Verification of the 3D Method of Characteristics Solver in OpenMOC

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ABSTRACT

The Method of Characteristics (MOC) has seen wide interest in full-core reactor physics analysis due to its computational efficiency and ability to easily treat complex geometries. Recently, the OpenMOC reactor physics code was extended to include 3D MOC capability. In this study, we present verification for the 3D MOC solver in OpenMOC and sensitivity of 3D MOC to the axial geometry discretization and axial track laydown. Results for the Takeda Model 1 benchmark show excellent agreement with the reference eigenvalues. A sensitivity study was conducted on a UO_2 quarter-assembly extracted from the C5G7 3D unrodded benchmark geometry in order to show the effect of the axial MOC parameters on the solution eigenvalue for a heterogeneous problem. The sensitivity results demonstrated that the solution accuracy was highly dependent on the axial source region discretization, but insensitive to axial spacing between tracks below $\sim$0.2 cm. Using the equal angle quadrature set, at least 10 and 18 polar angles were required to converge the problem to with 100 and 10 pcm, respectively. These results both verify the 3D MOC solver in OpenMOC and provide insights into the axial MOC parameters required to solve heterogeneous problems with 3D MOC.

Key Words: **3D MOC, Verification, Neutron Transport**

1. INTRODUCTION

There has recently been a shift to replacing the legacy diffusion theory based reactor physics codes with modern codes that more explicitly model the physics and yield higher accuracy solutions. The Method of Characteristics (MOC) has long been used in lattice physics analysis for cross section generation. Full-core analysis using MOC has typically followed a 2D/1D approach due to the computational costs of explicitly solving the full 3D MOC problem [1–4]. This approach uses 2D MOC in the radial direction and low order diffusion in the axial direction to couple the radial planes. While the 2D/1D approach has produced good results for many full-core problems, it is limited to problems that are relatively homogeneous in the axial direction.

Recently, there has been an expanded interest in solving the full 3D MOC problem with codes including MPACT [5, 6], DRAGON [7], and CRX [8]. However, scaling 3D MOC to full-core LWR geometries is still an open challenge due to the high memory and compute requirements [6, 9]. Progressing towards this goal is our primary motivation and this paper seeks to verify the accuracy of our implementation of a 3D MOC solver in OpenMOC, an open-source Method of Characteristics code developed at MIT. Additionally, this paper seeks to provide further insight into the MOC problem specifications required for heterogeneous geometry problems. We begin with a brief description of the key components of our 3D MOC implementation. Next we present verification results for the Takeda Model 1 benchmark and sensitivity analysis results on the number of polar angles, source region discretization, and axial track spacing required to axially converge a 3D quarter assembly problem. Finally, we end with a discussion of the implications of our analysis and insights into further improvements that can be made to increase the performance of 3D MOC solvers.

2. IMPLEMENTATION

The 3D MOC implementation is an extension to the existing 2D MOC implementation in OpenMOC that has been well documented elsewhere [10–12]. Several important characteristics of the 3D MOC solver in OpenMOC are described below:

- **Track Generation:** In extending OpenMOC to 3D, a new track generation procedure was developed to create 3D tracks that minimize the memory requirement compared to other track generation methods, presented in a previous study [13]. Importantly, this analysis highlighted the deficiencies of the simplified Modular Ray Tracing (sMRT) method in that the axial track spacing must be on the same order as the radial track spacing. As we will show in Section 3.2, the axial track spacing can be much coarser than the radial track spacing while maintaining solution accuracy. OpenMOC has three options for track generation: simplified Modular Ray Tracking (sMRT), Modular Ray Tracing (MRT), and 3D Global Tracking (3DGT). All simulations performed in this study utilize 3DGT.

- **Quadrature Sets:** Many 3D MOC implementations have opted for product quadrature sets that uncouple the azimuthal angle quadrature from the polar angle quadrature. During the track generation procedure, polar angles need to be corrected from that of the requested quadrature sets because MOC requires that tracks exactly link at the boundaries with complementary tracks determined by the geometry boundary conditions [13]. In this study, we have implemented and tested the accuracy of five polar quadrature sets that couple with the standard constant-angle azimuthal quadrature set. These include equal angle, equal weight, Gauss Legendre, Leonard, and Tabuchi Yamamoto polar quadrature sets. The formulas for computing the weights of the equal angle and equal weight quadrature sets are described in the Handbook of Nuclear Engineering [14]. The weights for the Gauss Legendre, Leonard, and Tabuchi Yamamoto quadrature sets were taken from reference without modification [14, 15]. It is important to note that in our implementation, only the equal angle and equal weight quadrature sets modify the weights based on the corrected polar angles; the Gauss Legendre, Leonard, and Tabuchi Yamamoto quadrature sets all use the unmodified weights that are based on the desired polar angles. For a more complete description of how the polar angles are modified during the track generation procedure, we point readers to our previous paper on track generation for 3D MOC [13].

- **CMFD Acceleration:** CMFD acceleration was implemented in OpenMOC according to the specification for MOC acceleration by Smith [16] with one minor modification to increase performance and stability. It has been recognized that CMFD is unstable for many problems so in this specification damping on the diffusion coefficient correction term is used for stabilization. Additionally, since most geometries are relatively homogeneous in the axial direction, the height of source regions and CMFD mesh cells can be quite large. This results in source regions that can be optically thick in the axial direction, but optically thin radially. For this reason, Larsen's effective diffusion coefficient is used in generating the CMFD equations [12, 17].

- **3D Ray Tracing:** In order to reduce memory requirements of storing all MOC track and segment information, axial on-the-fly ray tracing has been implemented. This is accomplished by pre-generating a 2D xy-plane of segments that incorporates all radial detail at every axial level. During transport sweeps the 3D segments are reconstructed on-the-fly using 2D xy-segment lengths and 1D axial meshes. This strategy implicitly transforms geometries into an axially extruded representation. The resulting algorithm consumes far less memory with minimal computational overhead for common reactor physics problems [18].

3. RESULTS FOR 3D MOC SOLVER IN OPENMOC

3.1. Verification with Takeda Model 1 Benchmark

The Takeda Model 1 benchmark problems have been used to verify the MOC solver in OpenMOC with several different quadrature sets and problem parameters. The purpose of this verification is to confirm the accuracy of the MOC solver and show the impact of different quadrature sets on the solution accuracy.

The Takeda benchmark suite is a collection of homogenized, simplified reactor configurations for validating 3D transport codes [19]. In this study, the Takeda model 1 rodded and unrodded configurations were simulated. The reference data provided with Takeda benchmark specification has a relatively large uncertainty of +/- 60 pcm, so multigroup Monte Carlo simulations were run with OpenMC to decrease the uncertainty on the reference eigenvalue. Table 1 lists the reference values from the benchmark specification and the reference values computed using OpenMC. All comparisons made in this paper are with the OpenMC values due to their reduced uncertainty.

Table I. Takeda Benchmark published and computed reference eigenvalues.

	Takeda Model 1 Unrodded		Takeda Model 1 Rodded	
	Published	**Computed**	**Published**	**Computed**
*k_{eff}	0.9780 ± (60)	0.97732 ± (3)	0.9624 ± (60)	0.96242 ± (3)
*Results are reported as: k_{eff} ± (uncertainty in pcm).				

Figure 1 shows the difference between the computed and reference eigenvalue at convergence, Δk_{eff}, versus the number of polar angles for the five quadrature sets described in Section 2. In all cases, 32 azimuthal angles were used with an azimuthal spacing of 0.05 cm and polar spacing of 0.05 cm. The source region mesh was refined to equal volume cubes of side length 0.25 cm.

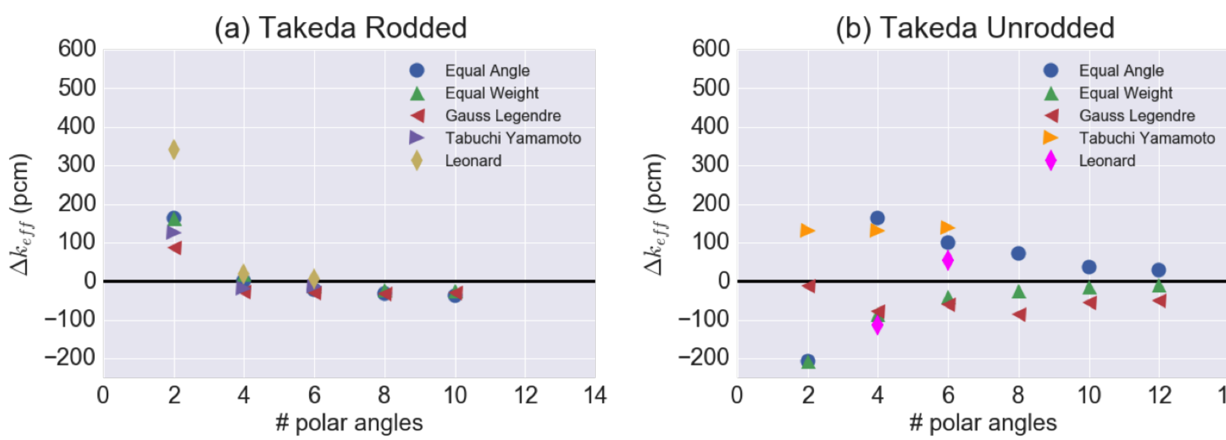

Figure 1. Plots of the residual error in k_{eff} for the Takeda Rodded (a) and Unrodded (b) configurations. As the number of polar angles is increased to 12 angles, the MOC solution converges to within 30 pcm of the reference eigenvalue for both problems.

The OpenMOC results show excellent agreement with reference values for both Takeda Model 1 benchmark problems. The homogenized regions make Takeda relatively easy to converge with only a few polar angles and in both cases only eight polar angles are required to converge the eigenvalues to within 100 pcm. The quadrature sets did not show significant differences in their accuracy on these small problems; however, the lack of heterogeneity between the fuel and moderator allow quadrature sets that perform poorly on real discretized LWR problems (e.g. Equal Angle Quadrature) to still achieve accurate results.

3.2. Sensitivity study on 3D C5G7 Benchmark

The C5G7 benchmark suite is a collection of quarter-core, heterogeneous-geometry simplified reactor configurations for verifying 2D and 3D transport codes [20]. In this study, the inner UO_2 assembly from the C5G7 3D Benchmark Unrodded case was studied. For simplicity, a quarter-assembly representation was used to allow the problem to be solved on single node with 160 GB memory. Figure 2 shows x-y, x-z, and y-z cut planes from the UO_2 assembly of the 3D C5G7 unrodded geometry.

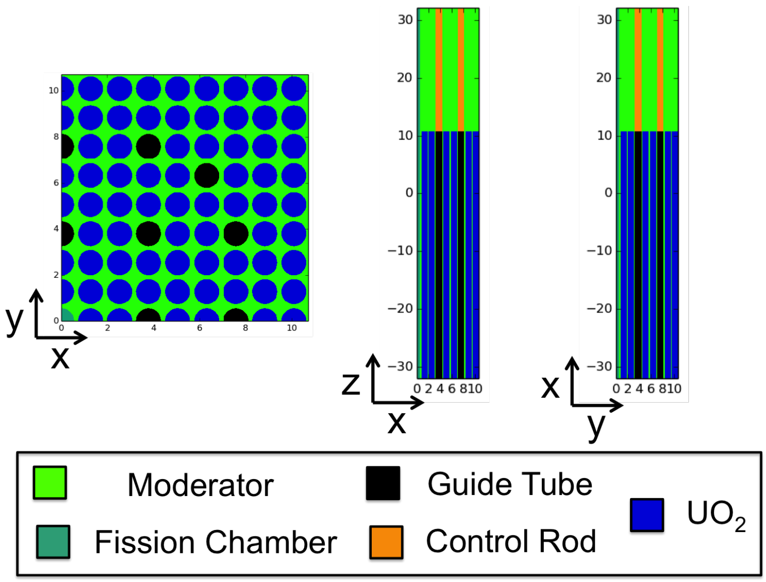

Figure 2. Plots of the x-y, x-z, and y-z cut planes colored by material for the UO_2 assembly of the 3D C5G7 unrodded geometry.

The radial discretization of each pin cell was kept relatively coarse with only four sector divisions to avoid excessive compute and memory requirements for converging the radial flux of the pins and because the requirements to radially converge the flux for the C5G7 and other LWR problems has been studied extensively with 2D MOC, including with OpenMOC [10]. The parameters required to converge the axial flux profile for 3D MOC is not well understood and it is thought that the axial track spacing can be significantly coarser than the radial track spacing due to the relatively homogeneous detail in the axial direction. The sensitivity study was therefore conducted on the flat source region (FSR) height, number of polar angles, and axial spacing between tracks. The case matrix of MOC parameters for the study is provided in Table II.

The case matrix from Table II was simulated and the eigenvalues were compared to the ultra-fine case with the 26 polar angles, 0.24 cm FSR height, and 0.025 cm axial track spacing. Figure 3 shows the difference in k_{eff} between each case and the ultra-fine case.

The polar angle convergence study in Figure 3a shows several important characteristics. For all FSR heights, the eigenvalue converges when 18 or more polar angles are used. This is significantly more than the 8 polar angles required to converge the eigenvalue for the Takeda benchmark problems and highlights the differences in MOC parameters required for solving problems with heterogeneous fuel and moderator regions. The FSR height has a significant impact on the eigenvalue with the 0.49 cm FSR height producing a $\sim$20 pcm bias compared with the cases with a 0.24 cm FSR height.

Table II. Parameters for 3D MOC sensitivity study.

Parameter	**Value(s)**
FSR height (cm)	0.24, 0.49, 0.97, 1.95
Number of polar angles	6, 10, 14, 18, 22, 26
Axial track spacing (cm)	0.025, 0.05, 0.1, 0.2, 0.4, 0.8
Radial track spacing (cm)	0.1
Quadrature set	Equal Weight
Number of azimuthal angles	16
Track generation method	3D Global Tracking

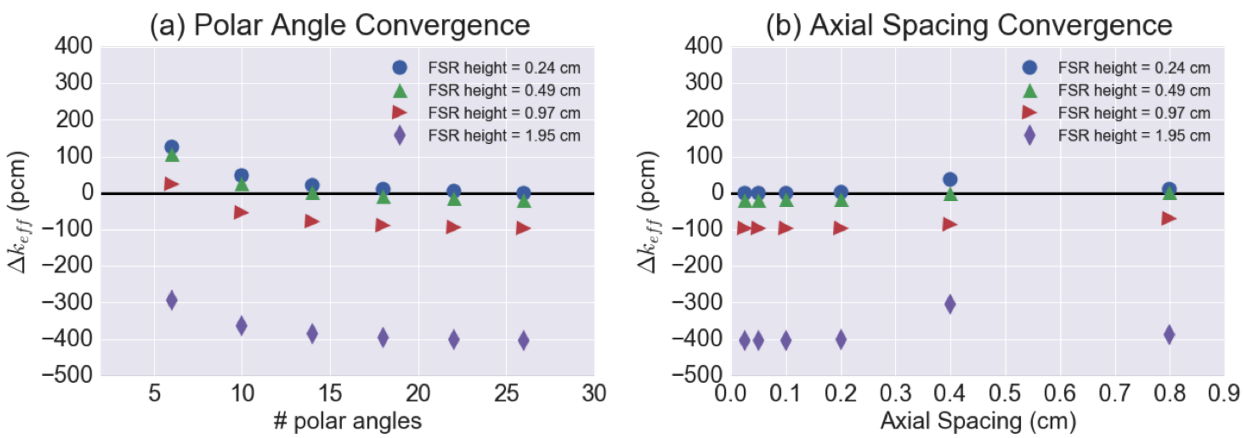

Figure 3. Plots of the difference in k_{eff} between each case and the ultra-fine case for polar angle and axial spacing convergence studies performed on the inner UO_2 assembly of the 3D C5G7 Benchmark Unrodded geometry.

The axial spacing convergence study in Figure 3b provides insight into the axial spacing required for a heterogeneous PWR problem. It is important to understand how much the axial track spacing can be coarsened while maintaining solution accuracy in order to minimize the memory and compute requirements of a problem. We have previously shown that the simplified modular ray tracking (sMRT) track generation method employed in MPACT limits the axial track spacing to be on the order of the radial track spacing [13]. For typical PWR problems, a radial track spacing of ≤ 0.05 cm is required to converge the radial flux profile. Therefore, if the axial track spacing can be several multiples of the radial track spacing, significant performance gains can be realized by going to a track generation method that allows the track spacings to be set (nearly) independently. Figure 3b shows that coarsening the axial track spacing to 0.2 cm results in ≤ 1 pcm change in the solution eigenvalue. Further increasing the axial spacing to 0.8 cm resulted in, at most, a 100 pcm change in the solution eigenvalue for all FSR heights tested.

4. DISCUSSION

One of the open questions in 3D MOC is what axial track spacing, source region discretization, and number of polar angles are required to converge a heterogeneous, full-core PWR problem. In a PWR geometry, the material composition is relatively homogeneous in the axial direction. Therefore, we would expect the axial MOC parameters to be relatively coarse compared to the radial MOC parameters (i.e. radial track spacing, number of azimuthal angles, and pin cell discretization). Some discussion on each axial MOC parameter is included below:

- **Polar Angles:** In 2D MOC, it is common to use between 6-10 polar angles (in [0,π]) with Tabuchi-Yamamoto or Gauss-Legendre quadrature sets. However, 2D MOC does not need to capture the axial heterogeneity due to partially inserted control rods, boundaries with the top and bottom reflector, and grid spacers. Resolving the flux around these features will likely require more polar angles than is used in 2D MOC. By solving a problem with partially inserted control rods (in the reflector region) and a top reflector boundary, we attempted to capture the sensitivity of axial MOC parameters with these effects included. Our results suggest that $\geq$18 polar angles are required when an equal weight quadrature is used. However, it is expected that fewer angles can be used when using quadratures sets better suited for 3D MOC, such as Tabuchi-Yamamoto or Gauss-Legendre.
- **Axial Spacing:** The axial track spacing for a 3D MOC problem is expected to be coarser than the radial track spacing due to the relatively homogeneous material composition in the axial direction. How much coarser is still an open question. Our results suggest that the axial track spacing can be *much greater* than the radial track spacing. Typically, the radial track spacing needs to be $\sim$0.05 cm to converge a 2D lattice problem. In our sensitivity study, increasing the axial track spacing to 0.2 cm had no significance on the eigenvalue and further increasing the axial track spacing to 0.8 cm resulted in, at most, a 100 pcm change in the eigenvalue. However, C5G7 has a relatively coarse group structure so the flux depressions caused by resonances are smeared out by the large group widths. Moving to a finer group structure would likely yield larger flux gradients near resonant absorbers that would require a finer axial track spacing to accurately model. Furthermore, our analysis only looked at k_{eff} whereas we are often more interested in control rod worths and pin powers, which are more sensitive to track laydown than global parameters like k_{eff}.
- **FSR Axial Discretization:** Typically, 8+ sector divisions, 3+ fuel rings, and 2+ moderator rings are required to accurately model the radial flux shape within pins of a lattice. In this study, we found that $\sim$0.25-0.5 cm height flat source regions were required to converge the eigenvalue for a lattice problem. Higher order source regions have been implemented in 2D MOC and shown to produce accurate results with no fuel or moderator rings [21]. Therefore, it is expected that higher order source approximations will allow axial source regions to be further increased in height to $\sim$1-2 cm. Currently, we are working on implementing quadratic axial sources in OpenMOC.

5. CONCLUSION

This study has verified the 3D MOC solver implemented in the OpenMOC neutron transport code using the Takeda Model 1 benchmark problem. The eigenvalue results show excellent agreement with the reference values for several quadrature sets. The results from our sensitivity study on the axial MOC parameters provide insight on the values of these parameters required to converge a 3D PWR lattice problem. Interestingly, our results showed that the axial track spacing can be increased to 0.2 cm with no significant impact on the eigenvalue and further increasing the axial track spacing to 0.8 cm resulted in, at most, a 100 pcm change in the eigenvalue. The eigenvalue showed some sensitivity to the number of polar angles and at least 18 polar angles were required to converge the eigenvalue to within 10 pcm of the ultra-fine case when using an equal-weight quadrature set. The axial source region discretization was required to be $\sim$0.25-0.5 cm in height to converge the eigenvalue when flat sources were employed. The insights provided in this study are valuable in helping answer the open questions in 3D MOC and validating our previous work on understanding the track generation procedure for 3D MOC. Furthermore, the lessons learned have led to new ideas for further improving the 3D MOC algorithm such as implementing higher order axial sources.

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