DYNAMIC IMPLEMENTATION OF THE EQUIVALENCE THEORY IN THE HETEROGENEOUS WHOLE CORE TRANSPORT CALCULATION

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ABSTRACT

The coarse mesh finite difference (CMFD) formulation is applied to the heterogeneous whole transport calculation as a means of efficient acceleration as well as simplified representation. A pin cell is chosen as the base coarse mesh which is much coarser than the intra-cell flat source regions. The CMFD formulation enables dynamic homogenization of the cells during the iterative solution process such that the heterogeneous transport solution can be preserved. Dynamic group condensation is also possible with a two-level CMFD formulation involving alternate multigroup and two group calculations. The two-dimensional method of characteristics (MOC) is used as the kernel to generate the heterogeneous solution and the CMFD solution provides the MOC kernel with much faster converged fission and scattering source distributions. Through the applications to various problems including different compositions, sizes, and energy groups, it is shown that the performance of the CMFD formulation is superior in that the number of the MOC calculations can be reduced below 10 while reproducing exactly the original transport solution. The merit of the CMFD formulation is greater for larger problems in which speedups of 100-300 are possible when compared to the unaccelerated case.

1. INTRODUCTION

Homogenization has been one of the primary approximations introduced in the reactor physics calculation. The equivalence theory[1,2] provides the basis of homogenization stating that an equivalent homogenized problem can be constructed for the heterogeneous problem by introducing additional degree of freedom such as the discontinuity factor. If these adjustment factors are calculated from the whole problem, the homogenized problem indeed has the same result as the original heterogeneous problem as far as the averaged properties are concerned. The problem in practical applications is however that these factors have to be calculated *a priori* for each prototypical part of the whole geometry. Thus there always exist errors associated with homogenization in the conventional two group nodal diffusion calculations.

The concept of discontinuity introduced for homogenization was later extended to the coarse mesh finite difference (CMFD) formulation, which is to construct an equivalent problem to a fine-mesh or higher order problem. However, in this case the discontinuity factor is determined dynamically for each coarse mesh surface employing the nonlinear iteration technique[3]. In most CMFD applications, the discontinuity factor is replaced with the coupling correction factor[4] or corrective nodal coupling coefficient. The CMFD formulation was proved to be a means of efficient acceleration as well as simplified representation.

As an effort to remove the errors associated with the homogenization and other approximations, the multigroup whole core transport calculation based on the method of characteristics (MOC) have been studied [5-8]. In this type of calculation, the heterogeneity within the pin cell is kept explicitly. If the pin cells can be homogenized consistently during the solution process such that the averaged properties of the heterogeneous solution can be preserved, it is possible to establish a simplified representation of the problem. Furthermore, by extending the idea of the equivalence theory to the energy space and angular space, a consistent lower order formulation in the form of a pin-cell homogenized, few group, diffusion-like, finite difference scheme would be possible. This simplified lower order formulation is much easier to solve and its solution can be used to accelerate the original higher order solution as the CMFD formulation does in the conventional nodal method. The authors proved in the preliminary work[8] that the CMFD formulation was indeed very effective in accelerating the multigroup whole core transport calculation. The number of ray tracing sweeps was reduced by more than a factor of 20 by employing the CMFD formulation compared to merely Chebyshev accelerated MOC calculation and the CMFD formulation was 2 or 3 times more effective than the coarse mesh rebalancing (CMR) scheme. In the four level formulation employed in the CASMO-4 code[7], it seems that a similar concept as the CMFD formulation is meant by the "*transport corrected diffusion*" problem. However, the details of the implementation should be quite different.

The primary benefit of the CMFD formulation would be the acceleration performance. However, the CMFD formulation has another prime significance of simplified representation of the problem requiring far less computation in the subsequent calculations. Particularly in perturbed calculations such as transient and depletion calculations in which the spectra and intra flux shapes vary slowly, the CMFD parameters such as corrective nodal coupling coefficient and the spectrum of the homogenized region determined for the base state can be used directly in the perturbed state, without requiring expensive reevaluation of such parameters through higher order kernels such as MOC or NEM. This idea was proved in a group of multigroup nodal rod ejection transient calculations in Hexagonal geometry[9], in which two group hexagon based CMFD solution was used at most time steps and multigroup hexagonal kernel calculations were rarely performed.

This paper is to elaborate the CMFD formulation for the heterogeneous whole core transport calculation, which is to implement dynamically the equivalence theory for both efficient acceleration and simplified representation. In the next section, a pin-cell based two-group CMFD formulation with a multigroup MOC kernel is presented which provides the basis of the DeCART (Deterministic Core Analysis based on Ray Tracing) heterogeneous whole core transport code. It involves the definitions of the CMFD parameters and the prolongation and restriction operations for the alternate CMFD and MOC calculations. An efficient nonlinear iteration logic for control of the three levels of calculations (two-level CMFD and MOC) is also introduced. In the third section, the performance of the CMFD formulation is examined in the aspects of convergence characteristics and computing time for various problems with different compositions, sizes and energy group structures. Section 4 concludes the paper.

2. TWO-GROUP CMFD FORMULATION WITH MULTIGROUP MOC KERNEL

In multigroup MOC transport calculations for heterogeneous configurations involving fuel pellet and cladding regions, the computational meshes should be chosen to be fine enough to capture the regional dependence of the angular flux within a pin. Thus a pin cell involves tens of fine meshes and it can be regarded *coarse* relative to the regional fine meshes cell as illustrated in Figure 1. In this regard, the pin cell can be taken as the base coarse mesh in the CMFD calculation for MOC acceleration, unlike the assembly sized coarse meshes used in the nodal diffusion calculations. In order to formulate a CMFD problem under this circumstance, one needs homogenized cell group constants (including diffusion coefficients) and cell coupling coefficients that relate the cell interface current with the two adjacent cell average fluxes. These CMFD parameters can be determined from a partially converged MOC solution that yields regional scalar fluxes as well as net interface average currents. The multigroup CMFD parameters can be further condensed to a two-group system which would be solved very quickly to catch up efficiently the fission source distribution and eigenvalue of the problem.

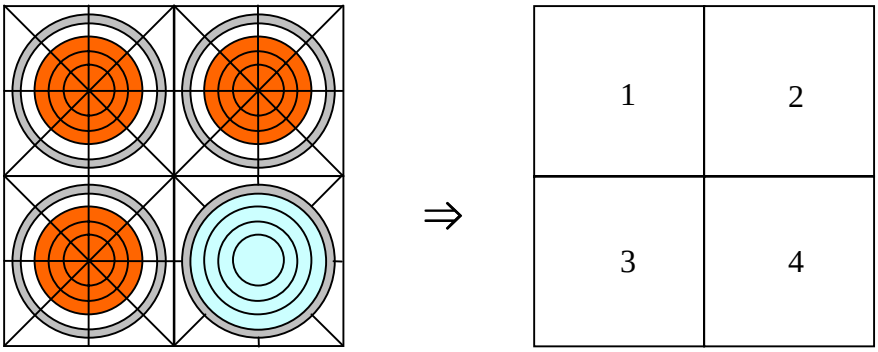

Figure 1. Flat Source Regions within Heterogeneous Cells and Homogenized Cells

The cell average fluxes resulting the partially converged CMFD solution is then to be used to update the fission and scattering source distributions for the subsequent MOC calculation. In the reconstruction of the regional source, the spatial shape of the scalar flux within a cell determined in the previous MOC calculation is used. Only the level of the scalar flux is adjusted according to the CMFD-determined cell average flux. Similarly, the net current information obtained at the problem boundary by the CMFD solution is used to update the boundary incoming angular fluxes for the MOC calculation. The shape of the incoming angular flux determined from the outgoing current and the boundary condition in the previous MOC calculation is retained in the update of the boundary incoming current. The alternate execution of the homogeneous CMFD calculation and the heterogeneous MOC calculation continues until convergence is reached. This section provides specific details of the cell-based two-group CMFD formulation outlined above starting with a brief description of the multigroup MOC kernel which is the most essential component of the CMFD formulation that maintains the superior accuracy of the MOC calculation.

2.1 Multigroup MOC Kernel

In the DeCART code, a cell-based modular ray tracing module is used. It will be augmented later by a whole ray tracing module in the later code versions. In each MOC update, the group sweep is performed at the outermost level. In the group sweep, each within-group problem is solved by the ray tracing module implementing the MOC, given the fission and scattering sources at each region and

the incoming angular fluxes at the problem boundary. The solution of the within-group MOC problem consists of the scalar flux at each region, the surface averaged net current at each cell surface and the outgoing angular fluxes at the problem boundary. The scalar flux is used to update the scattering source of the subsequent group while the fission source is updated only after the completion of the group sweep. After the group sweep over the entire groups, one or two upcattering sweeps are performed for the groups in which upscattering sources are present (two if the number of groups is greater than 10, one, otherwise). For instance, for a seven group problem, 11 within-group ray tracing calculations are performed per MOC update. The typical intracell regions defined in DeCART are as shown in Figure 1 which shows a 48 region cell as well as a 13 region cell. The ray discretization normally involves 4 azimuthal angles in one quadrant and 2 polar angles per hemisphere and 0.5 mm ray spacing. The solution accuracy can be enhanced by refining the intracell regions as well as the ray discretization.

2.2 Equivalence by CMFD Formulation

Suppose that a converged multigroup MOC solution is available for a heterogeneous configuration. Then would it be possible to represent the original problem with a finite difference formulation employing homogenized and furthermore condensed group constants including diffusion coefficients and to generate the same solution in the average sense? The answer is yes and it is possible by the CMFD formulation which imposes the conservation of the surface currents as well as the volumetric reaction rates through consistent homogenization.

For a heterogeneous cell such as the ones shown in Figure 1, the homogenized group constants can be obtained through flux volume weighting to conserve the reaction rate as follows when the heterogeneous solution is available:

$$\overline{\Sigma}_{\alpha g}^{i} = \frac{\sum_{k\in i} V^k \Sigma_{\alpha g}^k \phi_g^k}{\overline{\phi}_g^i V^i} \quad \text{and} \quad \overline{D}_g^i = \frac{\overline{\phi}_g^i V^i}{3\sum_{k\in i} V^k \Sigma_{trg}^k \phi_g^k}, \tag{1}$$

where indices *i, k,* and *g* represent the cell, region, and group numbers, respectively. $\overline{\phi}_g^i$ is the cell average flux. Using these homogenized group constants only in the finite differenced homogenized problem would not yield the same node average flux distribution. The equivalent finite differenced problem can be established only when the interface current of the transport reference solution is retrieved by the *coarse mesh* finite differenced interface current relation which reads:

$$\overline{J}_g^{i,s} = -\tilde{D}_g^{i,s}\left(\overline{\phi}_g^{i,s} - \overline{\phi}_g^i\right) - \hat{D}_g^{i,s}\left(\overline{\phi}_g^{i,s} + \overline{\phi}_g^i\right) \tag{2}$$

where index *(i,s)* means the *s*-th side of the *i*-th cell and thus $\overline{\phi}_g^{i,s}$ is the cell average flux of the *s*-th side neighbor of Cell *i* and $\overline{J}_g^{i,s}$ is the surface average net current at the *s*-th side surface of Cell *i*. Among the two coupling coefficients in Eq. (2), the first one is determined from the diffusion coefficients and cell width using the ordinary finite difference relation, whereas the second one is determined from the reference solution in order to force the interface current obtained by Eq. (2) to be same as the reference value. It is thus obtained as:

$$\hat{D}_g^{i,s} = -\frac{\overline{J}_g^{i,s} + \tilde{D}_g^i\left(\overline{\phi}_g^{i,s} - \overline{\phi}_g^i\right)}{\overline{\phi}_g^{i,s} + \overline{\phi}_g^i}. \tag{3}$$

Using the CMFD current relation given by Eq. (2) together with the group constants defined in Eq. (1) and the correctional coupling coefficient of Eq. (3), the nodal neutron balance in each cell can be guaranteed and thus the resulting solution of the CMFD problem can be the same as the original solution as far as the average fluxes (and the eigenvalue as well) are concerned. In the real applications, the reference solution to be used in Eqs. (1) and (3) is replaced by a partially converged heterogeneous MOC solution which is to be iteratively updated.

The equivalent CMFD problem involves much fewer unknowns and has a regular matrix structure. Therefore it can be solved much more quickly than the original heterogeneous transport problem with the aid of well established linear system solution methods. The solution of the CMFD problem for a given set of the CMFD parameters (the group constants and coupling coefficients) is a new cell average flux distribution (and new eigenvalue as well) unless the fully converged heterogeneous solution is used to obtain the CMFD parameters. The new flux distribution will be used to update the regional source and boundary incoming angular fluxes for the heterogeneous problem.

2.3 Prolongation

In each ray tracing calculation, the regional source distribution and the incoming angular fluxes at the problem boundary are to be given. Since only the cell average values of the scalar flux and the surface averaged net currents are available from the CMFD problem, *prolongation* operations are needed to map the lower dimensional space vector to the higher dimensional space vector. This can be performed by using the spatial and angular *shapes* that were determined at the previous MOC calculation. Specifically, the regional scalar flux and the boundary outgoing angular fluxes are updated using the following relations:

$$\phi_g^{k,l+\frac{1}{2}} = \frac{\phi_g^{k,l}}{\bar{\phi}_g^{i,l}} \bar{\phi}_g^{i,l+\frac{1}{2}} \tag{4}$$

and

$$\varphi_{g,m}^{p,l+\frac{1}{2}} = \frac{\varphi_{g,m}^{p,l}}{\bar{J}_g^{i,s,l}} \left(\tilde{D}_g^i - \hat{D}_g^i \right) \bar{\phi}_g^{i,l+\frac{1}{2}} \tag{5}$$

where $\varphi_{g,m}^{p,l}$ is the angular flux of Group g and Angle m at a Point p on a boundary surface s of a boundary cell i at the l-th MOC update. The incoming angular flux is determined from the outgoing angular flux of Eq. (5) and the boundary condition.

2.3 Two-Level CMFD Solver

The multigroup CMFD problem formulated by using the CMFD parameters defined by Eqs. (1) and (3), and the interface current relation of Eq. (2) can be solved by the fission source iteration method that involves the group sweep and within-group inner iteration. However, since the cell-based CMFD problem is in fact a fine-mesh problem, the repeated multigroup solution by the fission source iteration requires a nontrivial amount of computational load. In order to relieve this computational burden, an equivalent two-group CMFD formulation can be employed by extending the concept of spatial CMFD formulation to the energy space as presented in Reference 9. One of the benefits of introducing the two-group CMFD formulation is to use the existing efficient two-group solvers

developed for diffusion problems and the other is that the eigenvalue acceleration is easy with the Wielandt eigenvalue shift method. In the DeCART code, the BiCGSTAB algorithm with the BILU3D preconditioner [10] is used for the solution of both within-group and two-group problems. Although the BILU3D preconditioner was developed for coarse mesh problems, it turned out that the preconditioner worked very well for high energy group problems as well as the two group problems for the cell-pitch sized *fine* mesh problems.

2.4 Nonlinear Iteration Control

In the CMFD calculation, periodical updates of the CMFD parameters through the higher order space calculation are required and this is referred to as the nonlinear iteration. With the two-level CMFD formulation introduced, an additional level of update is needed for the two group CMFD parameters. Since it is not necessary to generate a fully converged solution for each set of CMFD parameters, there should be an efficient control logic to drive the CMFD calculation by monitoring convergence. In the DeCART code, partial convergence of each CMFD solution is determined by monitoring the relative residual which is the *l*2 norm of the residual vector of the linear system consisting of the multigroup CMFD cell balance equation. Specifically, the element of the residual vector is defined as:

$$r_{g,i}^{n} = \left(M\phi^{n}\right)_{g,i} - \lambda_{n}\chi_{g,i}\psi_{i}^{n} \tag{6}$$

where indices *n*, *g*, and *i* are the iteration, group and cell numbers, respectively and ψ_i^n is the total fission source within the volume of Cell *i* at the n-th iteration step. Because the imbalance given by Eq. (6) is defined for each group as well as each cell, the norm of the residual for the multigroup case is larger than the two-group case. In the denominator of the residual norm, the *l*2 norm of the group wise fission source ($\chi_{g,i}\psi_i^n$) is used. Figure 2 shows the nonlinear iteration control logic employed in the DeCART code that uses the relative residual as the exit condition at various levels.

3. EXAMINATION OF CONVERGENCE PERFORMANCE

The performance of the two-level CMFD formulation was examined for various test problems ranging from single assembly to typical PWR problems. The assembly configurations and the 7 group cross section data for each composition were taken from the KAIST 2A benchmark problem [11] which involved various types of assemblies such as rodded Uranium oxide or MOX as listed in Table 1. In addition to the 7-group cross sections, 35-group cross section sets were generated for the same assembly configurations by a lattice physics code to examine the group dependence. The convergence was first examined for the single assembly problems with the reflective boundary condition, and secondly for the core problems with different sizes, and finally for the 35- group KAIST 2A problem. For each problem, the reference solution was generated by converging the solution very tightly (i.e. global relative fission source *l*2 norm less than 10^{-10}) and this solution was used to compute the *true* error of each solution iterate. The unaccelerated case which employed only the MOC calculations and the power iteration was performed in parallel with the CMFD case to ensure solution convergence and to compare the performance.

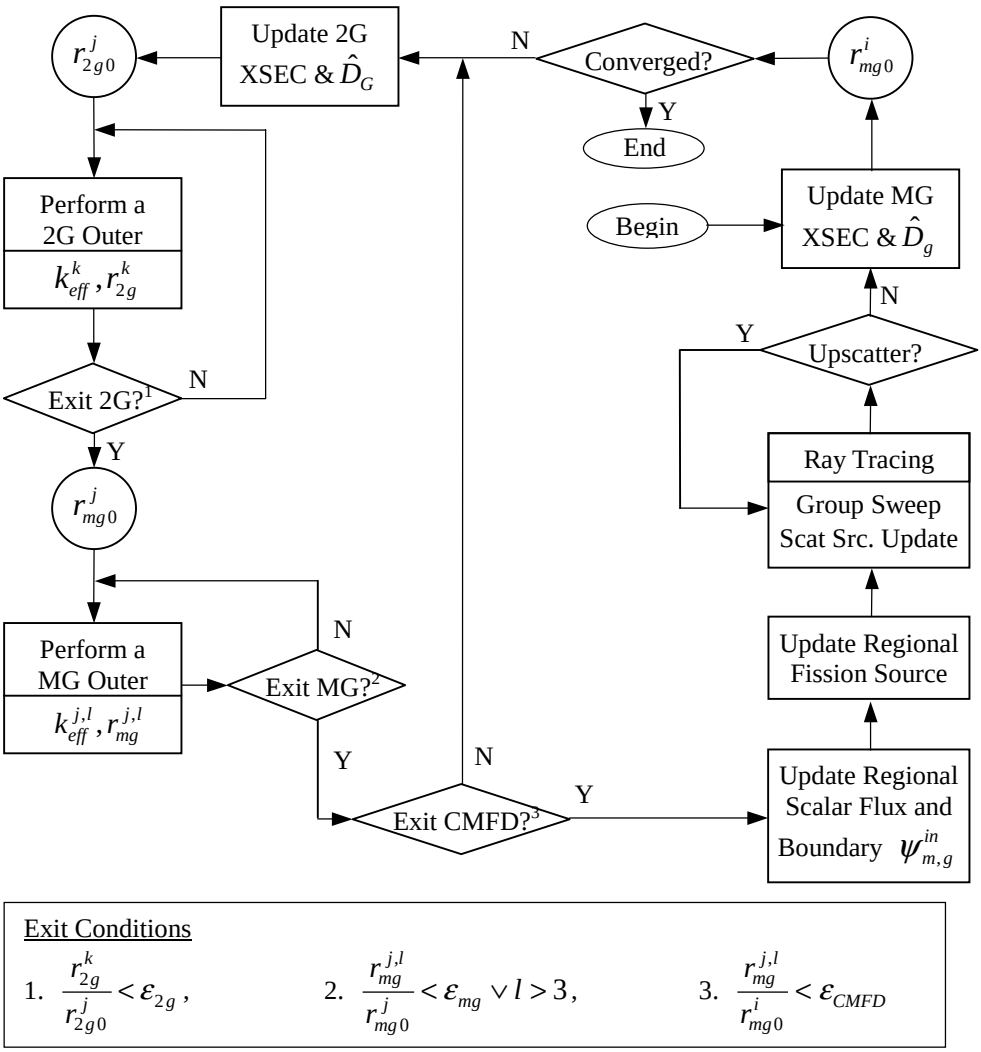

Figure 2. Calculation Flow and Control Logic of the DeCART Code

Table 1. Summary of the Assembly Cases

Assembly Type		k_{eff}	Unaccelerated Case, N_{MOC}	CMFD Formulation		
ID	Configuration			N_{MOC}	N_{MG}	N_{2G}
1	UO_2	1.09948	95	5	29	26
2	Rodded UO_2	0.83131	97	7	34	33
3	Gd Poisoned UO_2	1.04363	95	6	35	31
4	Zonned MOX	1.17308	83	7	42	34
5	Gd Poisoned MOX	1.13322	84	6	35	29

3.1 Convergence for the Base Case

The convergence of k_{eff} for the 7 Group KAIST problem is shown Figure 3. The eigenvalue is updated at every two-group and multigroup CMFD outer iteration. As shown in Figure 3, the eigenvalue stabilizes very quickly around the converged value (0.98397) only after three MOC updates. Compared with the unaccelerated case as shown in Figure 4, the CMFD formulation is roughly 100 times more effective in that only 7 MOC updates are required to reach the true global fission source error of 10^{-5} whereas about 700 MOC updates are for the unaccelerated case. Yet, the local solution converge indeed to the same value as shown in Figure 5 which shows regional group scalar fluxes at an interior cell and angular fluxes at a boundary point. During the convergence, two-group (marked with red circles) and multi-group (marked with black squares) CMFD solutions frequently adjust quite effectively local and global neutron balances as indicated by the fission source error and residual convergence in Figure 6. The large drop in the multigroup residual after the two-group CMFD updates shown in Figure 6 indicates that the two-group formulation is quite effective in accelerating the multigroup solution. The computation time for the CMFD calculations is however trivial compared to the MOC calculation (Table 3) even though fewer than 10 MOC updates are required.

The rapid essential convergence shown in Figure 3 and the steady exponential error reduction in the later iteration steps mean that only a few heterogeneous MOC calculations are sufficient to catch up most of the spectral, spatial coupling, and transport effects. This would be possible because fission and scattering source distributions determined from the prior CMFD calculation provides much better source information than what can be obtained with the MOC alone.

3.2 Convergence Sensitivity

The sensitivity of the convergence characteristics of the CMFD formulation on composition, core size, and the number of groups is examined. In this sensitivity study, the number of iterations required to reach the true fission source convergence of 10^{-5} is compared. As shown in Table 1, which lists the single assembly cases with different compositions, the number of MOC updates is somewhat independent of the fuel composition and it stays around 7, which amounts to a factor of 13 saving compared to the unaccelerated case (~90 MOC). Note that this saving at the assembly level is not so great.

For the core size sensitivity, five quarter-core problems are constructed with different numbers of fuel assemblies. For consistency with the KAIST 2A problem, the symmetry axis is placed at the assembly edge, not at the centerline. The numbers of fuel assemblies along one axis are 1, 3, 5, 7, and 9, respectively for the five quarter-core problems. The third case (5 FAs along the axis) is the same as the KAIST 2A problem. Similarly to this core, the cores are reflected with a row of reflector except for the first core. The results for the five cores are listed in Table 2. As shown in this table, the convergence of the CMFD formulation does not reveal any significant dependence on the problem size. The number of MOC updates stays around 7 just like the assembly case. However, the unaccelerated case suffers significantly from the increased size.

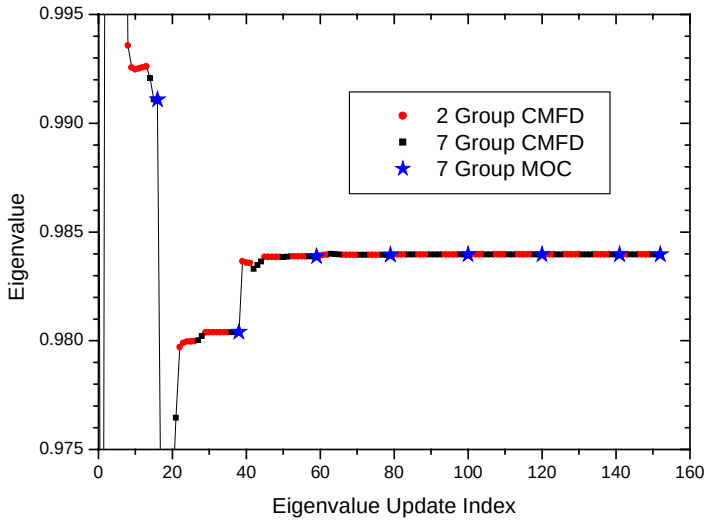

Figure 3. Convergence of Eigenvalue for the KAIST 2A Problem

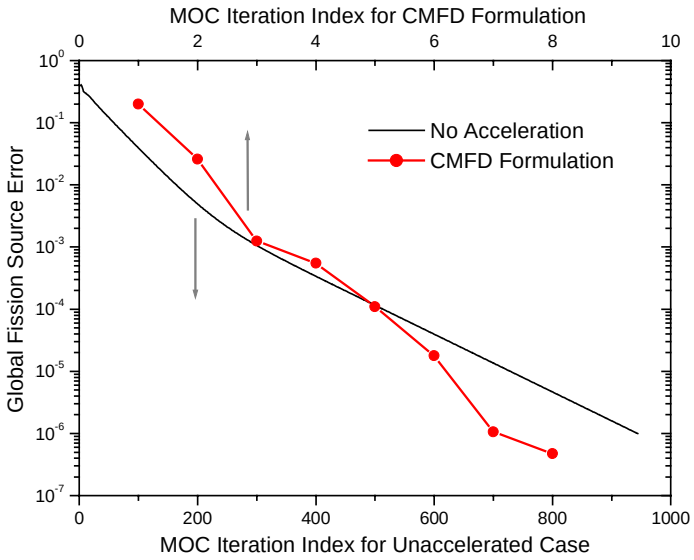

Figure 4. Global Fission Source Error Reduction Behavior

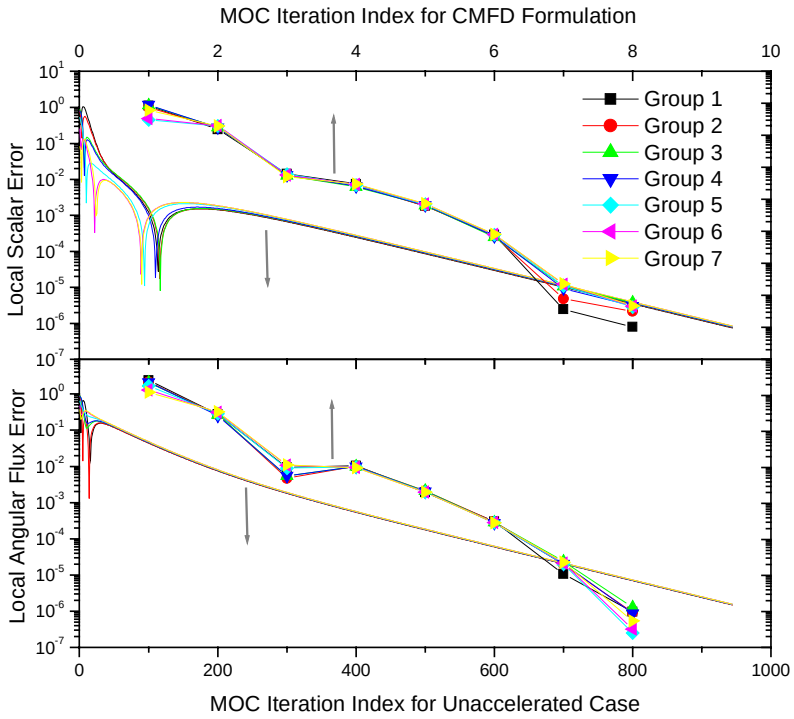

Figure 5. Convergence of Local Scalar Flux and Boundary Angular Flux

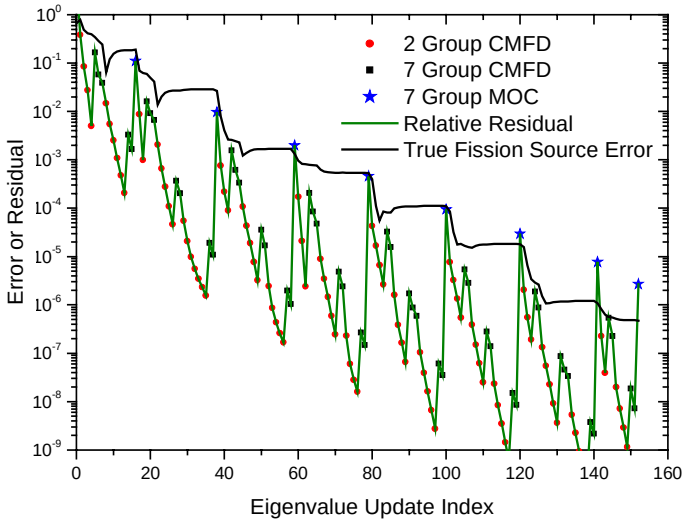

Figure 6. Various Level Residual Reduction Behavior for the 7 Group Problem

Table 2. Performance Comparison for the Core Cases

Groups	Problem Size		Unaccelerated Case		CMFD Formulation		
	N_x	# of FAs	Dominance Ratio	N_{MOC}	N_{MOC}	N_{MG}	N_{2G}
7	1	1	0.9076	115	6	29	28
	3	4	0.9712	370	7	44	52
	5	13	0.9894	729	7	46	88
	7	30	0.9915	1079	6	38	70
	9	52	0.9945	1739	6	39	75
35	5	13	0.9873	534	9	111	118

As indicated by the dominance ratio which was obtained as the ratio of the true errors of the two successive iterates the eigenvalue separation becomes very small as the problem size increases. In the physical point of view, it takes much longer to propagate the boundary information to the core interior in the plain power iteration case for a larger core. However, with the CMFD formulation, the boundary information is instantaneously propagated to the interior so that rapid convergence is possible. Due to this fact, the speedup is over 100 for the practical core cases. For the largest problem here, even a speedup of 290 is achieved.

The two-level CMFD formulation works as well for the 35 energy group case although the number of MOC updates is slightly larger than the 7-group case and more multigroup updates are required in the CMFD problems as indicated at the final low of Table 2. Nonetheless, the two-group CMFD is still quite effective in reducing the multigroup CMFD error once a few MOC calculations are performed as shown in Figure 7. Another thing to note in Figure 7 is that in the 35-group case, the multigroup residual (marked with blue stars) is much larger than the true fission source errors. This is due to that the groupwise component of the residual given by Eq. (6) is used and it increases with the number of groups. Therefore, a relaxed convergence criterion needs to be used if the convergence check is made solely with the residual. Otherwise, the fission source difference between the two successive iterates can be used.

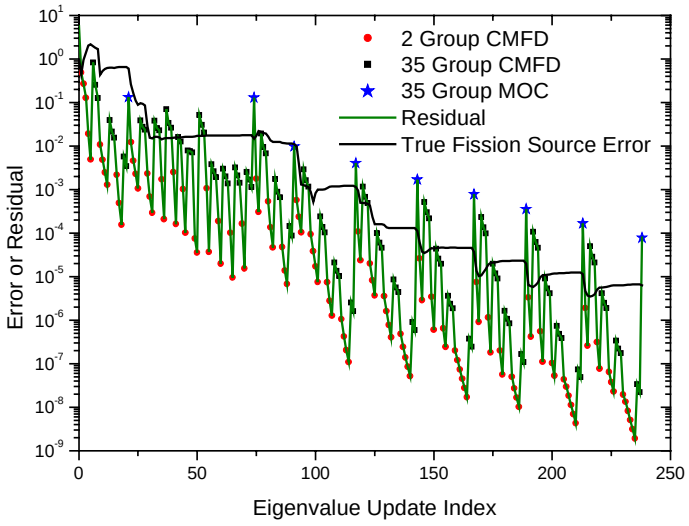

Figure 7. Various Level Residual Reduction Behavior for the 35 Group Problem

3.3 Computing Time

The computing times measured on a 1 GHz Pentium III PC are listed in Table 3 for the three primary modules of the DeCART code. In the test cases, 48 flat source regions are used in the fuel cells with 4 azimuthal angles in a quadrant, 2 polar angles in the half, and 0.5 mm ray spacing. The first thing to note in the table is that the total computing time for a typical PWR quarter core problem containing 52 FAs is about 20 minutes on a PC so that the whole core transport calculation is affordable. This is possible primarily due to the reduction in the number of the MOC updates achieved by the CMFD formulation. Nonetheless, the time for the MOC calculation is still dominating by taking more than 85% of the total computation time. In fact, the MOC module was optimized by representing the exponential functions with a precalculated table [8]. Yet, the time for ray tracing is dominating due to the huge number of rays and regions involved. Compared to the MOC time, the CMFD time for the fine mesh calculation is trivial. In this regard, there is no motivation for employing coarser level CMFD formulation involving, for example, assembly sized meshes.

Table 3. Computing Time Breakup

Module	KAIST 2A (5x5, 13 FAs)			Typical PWR (9x9, 52 FAs)		
	Number of Calls	CPU Time, sec	Fraction %	Number of Calls	CPU Time, sec	Fraction %
2G CMFD	75	15.8	5.8	86	54.1	4.2
MG CMFD	39	18.7	6.9	44	66.5	5.2
MG MOC	6	234.4	86.2	7	1156.7	89.9
Total		272.0			1287.3	

4. CONCLUSIONS

The CMFD formulation enables dynamic homogenization of the cells in the heterogeneous whole core transport calculation. As proved through the applications to various test problems, the heterogeneous transport solution is reproduced exactly while the number of MOC updates is reduced significantly. Dynamic group condensation is also possible with a two-level CMFD formulation involving alternate multigroup and two group CMFD calculations. The two-group CMFD formulation with the multigroup MOC kernel theory is therefore a very efficient means of accelerating the heterogeneous whole core transport calculations requiring only fewer than 10 MOC updates in practical 2D PWR whole core calculations. It also provides a simplified representation of the problem which can be utilized in the subsequent perturbation calculations such as transient and depletion.

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