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VERIFICATION OF THE SHIFT MONTE CARLO CODE WITH THE C5G7 REACTOR BENCHMARK

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ABSTRACT

Shift is a new hybrid Monte Carlo/deterministic radiation transport code being developed at Oak Ridge National Laboratory. At its current stage of development, Shift includes a parallel Monte Carlo capability for simulating eigenvalue and fixed-source multigroup transport problems. This paper focuses on recent efforts to verify Shift's Monte Carlo component using the two-dimensional and three-dimensional C5G7 NEA benchmark problems. Comparisons were made between the benchmark eigenvalues and those output by the Shift code. In addition, mesh-based scalar flux tally results generated by Shift were compared to those obtained using MCNP5 on an identical model and tally grid. The Shift-generated eigenvalues were within three standard deviations of the benchmark and MCNP5-1.60 values in all cases. The flux tallies generated by Shift were found to be in very good agreement with those from MCNP.

Key Words: Monte Carlo, verification, C5G7, eigenvalue.

1. INTRODUCTION

Shift is a radiation transport package being developed within the Denovo [1] framework for implementation as a hybrid code, utilizing the capabilities of both deterministic and Monte Carlo codes. Also, recognizing the need for parallel computing in the Monte Carlo radiation transport community and the difficulty to retrofit currently used codes to adequately take full advantage of parallel resources, Oak Ridge National Laboratory is developing Shift to be massively parallel. Shift supports multiple parallel decompositions ranging from full domain replication, full domain decomposition, domain decomposition with overlapping regions, and multiple-set-overlapping domain (MSOD) decomposition [2]. Shift is written in C++ and is designed to allow multiple physics and geometric representations in the Monte Carlo transport components without code modification. Thus, for example, multigroup and continuous energy physics can be

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supported without changing the core transport mechanics; all of the physics-dependent operations are encapsulated in the physics abstraction. Currently, Shift supports KENO and Reactor-Tool-Kit geometry packages and simple multigroup physics. Implementations are under development that will allow MCNP [3] physics and geometry support in the immediate future. Finally, because Shift is written in the same code base as the Denovo S_N solver, it can efficiently access the deterministic code mesh generation and solver mechanics to enable integrated hybrid capability.

The objective of the verification effort performed in this work is to ensure that the Monte Carlo component of the code is working correctly. This would also verify that any changes made to other parts of the code (i.e., geometry) had been implemented correctly. To rigorously assess the validity of the Monte Carlo package, a challenging problem with a significantly non-uniform fission source was selected. The results were then compared against those found in the benchmark report as well as results from MCNP5 with the same model. Additionally, flux tally comparisons between MCNP and Shift were performed.

2. BENCHMARK PROBLEM

The benchmark problems chosen for this verification study were the two-dimensional (2D) and three-dimensional (3D) C5G7 benchmark problems [4, 5]. The 2D C5G7 problem was created by the Organisation for Economic Co-operation and Development Nuclear Energy Agency (OECD/NEA) to benchmark radiation transport codes in a limited-scale light water reactor problem that avoids assembly or full pin-cell homogenization. References 4 and 5 provide reference Monte Carlo solutions as well as solutions obtained by benchmark participants using a variety of codes.

The benchmark models consist of 16 light-water-moderated 17×17 fuel assemblies with Uranium Oxide (UO_2) and mixed oxide (MOX) assemblies distributed in a checkerboard pattern and surrounded on all sides by a light water reflector. The core has quarter-core radial and half-core axial symmetry; thus, the models are one-eighth core with three reflective boundary conditions, as shown in Appendix A. Each assembly has a fission tube in the center grid-cell as well as 24 guide tubes for control rods, which are used in the 3D model, as shown in Appendix B. The MOX assemblies have pin-cells with three different levels of enrichment (4.3%, 7.0%, and 8.7%). The fuel rods, fission chamber, guide tubes, and in the 3D cases, the control rods have been homogenized. The fuel rod, guide tube, and fission chamber radii are all 0.54 cm with lattice pitch of 1.26 cm.

The 2D case was built as a 1-cm-thick horizontal slice with reflective boundary conditions on the top and bottom. In the 3D cases, the fuel assemblies are divided into three equal-length (14.28 cm) axial sections, shown in Appendix C. In the “Rods Out” case, the control rod arrays reside in the reflector region above the fuel assemblies. In the “Rodded A” case, the control rod array is inserted one-third of the way into the center-most fuel assembly (UO_2). In the “Rodded B” case, the control rod arrays are inserted two-thirds of the way into the center-most fuel assembly and one-third of the way into the two MOX assemblies. As the core is reflected axially, these cases simulate the control rods being inserted from the top as well as the bottom.

The materials are described by multi-group cross sections. The group structure is available in Appendix D. The benchmark specification also includes an MCNP-format cross section file containing macroscopic cross sections (atom density of all materials was set to 1 atoms/b-cm). The normalized cross sections were manually entered into the Shift input. The benchmark paper also provides pin power results, but these have not yet been compared.

Inputs for both MCNP and Shift were generated by the authors. MCNP5 version 1.60 was used. The models were built based on the dimensions given in References 4 and 5.

3. METHODOLOGY

Determining whether or not the fission source has converged is difficult in any Monte Carlo problem. MCNP has several built-in calculations to monitor source convergence; however, source convergence can never truly be guaranteed. MCNP calculates the Shannon entropy of the fission source in each cycle and recommends a minimum number of cycles that should be skipped in order to ensure that the entropy metric has converged before collecting statistics. In all cases performed, the initial fission source was uniformly distributed across the fuel assemblies. The maximum number of inactive cycles suggested for all cases based on the Shannon entropy was approximately 450, so 500 inactive cycles were simulated in each case. To obtain highly converged estimates of both the eigenvalue and flux tallies, 300,000 histories per cycle were simulated. This results in 210 million active histories, as compared to the 300 million used in the 2D benchmark and 500 million used in the 3D benchmark. For convenience, both MCNP and Shift were executed in parallel using domain replication.

The comparisons made between the published benchmark and Shift results were limited to eigenvalues. The differences between the benchmark, Shift, and MCNP eigenvalues were calculated in percent mille-k (pcm, $10^{-5}\ \Delta k$). More detailed comparisons were made between the MCNP and Shift models. Both codes performed normalized flux tallies over every individual pin-cell within the assemblies and further subdivided, in the 3D cases, between the three axial levels used in the benchmark. This resulted in 3468 tally cells for each of the 3D cases and 1156 tally cells for the 2D case along with associated uncertainties. The tallies were similarly normalized to allow for a direct comparison. Relative percent differences were calculated using equation 1.

$$Rel.\%\ Diff. = 100 \times \left|\frac{\varphi_{MCNP} - \varphi_{Shift}}{\varphi_{MCNP}}\right| \tag{1}$$

This metric was used due to its scalability and potential for discerning bias. Comparison between the results from the two codes also required propagation of their respective errors (Equation 2).

$$\sigma_{Total} = \sqrt{{\sigma_{MCNP}}^2 + {\sigma_{Shift}}^2} \tag{2}$$

4. RESULTS

Table I presents eigenvalue results from the published benchmark and the MCNP and Shift codes, along with the associated standard deviations and the results of the propagation of error calculations. Also shown in Table I are the differences in pcm.

Table I. Benchmark, MCNP, and Shift eigenvalue results for the 2D and 3D C5G7 problems

Case	Source	Eigenvalue	Std. Dev. [pcm]	Error Propagation Std. Dev. [pcm]	vs. benchmark [pcm]	vs. MCNP [pcm]
2D	**Benchmark**	1.18655	3	-	-	-
	MCNP	1.18651	5	8.34	4	-
	Shift	1.18652	7		3	-1
Rods Out	**Benchmark**	1.14308	3	-	-	-
	MCNP	1.14298	5	8.30	10	-
	Shift	1.14310	7		-2	-12
Rodded A	**Benchmark**	1.12806	3	-	-	-
	MCNP	1.12822	5	8.01	-16	-
	Shift	1.12807	6		-1	15
Rodded B	**Benchmark**	1.07777	3	-	-	-
	MCNP	1.07773	5	8.30	4	-
	Shift	1.07759	7		18	14

Shift currently implements only a track-length estimator for the eigenvalue, whereas MCNP implements track-length, absorption, collision, and a combined estimator. Nonetheless, the differences between eigenvalues in all cases are less than three standard deviations calculated with the propagation of error. Moreover, the difference in the magnitude of the estimated standard deviations calculated by Shift and our MCNP simulations are relatively small. This statistical agreement between the eigenvalue results from MCNP and Shift supports further comparison between flux tallies from the two models.

The relative percent differences in flux tallies between Shift and MCNP were calculated. Both Shift and MCNP use track length estimators for flux tallies. While comparisons to the pin power results in the benchmark paper were not performed, a comparison of pin-wise flux tallies between Shift and our MCNP results was performed. This comparison is of a much finer scale than the flux tally results provided with the benchmark, which only presented the maximum and average pin power results for various regions of the core. The range of relative percent

differences for each case is shown in Table II along with the fraction of the tally results that fell within three standard deviations of the MCNP result.

Table II. Comparison of MCNP and Shift tallies

Case	Range of relative % differences in flux tally	Tallies within 3σ
2D	-0.456 – 0.492	98.01%
Rods Out	-1.23 – 1.09	98.41%
Rodded A	-1.35 – 0.846	97.95%
Rodded B	-1.53 – 0.965	96.80%

The flux tallies reported by Shift are within 2% of the values reported by MCNP. The target value for the uncertainty analysis is to have 99.8% within three standard deviations, assuming a Gaussian distribution. Unfortunately, none of the cases have achieved this. However, it is reasonable to suspect that the cause of fewer-than-expected tallies falling within three standard deviations is small differences in the degree of fission source convergence and/or an underestimation of the tally uncertainties due to cycle-to-cycle correlations. Figure 1 shows the relative percent difference in the flux tallies from the upper axial slice of the fuel assemblies of the Rodded B case. This section was selected because it displays the greatest differences. As the figure shows, there are no tallies with a difference greater than 2% from the MCNP results, but most are well below that.

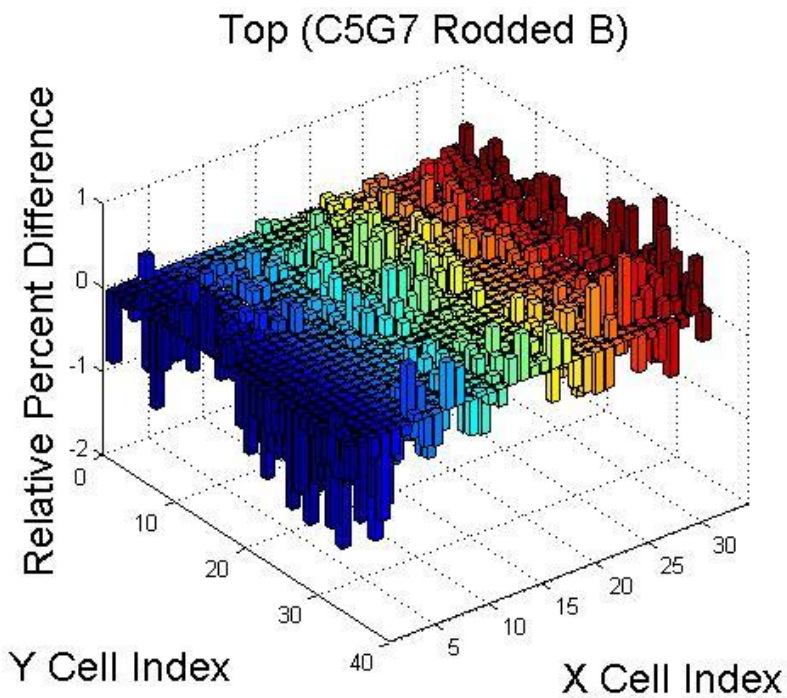

Figure 1. Relative percent difference of flux tallies in top section of Rodded B case between Shift and MCNP.

In Fig. 1, the center of the core is in the back corner. The largest differences are in the low-flux regions near the reflector, where the uncertainties are the highest. However, there appears to be a systematic difference in the tally results along the x-dimension of the model. Given that this is a rodded case of a high-leakage core model with both UO_2 and MOX fuel assemblies, the differences may be attributed to different degrees of fission source convergence within this axial slice. More computational effort would be required determine if this is, in fact, the case.

5. CONCLUSION

The eigenvalues between Shift, MCNP, and the benchmark reference all agreed within 18 pcm. An acceptable number of tallies fell within the combined standard deviations of the two codes, taking into consideration the cycle-to-cycle correlation and potential for an unconverged source inherent in any Monte Carlo eigenvalue problem. The observed agreements indicate that the Shift Monte Carlo package gives reasonable results for the benchmark problem examined in this study.

Further comparison with the benchmarks' pin power results will be performed in the future. Larger scale benchmark problems will be used as well. Finally, more detailed studies comparing Shift with currently available Monte Carlo codes such as MCNP in highly parallel environments will be performed, especially utilizing the domain decomposition capability of Shift.

ACKNOWLEDGMENTS

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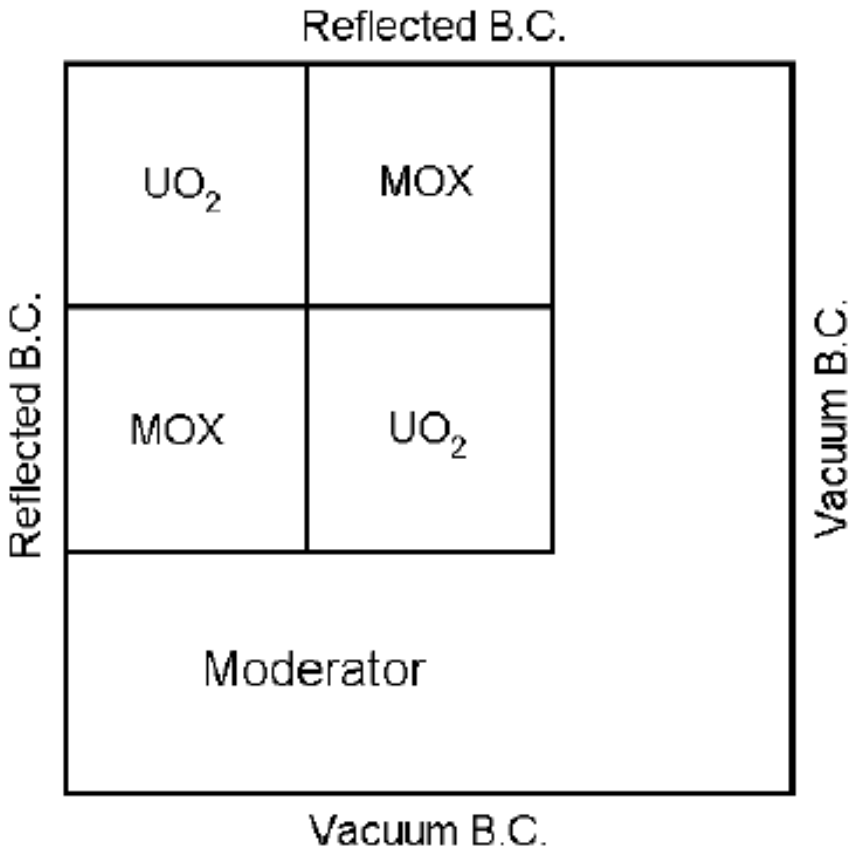
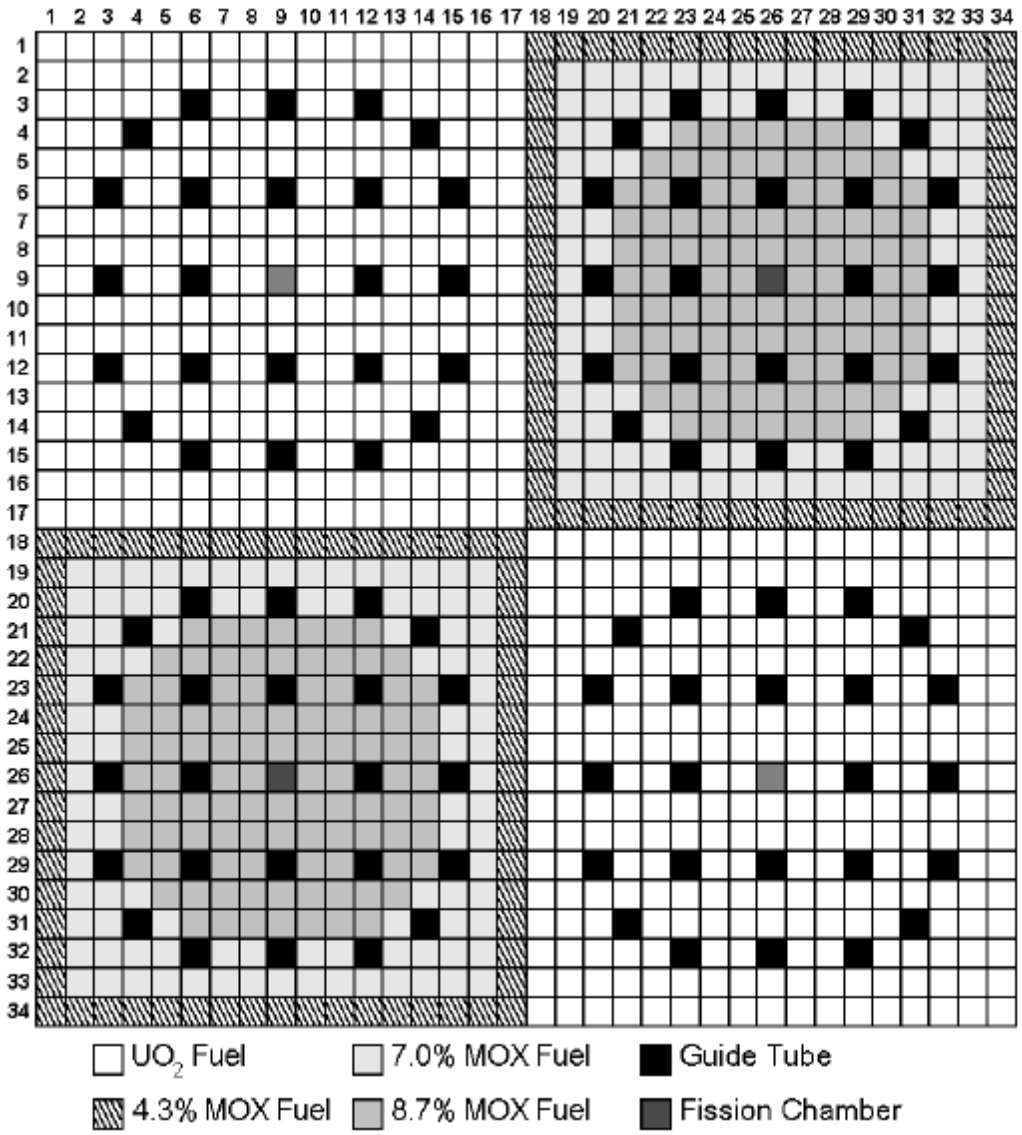
APPENDIX A

Core configuration of the 2D C5G7 benchmark problem.



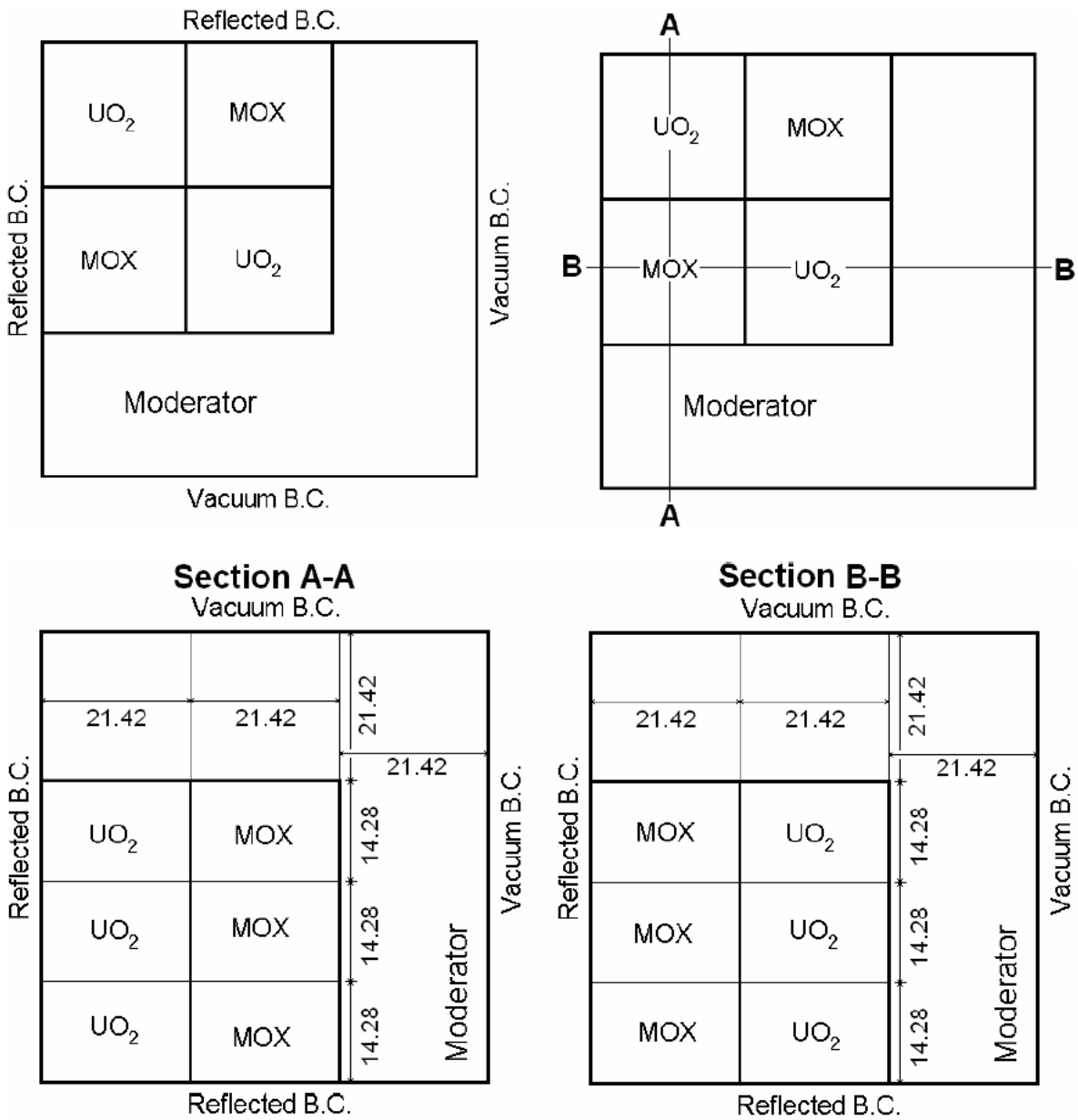
APPENDIX B

Configuration of the fuel rods of different fuel types, guide tubes, and fission chambers in the 2D and 3D C5G7 benchmark problem.



APPENDIX C

Configuration and division of the fuel assemblies in the 3D C5G7 benchmark problem.



APPENDIX D

Group structure for the C5G7 problem. Low energy cutoff is 10 μeV.

Group	Upper Energy
1	20 MeV
2	1 MeV
3	500 keV
4	3 eV
5	0.625 eV
6	0.1 eV
7	0.02 eV