

## **Application of a Heterogeneous Coarse Mesh Transport Method to a MOX Benchmark Problem**

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**Abstract** – Recently, a coarse mesh transport method was extended to 2-D geometry by coupling Monte Carlo response function calculations to deterministic sweeps for converging the partial currents on the coarse mesh boundaries. More extensive testing of the new method has been performed with the previously published continuous energy benchmark problem, as well as the multigroup C5G7 MOX problem. The effect of the partial current representation in space, for the MOX problem, and in space and energy, for the smaller problem, on the accuracy of the results is the focus of this paper. For the MOX problem, accurate results were obtained with the assumption that the partial currents are piecewise-constant on four spatial segments per coarse mesh interface. Specifically, the errors in the system multiplication factor and the average absolute pin power were 0.12% and 0.68%, respectively. The root mean square and the mean relative pin power errors were 1.15% and 0.56%, respectively.

**Keywords** – *Heterogeneous Coarse Mesh Transport, Transport Theory, MCNP, Benchmarks*

### **1. Introduction**

In a recent paper [1], a heterogeneous coarse mesh method was adapted to Monte Carlo simulations for 2-D calculations based on a methodology previously developed for the 1-D discrete ordinates approximation [2-3]. The original 1-D method centered around an expansion of the angular flux within each coarse mesh in surface Green's functions (SGFs), along with high-order variational techniques based on an original principle. In more recent work, the SGFs were replaced by responses to incident fluxes equal to the discrete Legendre polynomials in angle, which greatly reduced the number of response functions needed to achieve highly accurate results in 1-D reactor problems. The non-variational 2-D Monte Carlo method was developed to demonstrate the robustness and applicability of the coarse mesh transport method. It couples Monte Carlo response function calculations with deterministic sweeps for converging the partial currents on the coarse mesh boundaries.

In Section 2, the 2-D method is briefly described. In Section 3, the effect of the partial current representation in space and energy on the results for a small benchmark problem is

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studied. A similar investigation of the spatial representation for the MOX benchmark problem is presented in Section 4. Concluding remarks and directions of future effort can be found in Section 5.

## 2. Coarse Mesh Transport Method

The coarse mesh solution is obtained by iterating on the partial currents at the coarse mesh surfaces. The system eigenvalue ( $k$ ) is held constant during the current iterations, and is updated between outer iterations. Each coarse mesh is characterized by a set of responses that relate quantities of interest within a coarse mesh (*e.g.*, rod fission densities) to incident currents. The responses are estimated from a series of fixed source Monte Carlo simulations for each unique coarse mesh. The fission source, reduced by the fixed system eigenvalue estimate, is included in these simulations so that the separate calculation of responses to in-volume sources is avoided. As a result, the response functions must be updated in every outer iteration. In the 1-D approach, very accurate results were achieved when the response function updates were accomplished by linear interpolation on  $1/k$ . This avoids expensive iterations between the fine and coarse mesh calculations. In this paper, outer iterations were avoided in order to explore the impact of the partial current representation on the solution accuracy. Therefore, the results do not include the impact of residual eigenvalue errors associated with actual outer iterations. We did however verify the convergence on  $k$  for the MOX problem with a spatial segmentation of two for which the results will be briefly stated in Section 4.

### 2.1 Response Functions

A modified version of MCNP4B2 [5] was created to implement the fission source scaling factor discussed in the previous section. Response functions were calculated for each different coarse mesh (*e.g.*, fuel assembly) by imposing vacuum boundary conditions and a fixed source of one neutron per second entering one side of the system. A response function relates a quantity of interest, like an exiting surface current or the fission density of a region, with the incoming surface currents as shown in Figure 1. It is assumed that the currents transmitted between coarse meshes are uniformly distributed in energy within several bins (for continuous energy problems) and are cosine distributed in the entering and exiting angular half-spaces.

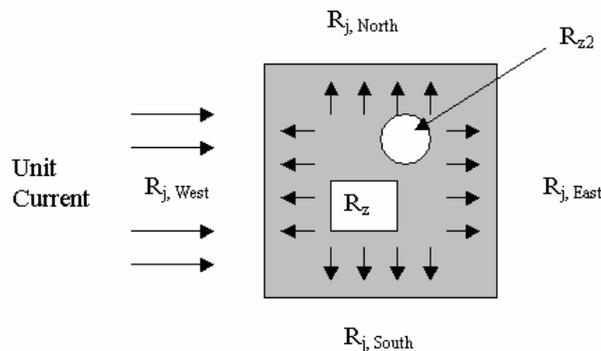


Figure 1: Response function generation for a given coarse mesh

In previous work [1], the partial currents were assumed to be spatially constant on individual coarse mesh boundaries (*e.g.*, the coarse mesh in Figure 1 is considered to have four boundaries). In this work, the partial currents will be treated as piecewise-constant on an arbitrary number of equal-width spatial segments per boundary. The change in the accuracy of the solution with the numbers of spatial segments will be studied. For the continuous energy problem, the effect of increasing the number of energy bins will also be studied.

## 2.2 Coarse Mesh Calculation

Once the response functions for each unique coarse mesh are computed, a sweeping technique, as developed in [3], is used to calculate the outgoing currents of each coarse mesh and the fission density in each fuel pin. Letting  $J$  represent the entering currents and  $R_z$  the response functions for a given property  $Z$  (*e.g.*, rod fission density, exiting current, *etc.*), that property can then be calculated by

$$Z = \sum_E \sum_S J^- R_z \quad (1)$$

where summations are performed over all energy groups (or bins)  $E$  and every coarse mesh boundary segments  $S$ . The exiting currents that are calculated for a given coarse mesh become the entering currents of the adjacent meshes. In a single inner iteration, the exiting currents are calculated for each coarse mesh, and successive iterations are performed until the currents converge. When the inner iterations are complete, a new multiplication factor is estimated as the ratio of gains to losses

$$k = \frac{\sum_E \sum_S \sum_M J^- R_{nf}}{\sum_E \sum_S \sum_M \{J^- (R_{ab} - 1) + J^+\}} \quad (2)$$

where  $R_{nf}$  is the neutron production rate in each coarse mesh and  $R_{ab}$  is the absorption rate,  $J^+$  is the exiting current and the additional summation is over all coarse meshes  $M$ .

## 3. First Benchmark Problem

In order to verify the importance of the energy and spatial refinements, the method was first applied to a small problem consisting of four coarse meshes with specular reflective boundary conditions, from reference [1], which is illustrated Figure 2.

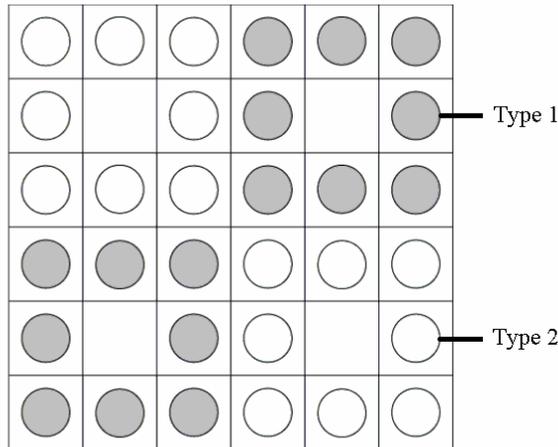


Figure 2: Small four coarse mesh problem

This problem is composed of two unique coarse mesh types that differ in fuel enrichment (type 1: 2% enriched  $\text{UO}_2$ ; type 2: 1% enriched  $\text{UO}_2$ ). The diameter of each fuel rod is 0.82 cm and the rod pitch is 1.26 cm, which is representative of a PWR fuel assembly. Each coarse mesh contains eight fuel rods in a 3 by 3 array with overall dimensions of 3.78 cm by 3.78 cm. A 50 million history reference calculation of the system eigenvalue and fission densities (FDs) was performed with an unmodified version of MCNP4B2. The reference eigenvalue for this problem was found to be  $1.17406 \pm 0.00006$ .

In reference [1], response functions were computed in 12 energy bins with one spatial segment per coarse mesh edge. Table 1 shows the effect of increasing the number of energy bins and spatial segments to 45 and 2, respectively, on the multiplication constant and rod fission density error.

Table 1: Benchmark #1 ( $k_{\text{ref}} = 1.17406$ )

<b>E / S</b>	<b>k</b>	<b>%k</b>	<b>avg err.</b>	<b>RMS</b>
12 / 1	1.16240	-1.0	1.27	1.55
12 / 2	1.16195	-1.0	1.09	1.34
45 / 1	1.16595	-0.69	0.81	1.03
45 / 2	1.16958	-0.57	0.33	0.43

E / S: Energy bins / Spatial segments

k: Eigenvalue

%k:  $(k - k_{\text{ref}}) * 100 / k_{\text{ref}}$

avg err.: average relative error of the rod FDs

RMS: root mean square of the relative error of the rod FDs

The approximation of 12 energy bins gives reasonable accuracy in the rod fission densities with an average error of 1.27% and the k value with a relative error of  $-1.0\%$ . The spatial refinement for the same energy structure has no effect on the k value but does reduce the average

relative error of the FDs to 1.09%. By refining the energy group structure to 45 groups, we observe an appreciable gain in accuracy for both the  $k$  value and the rod FDs. The error in  $k$  is reduced to  $-0.7\%$  and the average error on the rod FD drops to  $0.81\%$ . This indicates the strong energy dependence of this particular problem. Increasing the spatial refinement further improves the 45 energy group results. The  $k$  value is underestimated by  $-0.57\%$  and both the average and the RMS errors for the rod FDs are considerably reduced to  $0.33\%$  and  $0.43$ , respectively. The continuous energy nature of this problem may limit the gain in accuracy from the spatial refinement, since the energy dependence seems to be the dominant factor.

#### 4. MOX Benchmark

The second benchmark problem consists of a more rigorous representation of a light water reactor due to its size, the presence of a surrounding reflector region and the presence of a higher degree of heterogeneity.

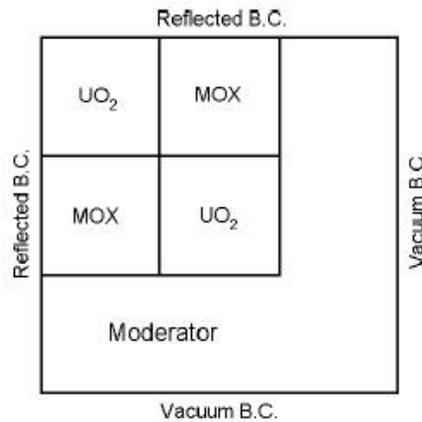


Figure 3: Two-dimensional MOX problem

This problem is composed of three different coarse mesh types: a MOX fuel assembly, a  $UO_2$  fuel assembly and moderator. The geometric data and seven-group cross sections for this benchmark as well as the reference solution were taken from reference [4]. The partial currents were treated as piecewise-constant on one, two, and four equal-width spatial segments per energy group per coarse mesh edge. The results are shown in Table 2.

Table 2: Benchmark #2 ( $k_{ref} = 1.18655$ )

S	k	%k	Avg RE	RMS
1	1.16503	-1.82	11.55	16.74
2	1.17868	-0.67	2.76	4.29
4	1.18803	0.12	0.68	1.17

The size and layout of this problem strongly suggest choosing a coarse mesh representing an entire fuel assembly. The coarse mesh is thus  $21.42$  cm by  $21.42$  cm. The results obtained with

one spatial segment are not very accurate, due to the size and heterogeneity of this problem. The average relative pin power error is 11.55% and the relative error in  $k$  is  $-1.82\%$ . By dividing the segments of each coarse mesh by two, the average relative pin power error, the RMS and the error on the  $k$  value were substantially reduced. Considering four spatial segments gives even better results. The average relative error drops to 0.68% and the RMS to 1.17%. The error in the  $k$  value is 0.12%. The accuracy of these results is comparable to some fine mesh codes used to solve this benchmark [4]. We note that the deterministic current iterations that actually solve the problem converge very fast. It takes between 4 and 5 seconds to solve the benchmark problem given a pre-computed set of response functions on a Pentium 2.8GHz PC. The outer convergence in  $k$  was verified for a case with two spatial segments. Convergence was achieved within 5 outer iterations with a  $10^{-5}$  criterion from an initial guess of  $k = 1$ . The relative error in  $k$  is  $-0.71\%$  with average and RMS pin power errors of 3.24% and 4.62% respectively.

## 5. Conclusions

More extensive testing of a coupled Monte Carlo/deterministic coarse mesh transport method was performed with the previously published continuous energy benchmark problem, as well as the multigroup C5G7 MOX problem. The effect of refining the representation of the partial currents transmitted across coarse mesh interfaces was studied. It was found that accurate results could be obtained by considering the partial currents to be piecewise constant on two to four spatial segments per coarse mesh boundary per energy group (or bin). The results for the continuous energy problem are limited by the assumption that the current is uniformly distributed within individual energy bins. A more sophisticated approach to the energy dependence seems to be required to achieve significant increases in accuracy for that problem. Regardless of the current representation, the deterministic iterations converge extremely fast (on the order of seconds) given pre-computed Monte Carlo responses.

The impact of residual eigenvalue error associated with actual eigenvalue iterations for the MOX problem was considered for a case with two spatial segments and showed to be minimal. Future work foresees the use of linear interpolation for response function updates. Additional avenues of future work include implementing a more sophisticated representation of the partial currents. For example, a spatial expansion in continuous polynomials may lead to higher accuracy with fewer response functions. The overall accuracy is then likely to be limited by the angular representation, especially with respect to the treatment of the azimuthal angle in 2-D problems. An expansion of the azimuthal dependence in low-order polynomials may result in significant gains in accuracy.

## 6. References

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