particles are tracked through the UM geometry, tallies can be made on the same mesh, this results in a mesh tally that is conformal to the geometry in an MCNP6 produced EEOUT file. Figure 4 shows the neutron flux shape captured by this mesh tally. Note that a script supplied with Attila4MC was used convert the data MCNP's EEOUT file format so that it could be plotted in TecPlot.

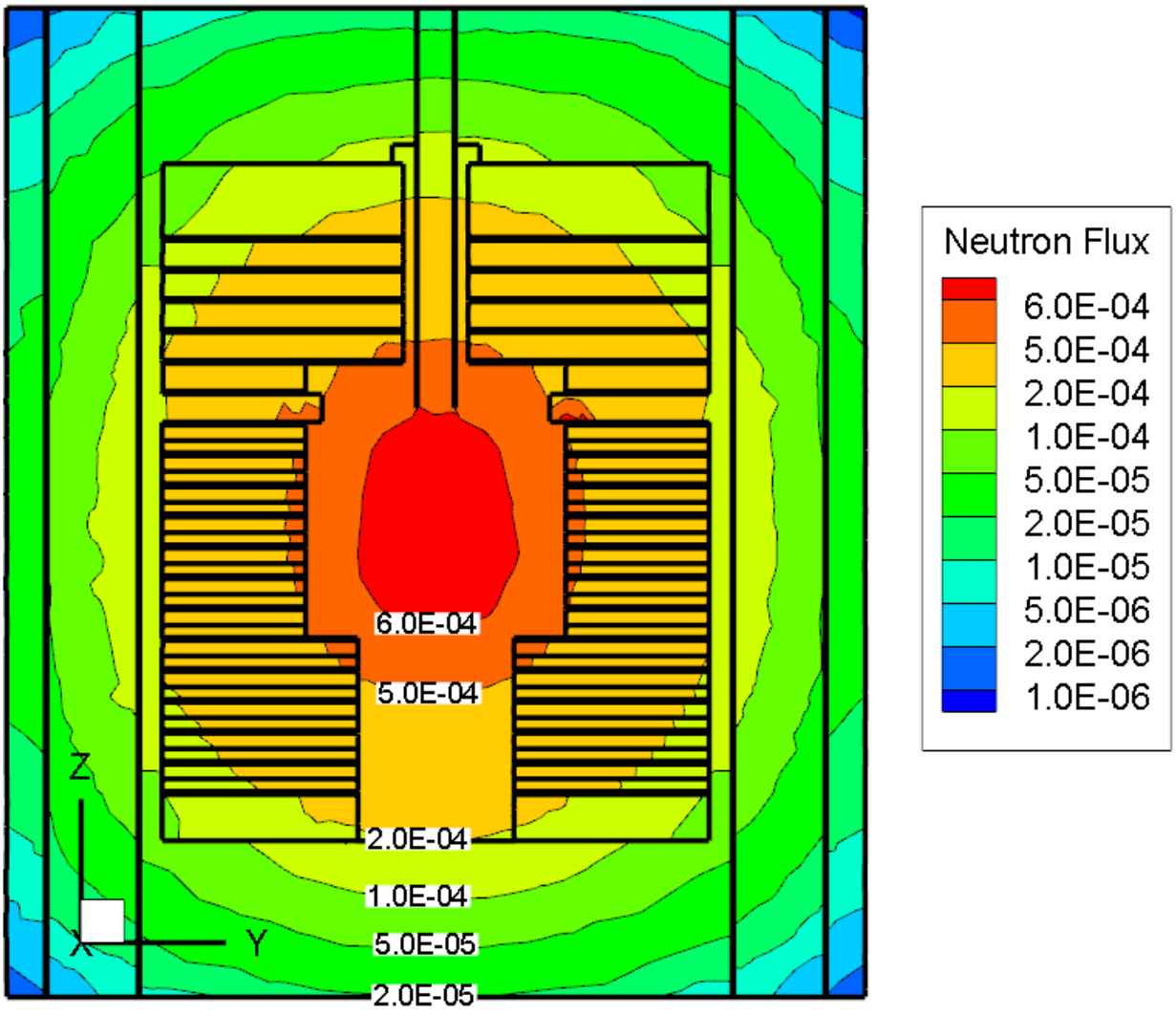

Figure 4 – Neutron Flux Results as Reported in the MCNP EEOUT Output Data and visualized with TecPlot

Once the considerations are taken into account for proper mesh generation there are several benefits of using UM geometries. As mentioned at the start of this section, state-of-the-art visualization of the model and its results improves an engineer's ability gain insight from the simulation while at the same time reducing risks associated with geometry errors. Additionally, for very detailed models it is possible to import existing drawings that contain complex geometries and create UM for use with MCNP6, potentially decreasing the time required to create input files. Another benefit is the possibility of linking UM geometries and results with meshes used with multi-physics packages, facilitating MCNP6 results used as input to further engineering/physics studies.

4. Calculation Details

A new feature added to MCNP6 is the ability to represent geometry with Finite Element Analysis (FEA) style Unstructured Mesh (UM), Reference (6). This new development enabled the marriage of two mature technologies namely: MCNP6 which defines the state of the art in continuous energy Monte Carlo radiation transport and Attila (also developed at Los Alamos National Laboratory) which is deterministic radiation transport code for unstructured mesh. The commercialization of Attila has yielded a graphical user interface (GUI) that provides a robust capability for unstructured mesh generation, materials definition with accompanying assignment to the mesh, source description, tally definition, along with valuable 3D visualization of both the geometry model and transport results. A recent development in the Attila GUI has enabled it to be used for both the Attila deterministic solver as well as the generation of mesh geometry and MCNP6 input files. While not necessary for the Big Ten benchmark presented in this report, it is worth noting that these complimentary methods also allow automatic hybrid deterministic/Monte Carlo variance reduction utilization the Consistent Adjoint Driven Importance Sampling (CADIS).

The combination of these capabilities have been collected into a new product called Attila4MC, Reference (7). Note that this work uses the current production versions of both codes namely: MCNP6.2 and Attila4MC 10.0. This section describes the process involved in constructing the MNCP6 input file and accompanying UM geometry file. Attila4MC has been designed to be CAD system agnostic, so the users can use whatever tool their institution provides so long as it can generate CAD files in either Parasolid (.x_t) or ACIS (.sat) formats. SpaceClaim is the recommended CAD package for use with Attila4MC as it has been specifically developed to support the geometry modeling needs of engineering analysis software. The Parasolid (.x_t) format is typically preferred as experience has shown that it tends to do a better job of maintaining meta data such as part and assembly names specified in the CAD model upon export. The Attila4MC mesh generation tool currently only supports 1st order tetrahedral mesh elements that are body fitted to the CAD geometry because it is tied to what the Attila solver supports. Note that MCNP6 can support 1st or 2nd order tetrahedral, pentahedral or hexahedral mesh element types, Reference (8).

Mesh Generation Parameters

The Attila4MC mesh generator comes with a series of advanced features, including extrusion meshing, curvature and anisotropic mesh refinement. All of which aim to provide as good as possible representation to the base CAD geometry with as small of an element count as possible. The mesh generator also allows the user to specify both a global maximum mesh edge length and a maximum edge length for each meshed part. The global mesh size specified for the Big Ten geometry was 5 cm. Part specific maximum edge length parameters were used for the control rods: 4 cm for the six Depleted Uranium (DU) control rods located within the reflecting region of the assembly and 1.5cm for the 10% enriched uranium control rod located on axis. Curvature refinement was also enabled for this problem with a diameter to height ratio of 0.02 with a minimum edge length parameter set to 1cm. This resulted in a mesh with 285,322 tetrahedral elements with 49,382 node points. This mesh representation is shown below in Figure 5.

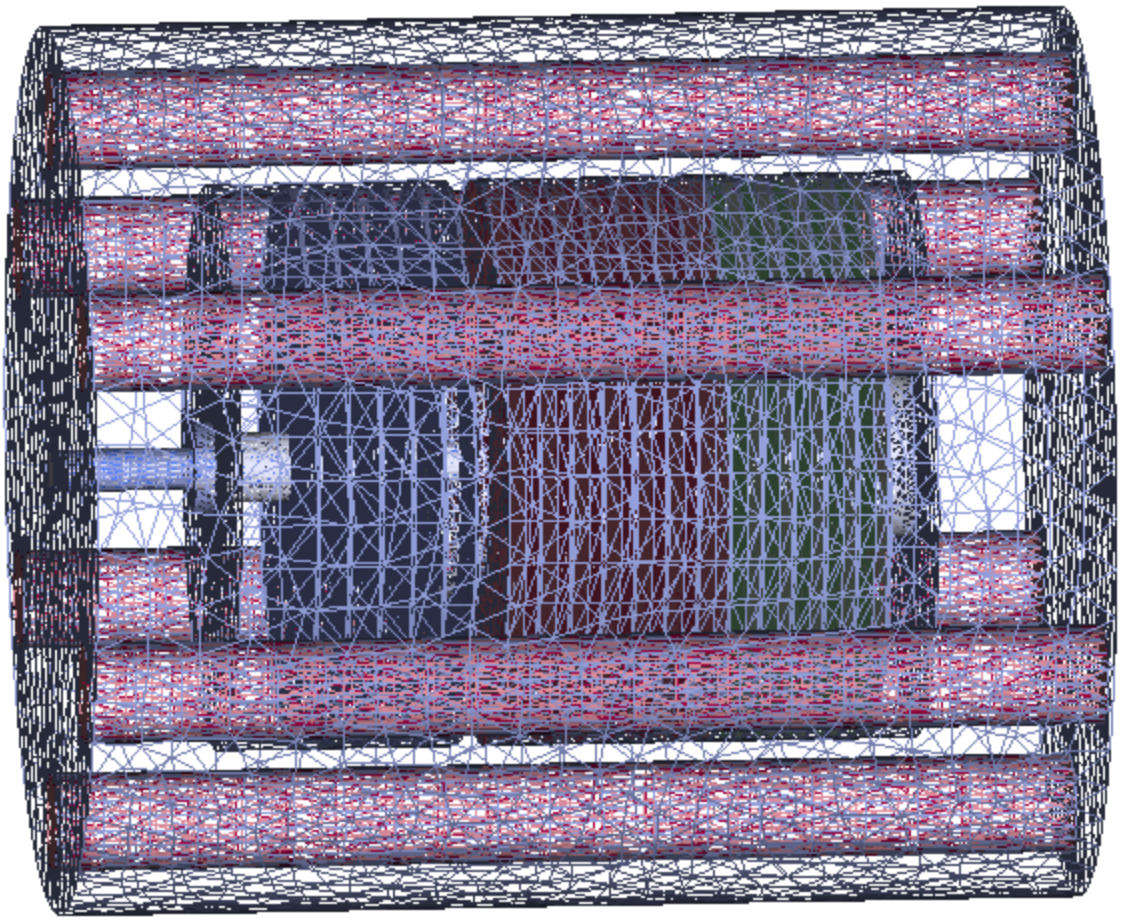

Figure 5 – 1st Order Tetrahedral Mesh Representation of the Big Ten Assembly Produced by Attila4MC

Pre-faceting

The goal of this meshing procedure was to represent geometry in the CSG and CAD geometries as closely as possible so that the physical properties of the assembly could be maintained with a reasonable mesh size. To represent the thin annular gaps between the control rods and their stainless steel sleeves as precisely as possible with a first order (linear) element type, the true cylindrical shape of the control rod geometry was replaced with 20-sided extruded polygons as shown below in Figure 6. Figure 7 shows a close up of the meshes that would be produced (with the same parameters as described above for the global Big Ten model) for a true cylindrical geometry versus a pre-faceted geometry. The pre-faceted geometry required approximately an order of magnitude less mesh elements to represent the control rod and its sleeve while doing an equivalent job representing the circular cross-section of the geometry while at the same time preserving the precise gap thickness all the way down the control rod's length. In setting up mesh geometries for criticality calculations one of the most important considerations is the preservation of mass especially for the active components. Table 1 provides a component by component breakdown of the volume and mass quantities for the meshed and CAD geometries. Note that to the significant digits shown the total system masses are identical and the active volumes agree to within about a third of a percent.

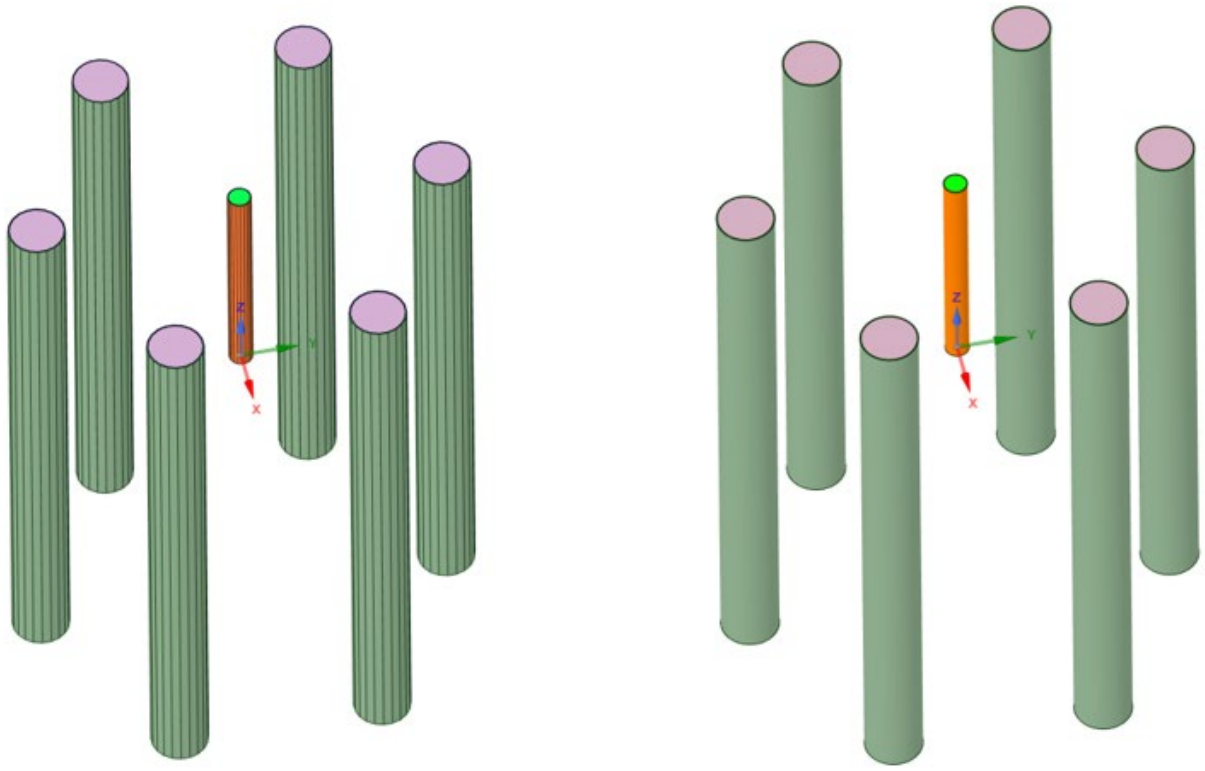

Figure 6 – Pre-faceted Control Rod Geometry Compared to True Cylindrical Geometry

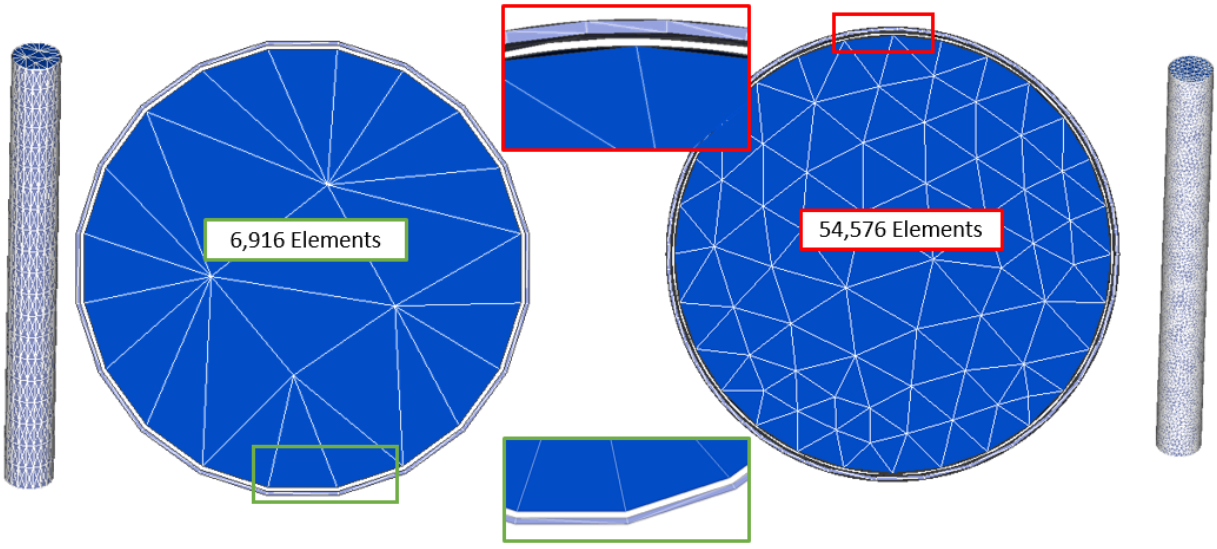

Figure 7 – Comparison of Pre-faceted and True Cylindrical Geometry Post Meshing

Density Adjustment to Maintain Critical Mass

Another calculational detail was parameterized in the Big Ten model to look at the effect of adjusting the density of cells in correspondence to the meshed volume. As discussed previously creating a mesh from a solid geometry does not necessarily preserve the volume of the represented geometry especially if that geometry has substantial curvature. Therefore a technique to adjust the density of cells using a ratio of the solid volume to the meshed volume results in a preservation of mass. In this problem three different options were examined. The first was keeping the density of all pseudo cells constant corresponding to the specified density for the experiment. This is termed the "nominal density" and is equal to the density used in the CSG model. The second option is to modify the density to keep the mass of all pseudo cells equal to the mass of the CSG cells. This is termed the "adjusted density". Finally, the third option is to adjust the density of the U93 and U10 cells, while maintaining all others cells at nominal density. Densities using this method are listed in Table 2. The results of MCNP6.2 kcode calculations using this method are listed in Table 5.

Table 1. Component Volume and Mass Comparison

Region Name	Meshed Volume (cc)	CAD Volume (cc)	% Diff	Mass Density (g/cc)	Meshed Mass (g)	CAD Mass (g)
DU-Reflector	3.51E+05	351175.8228	-0.10%	18.886	6.63E+06	6.63E+06
U-10	1.76E+04	17675.9671†	-0.36%	18.795	3.31E+05	3.32E+05
UnatPlate	9.24E+03	9262.6019	-0.29%	19.006	1.76E+05	1.76E+05
DU-Control Rod	3.62E+04	35844.1366†	0.86%	18.886	6.83E+05	6.77E+05
SS347-Sleeve	1.19E+03	1307.7464†	-9.08%	7.9999	9.51E+03	1.05E+04
SS304- Sleeve	4.14E+01	40.584†	2.05%	7.9998	3.31E+02	3.25E+02
Unat-Top	4.41E+04	44234.6605	-0.38%	19.049	8.39E+05	8.43E+05
U93-Top	3.81E+03	3819.16	-0.37%	18.852	7.17E+04	7.20E+04
Gap-Top	1.21E+00	1.2066	0.03%	0	0.00E+00	0.00E+00
Gap-Mid	3.92E+01	39.3264	-0.38%	0	0.00E+00	0.00E+00
U93-Mid	3.61E+03	3625.1456	-0.38%	18.852	6.81E+04	6.83E+04
Unat-mid	3.26E+04	32688.049	-0.40%	19.049	6.20E+05	6.23E+05
Gap-Bottom	2.60E+01	26.0625	-0.38%	0	0.00E+00	0.00E+00
U93-Bottom	3.68E+03	3690.6551	-0.39%	18.852	6.93E+04	6.96E+04
Unat-Bottom	2.76E+04	27730.4654	-0.39%	19.049	5.26E+05	5.28E+05
Gap-U10	9.15E+00	9.5638†	-4.34%	0	0.00E+00	0.00E+00
Gap-Control Rod	1.24E+03	1408.3621†	-11.83%	0	0.00E+00	0.00E+00
				Total	1.00E+07	1.00E+07

† True geometry CAD Volume NOT Pre-faceted CAD Volume

Table 2. Nominal and Adjusted Density for UM Pseudo Cells.

Region Name	Nominal Density (g/cm^3)	Adjusted Density (g/cm^3)
DU-Reflector	0.0477790	0.0478247
U-10	0.0476092	0.0477821
Unat-Plate	0.0480869	0.0482254
DU-Control Rod	0.0477790	0.0473708
SS347-Sleeve	0.0874931	0.0962311
SS304- Sleeve	0.0879737	0.0862043
Unat-Top	0.0481957	0.0483780
U93-Top	0.0482701	0.0484497
Gap-Top	0.0000000	0.0000000
Gap-Mid	0.0000000	0.0000000
U93-Mid	0.0482701	0.0484565
Unat-mid	0.0481957	0.0483897
Gap-Bottom	0.0000000	0.0000000
U93-Bottom	0.0482701	0.0484573
Unat-Bottom	0.0481957	0.0483850
Gap-U10	0.0000000	0.0000000
Gap-Control Rod	0.0000000	0.0000000

Homogenization

When using the UM method, it is generally of interest to use the smallest mesh that adequately captures the physics of interest. The primary purpose of UM in MCNP is to define the boundaries of materials, once this is accomplished, particles are tracked in a similar way inside the mesh elements as they would be in a normal CSG cell. That means that the mesh needs to be good enough to capture the shape of an object but does not necessarily need to be fine enough to capture flux gradients unless the flux profiles are to be visualized using the tallied flux data collected on the UM. For criticality calculations, the primary quantity of interest is the Eigen value for a nuclear assembly which indicates how the neutron population in that assembly will grow (k-effective > 1 for a super critical system), stay the same (k-effective = 1 for a critical system) or decay away (k-effective < 1 for a sub critical system). Because this k-effective value is determined by balancing neutron leakage and production terms for the whole system the mesh can be simplified as long as the distribution of material is adequately described.

In the UM used in the benchmark model discussed in the previous sections, the mesh size was driven up to over a quarter million elements because the thin (~3mm) fuel HEU plates, the natural uranium reflecting plates and the gaps between them were modeled explicitly which in turn set the local mesh edge length. The mesh size could be easily reduced by over half by replacing these thin interleafed layers with homogenized material zones in the CAD model then remeshing the new CAD with the same mesh parameters that were used in the previous model so the same critical mass is maintained. To do this as fairly as possible, this was done by combining similar annular rings (i.e. cylinder sections with the same inner and outer radius) yielding top middle and bottom homogenization zones in the active core as shown in Figure 8. Note that to keep the neutron reflector geometry a correct as possible the thick natural uranium plates on the top and bottom of the stack were maintained explicitly. Table 3 provides the atom fractions of the uranium isotopes (all with approximately 10% U-235) and mass densities of the homogenization zones determined by taking the volume weighted averages of the HEU, natural uranium plates and void gaps between them. The net result is a mesh model of the big ten assembly with 127,326 tetrahedral elements, which is over 55% lower element count than the explicit model which would therefore require less than half the amount of both memory and time to estimate the k-effective value in MCNP than required in the explicit UM model described above.

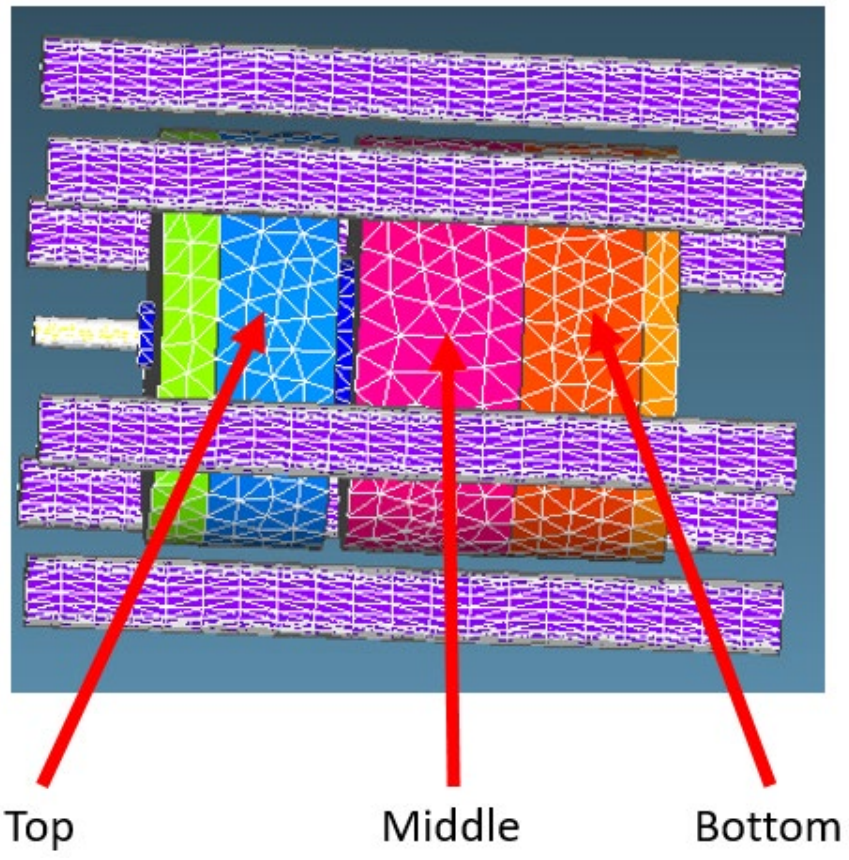

Figure 8 – Homogenized Version of the Big Ten Model with the External Depleted Uranium Reflector Hidden

Table 3. Uranium Atom Fractions of the three Homogenized Core Zones

Density (g/cc)	19.025	19.009	19.010
Isotope	Top Homogenization	Middle Homogenization	Bottom Homogenization
U-234	6.1231e-5	5.2060e-5	6.0800e-5
U-235	5.6301e-3	4.8029e-3	5.5912e-3
U-236	1.5648e-5	1.3199e-5	1.5534e-5
U-238	4.2496e-2	4.3283e-2	4.2497e-2

Independent Attila Check Calculations

One of the benefits of using the Attila4MC workflow for generating UM models for MCNP is that an independent check calculation can be made using the Attila discrete ordinance solver, which has forward, adjoint and Eigen value modes with a minimal extra effort. Attila solves the linear time independent form of the Boltzmann transport equation be discretizing phase space with a 1st order tetrahedral mesh for space, using angular quadrature sets to define what direction particles may stream or scatter and using multi-group formulation for energy. Eigen values searches were performed using both the explicit and homogenized versions of the UM geometry model that were created for the above MCNP6 calculations. The Radion15 general purpose shielding cross section set was used for both calculations as it had data for all four isotopes of uranium of interest to this problem as well as a uranium fission energy weighting function for its 22 neutron energy groups. Note that the Radion15 cross section set is based on ENDF/B-VI era nuclear data and was processed with both NJOY and TRANSX by Transpire Inc. In addition to the two separate geometry models evaluated, two separate angular quadrature and scattering order were evaluated. For the explicit fuel plate model, an S_{24} Triangular-Chebychev-Lobatto quadrature set was employed which has 618 angles uniformly distribute over the unit sphere along with a P_5 scattering treatment. For the homogenized fuel plate model, an I.K. Abu Shume biased quadrature was used that has 1056 angles concentrated on the z-axis poles along with a P_3 scattering treatment.

Figure 9 shows the neutron flux profiles for both the explicit and homogenized fuel plate models. Both of these results have very similar flux shapes as predicted by MCNP shown in Figure 4. Unlike the MCNP6.2 result, the flux profiles provided by default by Attila are scaled to account for the amount of material present in the model rather than being normalized. Table 4 provides a summary of the k-effective values predicted for the two versions of the model. The homogenized model provided a k-effective result that was slightly closer to the benchmark value of 1.0046±0.0002. Both of these k-effective values are slightly larger than predicted by MCNP6.2 but generally confirm Big Ten would be delayed super-critical as modeled.

Table 4. Big Ten k-effective results from Attila

Model	Converged k-effective value
Explicit Fuel Plate	1.020
Homogenized Fuel Plate	1.017

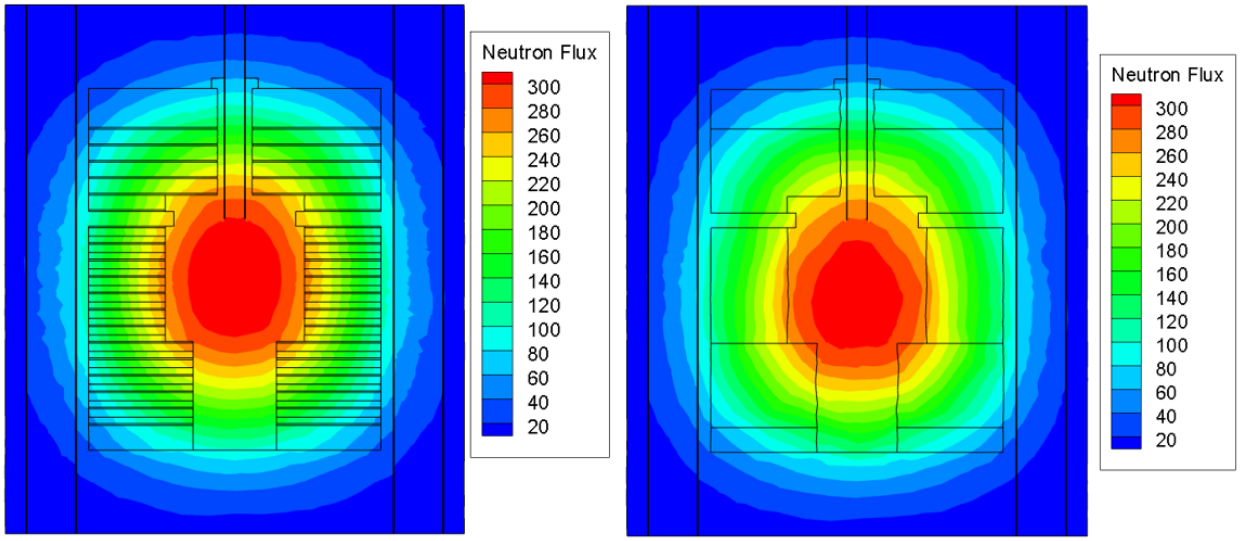

Figure 9 – Attila Predictions for Neutron Flux In Explicit and Homogenized Fuel Plate Models

5. Conclusions and Recommended Best Practices

The capability to use UM geometries with MCNP6 was discussed and presented for the Big Ten assembly (IEU-MET-FAST-007). The k-effective results obtained for Big Ten using various computational methods are within ~0.6% of one another and the experimental k-effective result for the detailed model 1.0046 +/- 0.0002.

Table 5. MCNP6.2 kcode results

	MCNP6.2 (Continuous Energy ENDF/B-VII.1)	MCNP6.2 (Continuous Energy ENDF/B-VIII.0)
CSG Model	1.00432 ± 0.00007	1.00414± 0.00008
UM Model-nominal density	1.00400 ±- 0.00007	1.00382 ± 0.00008
UM Model-adjusted density	1.00529 ± 0.00007	1.00512 ± 0.00008
UM Model-partial adjusted density	0.99909 ± 0.00007	0.99903 ± 0.00008

A comparison study using Whisper-1.1 shows that MCNP6.2 results from the CSG kcode calculation and the UM kcode calculation are neutronically similar to the same benchmarks in the Whisper library, and are therefore neutronically similar to one another.

Proper preservation of mass and volume are essential when using UM geometries for criticality safety calculations. Various techniques of mesh generation influence preservation of geometry while taking into consideration mesh efficiency, and those relevant to the Big Ten assembly were presented in this paper.

Recommendations for best practices to consider when using UM for criticality safety include:

- Check meshed mass and volume to ensure correct preservation, especially for fissile/fissionable materials and close fitting reflectors.
- When building a mesh, the mesh edge length parameter may be tailored to specific pieces where preservation of mass or volume is crucial. In the Big Ten model described in this paper a global mesh edge length of 5cm, with the exception of an edge length of 4 cm for the six Depleted Uranium (DU) control rods located within the reflecting region of the assembly and 1.5cm for the 10% enriched uranium control rod located on axis, was appropriate for general efficient meshing while specifically preserving of control rod geometry specifically.
- Curvature refinement is useful for pieces such as cylinders and spheres. In the Big Ten model described in this paper curvature refinement was enabled with a diameter to height ratio of 0.02 with a minimum edge length parameter set to 1cm.
- Consider representing cylinders as pre-faceted polygons when it is important to preserve gap distances and/or align concentric rings. In the Big Ten model described in this paper 20-sided polygons were used for the control rods and help preserve gap distances and mesh cylinders efficiently with a reduced number of mesh elements.
- If intending to use UM for criticality safety calculations conduct validation with the same method (UM geometries) to properly determine calculational margin and margin of subcriticality.

6. References

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