The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

IMPROVED MONTE CARLO ADAPTATION OF THE HETEROGENEOUS COARSE-MESH TRANSPORT METHOD

Benoit Forget and Farzad Rahnema
Nuclear and Radiological Engineering / Medical Physics Program
George W. Woodruff School of Mechanical Engineering
Georgia Institute of Technology
Atlanta, GA, 30332-0405
farzad.rahnema@nre.gatech.edu

ABSTRACT

Recently, a coarse mesh transport method that couples Monte Carlo response function calculations to deterministic sweeps was extended to 2D (x,y) geometry. The deterministic sweeps were used to converge the partial currents on the coarse mesh boundaries while dealing with the statistical uncertainties in a straightforward fashion. The initial formulation used the cosine-current angular distribution and the spatially flat-flux approximation. This method yielded satisfactory results on the C5G7 MOX benchmark, but knowing that the cosine-current approximation breaks down near regions with strong absorption or in the vicinity of the coarse mesh corners, a new formulation was sought. The angular and spatial approximations were replaced by orthogonal polynomial expansions (Legendre polynomials) to develop a better representation of the partial currents connecting each coarse mesh. The method was then tested on two benchmark problems: a small 2D one group problem and the C5G7 MOX problem. In the first problem, using a 2nd order expansion in all variables (space, polar angle and azimuthal angle) with two segments per edge, we obtain an average pin power, a root mean square and a maximum errors of 0.09%, 0.11% and 0.18%, respectively. The eigenvalue of the coarse mesh method differs from the MCNP reference solution by -0.06%. In the C5G7 MOX benchmark problem, using 2nd polynomials expansions in all variables, the eigenvalue error is 0.06%. The average pin power, the root mean square and the maximum errors are 0.51%, 0.65% and 2.18%, respectively.

Key Words: Heterogeneous Coarse Mesh Methods; Transport Theory; MCNP; Orthogonal Polynomial Expansions

1 INTRODUCTION

Recently the coarse mesh transport method of reference [1] was extended to 2-D(x,y) geometry by using the Monte Carlo code MCNP as the response function generator for the deterministic transport sweeps which converge the angular partial currents on the coarse mesh boundaries. The propagation of statistical uncertainties was accounted for in a straightforward manner. Because of the source sampling limitation in MCNP, the currents transmitted between coarse meshes were assumed to be cosine distributed in angle and piecewise-constant on an arbitrary number of equal-width segments [2, 3]. It was found that the cosine current approximation breaks down near regions with strong absorption [4] or coarse mesh corners and that spatially constant flux may require a very fine segmentation (e.g., near control blades).

In this paper, the cosine current and uniform surface flux (current) approximations are replaced by a polynomial expansion in both angles and space. Previous studies [5], using a modified version of MCNP [6], have successfully expanded the polar angle in 1-D using Double Legendre Polynomials (DP_n), which met the requirement of being orthogonal on the half-space.

We extended this idea to 2-D by not only expanding the polar angle but also the azimuthal angle and the spatial variable in Legendre polynomials. Section 2 contains the description of the expansion technique and its implementation in MCNP and coupling with the coarse mesh method. The method's accuracy and speed are evaluated in section 3. The evaluation is performed by considering a very simple and small 2-D problem and the C5G7 2-D MOX PWR benchmark problem. The conclusions and future directions are found in section 4.

2 DESCRIPTION OF THE METHOD

In recent papers [1-3], the coarse mesh method was developed with an imposed angular distribution (cosine-current) and flat current approximation on an arbitrary number of segments along each edge. This method gave good results for the 2-D MOX PWR benchmark problem, but the accuracy depended on the number of segments per edge. Results improved until four segments per edge were used. However, the accuracy began to deteriorate slightly as the number of segments was further increased without refining the angular shape of the current. It was clear that better approximation of the angular current was needed to improve the accuracy of the method.

Building on the ideas developed in reference [8] using a discrete polynomial expansion within a discrete-ordinates formulation of the coarse mesh method and the ideas developed in 1-D in reference 5 using continuous polynomial expansion within MCNP in a response matrix formulation, we extended the 2D coarse mesh method to allow for continuous polynomial expansion in space and angle. Each coarse mesh is characterized by a set of response functions relating the quantities of interest to an incident current. These responses are obtained for each unique coarse mesh by using MCNP to solve a series of fixed source problems in which the fission source is scaled by *k*. This formulation makes the response functions dependent on the global solution (*k* and the angular partial currents at the mesh boundaries). Since the global solution is not know *a priori*, the method is based on a two-level process with inner iterations performed on the partial currents of each coarse mesh (sweeps) and the outer iterations performed on the system *k* (or equivalently the response functions). As in the 1D case [8, 9], a linear interpolation scheme can be used to update the response functions between outer iterations. Experience with 1-D and 2-D benchmark problems have shown that the residual error in the converged local solution (e.g., fuel pin power distribution) is less than 1%. The statistical error of the response functions can be easily propagated through the deterministic sweeps.

2.1 Response Functions

Starting from the work in reference 5, we further modified MCNP4C to implement the fission source scaling factor, the surface source sampling on polynomials in space and angle and the tallying on the polynomial expansion coefficients. The spatial ($x \in \{0, \Delta_x\}$) and azimuthal angle ($\varphi \in \{0,\pi\}$) variables were expanded using Double Legendre polynomials while the polar angle variable ($\mu \in \{-1,1\}$) was expanded using Legendre polynomials. As was done before for the source sampling in [5, 8], the source was sampled by linear combinations of the Legendre expansions to avoid the presence of negative weights associated with expansions orders greater than zero.

A response function is defined as a function relating a given quantity to an incoming current, as shown in Figure 1. In this figure, R_j represents the exiting surface current response and the R_z denotes the response of a quantity of interest inside the coarse mesh, for example, the fission density inside the region. This consists of solving a fixed source problem with a given distribution (polynomial expansion) with vacuum boundary conditions for each unique coarse mesh.

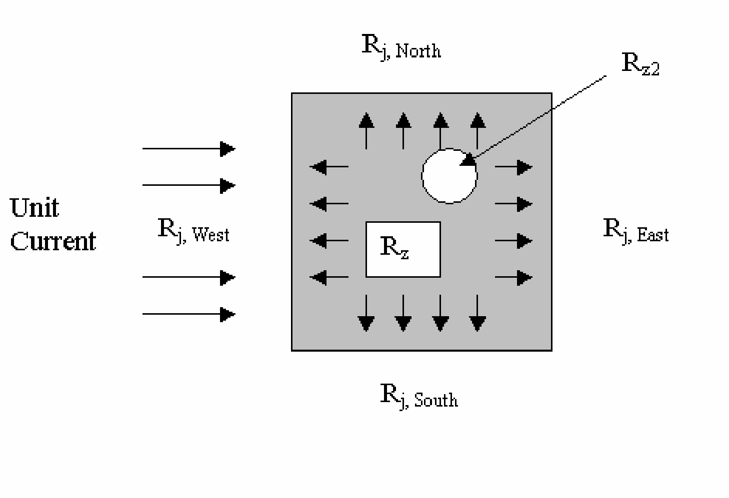

Figure 1: Response Function Generation for a Given Coarse Mesh

The values tallied in these simulations are the moments of the Legendre polynomials (or Double Legendre polynomials) on the exiting currents in each energy group on each boundary segment. The total rod fission densities and the total neutron production in the coarse mesh are also tallied.

2.2 Coarse Mesh Calculation

Once the response functions for each unique coarse mesh have been computed using the appropriate boundary condition (surface source), a deterministic sweeping technique [3, 10] is used to calculate the outgoing half-space currents from each coarse mesh and any other quantity of interest (i.e. fission density in each fuel pin). The exiting current J^+ (J^{out}) is calculated from the following relation between the current response function R_J and the entering current J^- (J^{in}) for each coarse mesh V_i

$$J_s^{out}(r,\hat{\Omega},E) = \sum_S \int_\Omega \int_r \int_E R_{J,s}(r' \to r, \hat{\Omega}' \to \hat{\Omega}, E' \to E) J_s^{in}(r',\hat{\Omega}',E') dE' dr' d\hat{\Omega}' \quad (1)$$

In the above equation, r represents the position of the neutron on a coarse mesh surface s (a line in the 2-D case), while $\hat{\Omega}$ is the unit vector in the direction of the neutron and E is the energy variable. The summation is performed over all surfaces and the integrals are performed over the entire energy range, the angular half-space and spatial limit of each surface (line). Equation (1) can be conceptually seen as a scattering kernel which redistributes neutrons in space, angle and energy. The exiting currents then become the entering currents of the neighboring cells. For other quantities, Z, whose final value does not depend on space and angle (i.e. fuel pin fission density), the following relation holds

$$Z = \sum_{S} \int_{\Omega} \int_{r} \int_{E} R_{Z,s}(r',\hat{\Omega}',E') J_s^{in}(r',\hat{\Omega}',E') dE' dr' d\hat{\Omega}' \quad (2)$$

3 RESULTS

In order to test the modifications associated with the polynomial expansions in MCNP and the coarse mesh code, two benchmark problems previously solved with the coarse mesh method will be used. The first benchmark is a simple 2-D problem that was solved very accurately and efficiently with the cosine-current version of the coarse mesh method. Its size makes it very practicable for debugging purposes because the problem is simple. The second benchmark is the C5G7 MOX problem [7] for which good results were obtained with the cosine-current version of the coarse mesh method. The high heterogeneity of this configuration will indicate beyond any doubts if the new formulation is an improvement over its predecessor.

3.1 Small 2-D Benchmark

This benchmark problem, illustrated in Figure 2, is composed of two unique coarse mesh types that differ in fuel enrichment (type 1: 2% enriched UO_2 ; type 2: 1% enriched UO_2). The geometrical description of this problem can be found in reference 3. The reference solution (the system eigenvalue and rod fission densities (FD)) was obtained with MCNP4B2 code [6]. The one group cross-sections [3] for the unique assemblies were generated by the collision probability code HELIOS [11]. The reference calculation was performed on a $1/4^{th}$ model of the system with five million histories. The eigenvalue was found to be 1.18471 ± 0.00021, and the relative uncertainties in the rod fission density (FD) results were less than 0.1%.

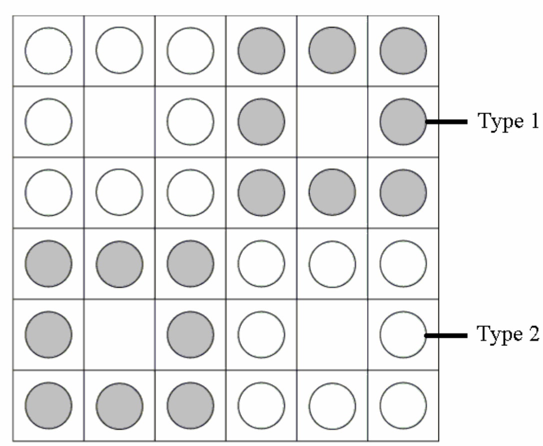

Figure 2: Geometrical Configuration of the Small 2-D Benchmark Problem.

Results using different combination of expansion orders in space and angle are compared to the reference solution in Table I. All the response function calculations were performed with two million particles on one segment per edge with the reference system eigenvalue as a scaling factor. These results thus represent the best case scenario where the outer iterations converge exactly to the true eigenvalue. The results with the cosine-current assumption taken from reference [3] are also presented in the last column to show the improvements achieved with the new formulation.

Table I: Results of the Small 2-D Benchmark Problem with One Segment per Edge.

	{0,0,0}[a] (%)	{0,1,1} (%)	{0,2,2} (%)	{1,2,2} (%)	{2,2,2} (%)	Cosine, FFA[b] (%)
RE[c] k	-0.89	-0.89	0.21	0.22	0.22	-0.16
AVG RE[d]	1.04	1.04	0.28	0.12	0.13	0.27
RMS[e]	1.08	1.09	0.35	0.16	0.15	0.32
MAX RE[f]	1.60	1.64	0.67	0.35	0.31	0.66
# RF[g]	2	8	18	36	54	2

[a] {…, …, ...} : Defines the expansion order as follows {spatial, polar, azymuthal}
[b] Cosine-Current distribution with Flat-Flux Approximation
[c] Relative Error of the eigenvalue (k)
[d] average relative error of the pin powers.

$$avg\ RE = \frac{\sum_N |e_n|}{N},$$

where N is the number of fuel pins and e_n is the calculated per cent error for the nth pin power, p_n.

[e] Root Mean Square Error of the pin powers

$$RMS = \frac{\sqrt{\sum_N e_n^2}}{N}$$

[f] Maximum pin power error
[g] Number of response functions used in the calculation

From the results in Table I, we see a consistent improvement with the increasing expansion orders. The {0,2,2} case leads to results comparable to the cosine-current distribution with the flat-current approximation. When the spatial expansion (1st order) is added to the previous case, the pin power errors decrease from 0.28 % to 0.12%. The maximum error also drops to almost half its value (0.67% to 0.35%). Increasing the spatial expansion order (2nd order) has no noticeable effect on the accuracy. The variations are believed to be within the statistical uncertainties associated with the stochastic response function generation.

The results in Table II differ from the previous table by having two segments per coarse mesh edge. This segmentation allows for different representations of the angular current along the same coarse mesh edge, thus giving a truer representation at low order. The response functions were also calculated with 2 million particles.

Table II*: Results of the Small 2-D Benchmark Problem with Two Segments per Edge.

	{0,0,0} (%)	{0,1,1} (%)	{0,2,2} (%)	{1,2,2} (%)	{2,2,2} (%)	Cosine, FFA (%)
RE k	-0.97	-0.98	-0.07	-0.06	-0.06	-0.16
AVG RE	0.91	0.82	0.13	0.09	0.09	0.12
RMS	0.95	0.84	0.15	0.10	0.11	0.14
MAX RE	1.25	1.18	0.28	0.16	0.18	0.26
# RF	4	16	36	72	108	2

* See legend of Table I for explanation of all the terms

We must point out is that the number of response functions is doubled in going from one segment to two segments per edge except for the cosine-current approximation. In the latter case, we made use of the symmetry along the half-plane of the coarse mesh to reduce the number of response functions. The use of symmetry in the polynomial expansions case is also possible. However additional coding work is required to allow for this option. The odd expansion order in both space and azimuthal angle do not allow for the use of symmetry but all other expansion orders do. For example, the number of response functions for the {2, 2, 2} case would be reduce to 84 from 108 by making use of the symmetry.

The results in Table II show once again a consistent improvement as the expansion order increases until we reach a point where the errors are believed to be within the statistical uncertainty of the results. The results for the {0,2,2} case are still close to the cosine-current representation, but as the spatial order is increased, greater accuracy is achieved. With a linear expansion in space (1^{st} order), the average error in the pin power distribution drops to 0.09%. The maximum error reduces to 0.16%. The eigenvalue error is also reduced to -0.06% compared to 0.16% for the cosine-current representation. The cosine-current approximation leads to very accurate results for a very low number of response functions, but this angular representation may not be valid for more complex problems. The goal of this benchmark problem was to show that the accuracy can be improved by polynomial expansion, but it remains to be shown that the added pre-computational time is worth the gain in accuracy.

3.2 C5G7 2-D MOX Benchmark

The C5G7 2-D MOX benchmark problem, shown in Figure 3, is a more realistic representation of a reactor configuration due to its size, geometry, and heterogeneity. The geometric data and seven-group cross sections for this problem as well as the reference solution can be found in reference 7. The problem is composed of three unique coarse mesh types: a MOX fuel assembly, a UO_2 fuel assembly, and water reflector.

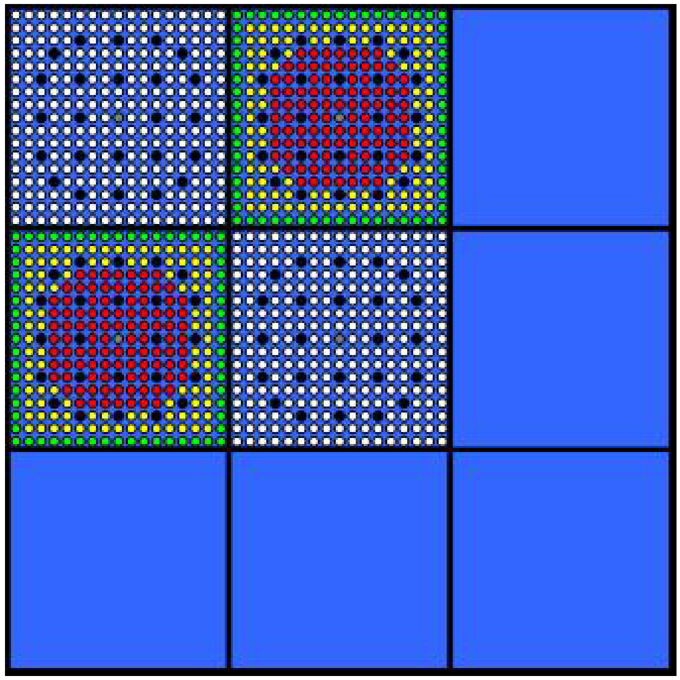

Figure 3: Geometrical Configuration of the C5G7 2-D MOX Benchmark Problem

This problem was solved by using a polynomial expansion on a different number of segments per edge. Table III contains the results for the case with one segment per edge. Table IV summarizes the results for the case with two segments per edge and Table V gives the results for the case with four segments per edge. The last case is consistent (in terms of the number segment per edge) with the best case obtained with the cosine-current distribution version of the coarse mesh code. All response functions were generated with ½ million particles. The reference system eigenvalue was used to scale the fission source. These results thus represent the best case scenario where the outer iterations converge exactly to the true eigenvalue.

Table III*: Results of the C5G7 MOX Benchmark Problem with One Segment per Edge.

	{0,0,0} (%)	{0,2,2} (%)	{1,2,2} (%)	{2,2,2} (%)	Cosine, FFA (%)
RE k	-2.11	-2.79	-0.04	0.05	-1.82
AVG RE	13.45	12.00	1.67	1.13	11.55
RMS	20.00	17.33	2.32	1.55	16.74
MAX RE	120.67	107.94	12.09	8.15	103.81
# RF	21	189	378	567	21

* See legend of Table I for explanation of all the terms

The results in Table III show clearly the advantage of using the polynomial expansion. Using the polynomial expansion in space as opposed to the flat current approximation contributes significantly to reducing error both in the pin power distribution and the eigenvalue. The 1st order spatial expansion has an eigenvalue error of -0.04% compared to the -1.82% obtained with the cosine-current distribution. The second order expansion in both angles gives results that are very similar to the cosine-current approximation results. Adding the spatial expansion greatly reduces the eigenvalue and pin power errors indicating the importance of a good spatial presentation in geometrically realistic reactor calculations.

Table IV*: Results of the C5G7 MOX Benchmark Problem with Two Segments per Edge

	{0,0,0} (%)	{0,2,2} (%)	{1,2,2} (%)	{2,2,2} (%)	Cosine, FFA (%)
RE k	-0.18	-1.00	0.05	0.05	-0.67
AVG RE	6.06	3.60	0.90	0.77	2.76
RMS	8.65	5.27	1.34	1.01	4.29
MAX RE	46.33	40.09	9.12	5.23	34.92
# RF	42	378	756	1134	42

* See legend of Table I for explanation of all the terms

In Table IV, we observe an excellent agreement in the pin powers and eigenvalue errors between the {0,2,2} case and the cosine-current results. Once again, the improvement is even greater when the spatial expansion is added. The eigenvalue error drops to 0.05% while the pin power errors are considerably lower.

Table V*: Results of the C5G7 MOX Benchmark Problem with Four Segments per Edge

	{0,0,0} (%)	{0,2,2} (%)	{1,2,2} (%)	{2,2,2} (%)	Cosine, FFA (%)
RE k	0.66	-0.25	0.06	0.06	0.12
AVG	5.47	1.28	0.59	0.51	0.68
RMS	6.94	1.87	0.88	0.65	1.17
MAX	23.51	11.96	6.39	2.18	6.99
# RF	84	756	1512	2268	84

* See legend of Table I for explanation of all the terms

The results presented in Table V are for the case with four segments per edge. As mentioned previously, this case is the only one for which the statistical uncertainty was computed (propagated). For the {2,2,2} case, the statistical uncertainty of the eigenvalue was 0.04% (or 1.1873 ± 0.0005) and the pin power uncertainty ranged from 0.22% to 0.42%. From reference 3, the statistical uncertainty on the pin power distribution of the cosine-current case ranged from 0.16% to 0.33%. Table V shows once again that good results are obtained with low order expansions in all three variables. For the {2,2,2} case, the eigenvalue error is 0.06% and the pin power average error is 0.51%. The most interesting result is the maximum (peak) pin power error which reduces from 6.99% in the cosine-current case to 2.18% in the {2,2,2} case.

Note that the location in which the maximum error occurs has changed. In the previous study, the lower right corner pin was always the one with the maximum error because of its location and its low power, but with the polynomial expansion, the distribution of errors is more evenly distributed as can be seen in Figure 4 for the case {2,2,2} with 4 segments per edge. This figure illustrates the four fuel assemblies as positioned in Figure 3. The use of the polynomial expansions gives a better representation of the distribution along the edge of each coarse mesh, which is why the error distribution is much flatter along the edges in comparison with the previous results [3]. Note that although the fuel pins are shown as squares in Figure 4, the coarse mesh method makes no approximation in modeling the geometry (i.e., the geometry is exactly modeled).

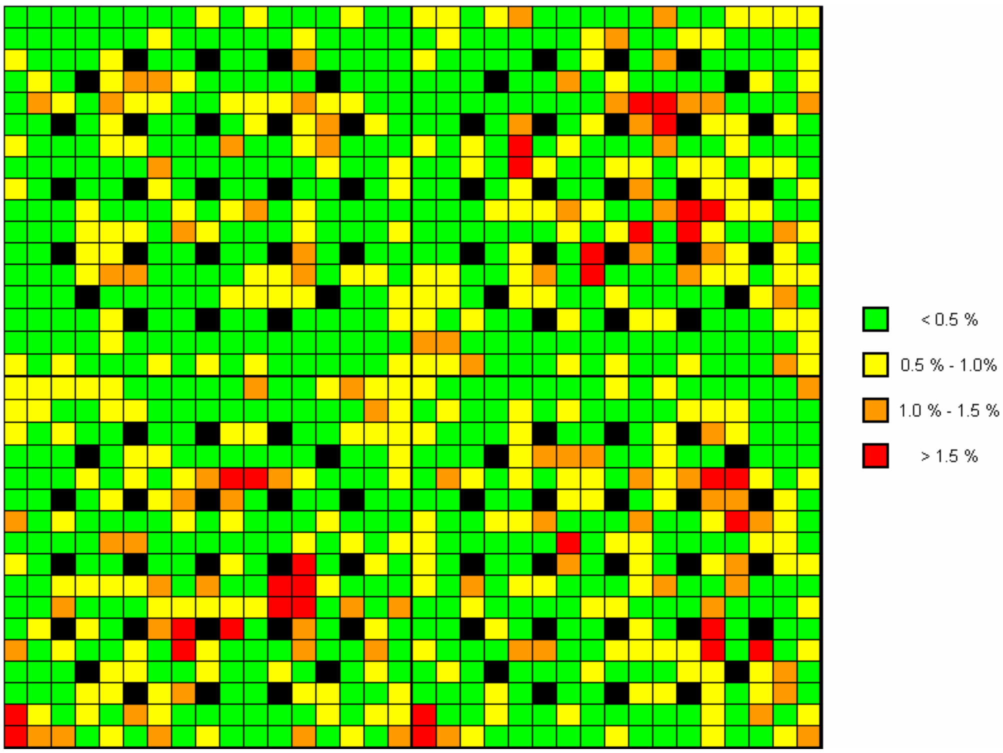

Figure 4: Relative Error Distribution of the Pin Powers of the C5G7 2-D MOX Benchmark for the {2,2,2} case.

For the {2,2,2} case, the new formulation of the coarse mesh method (polynomial expansion) took 280 seconds to converge on the partial currents (10^{-5} convergence criterion), while the cosine-current formulation took less than 2 seconds. The running time difference is caused by the difference in the number of response functions needed to solve the problem.

From the results of the three previous tables, we can see that low order polynomial expansions alone can not accurately account for the spatial and angular effects on large coarse meshes. The addition of the segmentation allows for a greater flexibility along the edge making each segment independent of the others. This can become very useful in meshes where there is a sharp gradient in the spatial and or the angular distribution of the flux or current along the surface of the coarse mesh (caused by the presence of nearby reflector, enrichment variation in the peripheral pins, and/or the presence of control rods). On segments closer to a given local perturbation polynomials are able to model more accurately the skewed (distorted) flux shape without being influenced by the smoother flux shape of the segments further away. In this paper, it is shown that the combination of segmentation with low order expansion works well. Use of higher order expansions is currently under investigation.

4 SUMMARY AND CONCLUSIONS

The heterogeneous coarse-mesh transport method was reformulated to replace the cosine-current angular and the spatial flat-current approximations by Legendre polynomial expansions in both space and angle. This new formulation was tested in a small 2-D one group and the C5G7 7-group MOX benchmark problems. It was found that the new method is more accurate than the cosine-current formulation when compared to the MCNP whole core reference solution.

Excellent accuracy in the first benchmark problem was achieved by using one segment per edge. Using two segments per edge improve the accuracy to within the statistical uncertainties of the method. The case with a 2^{nd} order expansion in all variables (space, polar angle and azimuthal angle) with two segments per edge had an average pin power, root mean square and maximum errors of 0.09%, 0.11% and 0.18 % respectively. The eigenvalue error for this case was -0.06%. The second benchmark problem, C5G7 MOX, was a much better test for the method because of its size, heterogeneity and geometric complexity. As expected, it was found that increasing the number of segments per edge yields better results for low order expansions. The case with the 2^{nd} order expansion in all variables (space, polar angle and azimuthal angle) and four segments per edge yielded the best results. The eigenvalue error was 0.06% in this case. The corresponding average pin power, root mean square and the maximum errors were 0.51%, 0.65% and 2.18% respectively. The accuracy of the eigenvalue and the peak pin power were greatly improved by the use of the polynomial expansion in comparison with the cosine-current approximation.

In order to complete the work in 2-D, one must increase the order of the expansion method. This should reduce the need for spatial segmentation and improve the angular approximation. In this paper, we have developed a Monte Carlo adaptation of the incident current response expansion method. The adaptation in conjunction with the use of continuous Legendre polynomials in MCNP to expand the angular interface partial currents will make it possible to extend the method to 3-D geometry in a practical manner. The development of the method in 3-D and its implementation is currently in the preliminary development stage.

5 ACKNOWLEDGMENTS

This work was supported by a contract from the Department of Energy under the Nuclear Energy Research Initiative. In addition, the first author was supported in part by a grant from the Natural Sciences and Engineering Research Council of Canada. The authors would also like to acknowledge the help received by Dr. David Griesheimer in modifying MCNP.

6 REFERENCES

1- S. W. Mosher and F. Rahnema, "Monte Carlo Adaptation of a Heterogeneous Coarse Mesh Transport Method," *Trans. Am. Nucl. Soc.,* **89**, 310 (2003).

2- B. Forget, F. Rahnema and S. W. Mosher, "Application of A Heterogeneous Coarse Mesh Transport Method to a MOX Benchmark Problem," *PHYSOR-2004 The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments*, April 25-29, Chicago, Illinois (2004)

3- B. Forget, F. Rahnema and S.W. Mosher, "A Heterogeneous Coarse Mesh Solution for the 2-D NEA C5G7 MOX Benchmark Problem," *Progress in Nuclear Energy*, **45**, No.2-4, 233-254 (2004).

4- P. Mohanakrishnan, "Angular Current Approximations in Neutron Transport Calculations Using Interface Currents – A Review," *Progress in Nuclear Energy*, **7**, 1-10 (1981).

5- D.P. Griesheimer and W.R. Martin, "Monte-Carlo Based Angular Flux Response Functions," *Trans. Am. Nucl. Soc.*, **89**, 370 (2003).

6- J. F. Briesmeister, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 4C," *Los Alamos National Laboratory*, LA-13709-M (2000).

7- E. E. Lewis, G. Palmiotti, T. A. Taiwo, R. N. Blomquist, M. A. Smith and N. Tsoulfanidis, "Benchmark Specifications for Deterministic MOX Fuel Assembly Transport Calculations Without Spatial Homogenization," *Nuclear Energy Agency* (2003).

8- Mosher, S.W., "A Variational Transport Theory Method for Two-Dimensional Reactor Core Calculations," Ph.D. Thesis, Georgia Institute of Technology (2004).

9- S.W. Mosher and F. Rahnema, "The Incident Flux Response Expansion Method for Heterogeneous Coarse Mesh Transport Problems", *Transport Theory and Statistical Physics*, submitted (2004).

10- S.W. Mosher and F. Rahnema, "An Intra-Nodal Flux Expansion for a Heterogeneous Coarse Mesh Discrete Ordinates Method," *Proc. of ANS Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew*, April 6-10, Gatlinburg, Tennessee (2003).

11- E.A. Villarino, R.J.J. Stamm'ler, A.A. Ferri, A.A. and J.J. Casal, "HELIOS: Angularly Dependent Collision Probabilities", *Nuclear Science and Engineering,* **112**, 16 (1992).