Multi-Grid Acceleration Scheme for Neutron Transport Calculations using Optimally Diffusive CMFD Method

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Multi-Grid Acceleration Scheme for Neutron Transport Calculations using Optimally Diffusive Coarse Mesh Finite Difference Method

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INTRODUCTION

High fidelity neutronic analysis of a reactor system requires accurate prediction of spatial and energy distribution of neutron flux through solution of the neutron transport equation on faithfully modelled problem geometry with minimum assumptions. The increasing complexity and heterogeneity of advanced reactor designs also makes it necessary for an appropriate treatment of anisotropic transport in strongly absorbing and streaming media. Despite such requirements, the solution of neutron flux distribution in practical systems must be obtained within a feasible time and reasonable computational burden. Method of characteristics (MOC), proposed by Askew [1], can satisfy all of the above requirements.

Despite all the advantages associated with it, any application of the MOC formulation to practical problems requires numerous iterations and long computing times as it is extremely inefficient and slow to converge for problems with large dominance ratio or high scattering to transport cross-section ratio. Thus, use of an effective acceleration technique to speed up the solution becomes necessary. Among the acceleration techniques, two methods and their variants have been very popular due to their simple implementation. Coarse mesh rebalance (CMR) [2][3] adjusts the average amplitude of flux over a coarse mesh without altering the fine spatial and angular flux distribution within the coarse mesh. Although CMR is simple and flexible to coarse mesh geometry, it loses efficiency and may even diverge for meshes that are optically too thin or thick, and for highly scattering problems [4]. The coarse mesh finite difference (CMFD), proposed by Smith [5], is a non-linear iteration method based on the finite difference formulation by preservation of the interface currents between coarse meshes. It is generally much faster and effective than the CMR method and shows better convergence behavior [6], but restricts the calculation geometry to finite difference discretization, i.e., rectangular or triangular coarse meshes. Apart from this drawback, CMFD also fails to converge for optically thick coarse meshes. However, partial current based CMFD (pCMFD) [7], which preserves partial currents at coarse mesh interfaces, ensures convergence for coarse meshes of any size but at the cost of convergence speed in cases where CMFD converges [8].

This paper presents the implementation of an acceleration scheme based on the optimally diffusive coarse mesh finite difference (odCMFD) method in code DIAMOND [9][10], an MOC-based neutron transport solver for 2D heterogeneous rectangular assemblies. This scheme has been chosen because of its unconditional stability with respect to optical thickness of the coarse mesh, like the pCMFD, and its convergence speed which is equal to or only marginally slower than the conventional CMFD, as demonstrated by Zhu et al [11][12]. Description of the odCMFD methodology and its performance results for validation problems using DIAMOND have been provided in the following sections of this paper. It has also been shown that "real" performance gain offered by the odCMFD acceleration in terms of time closely follows the behavior of the conventionally used metric, reduction in the number of transport iterations.

OPTIMALLY DIFFUSIVE CMFD SCHEME

The odCMFD scheme was proposed by Zhu et al. [11] based on the idea of an "exact" diffusion coefficient developed by Larsen [13] to maintain consistency between the solutions obtained from a low order diffusion solver and S_N transport solver in planar geometry with quadratic sources. Zhu et al [11] combined the idea of this "exact" diffusion coefficient given by Larsen [13] with that of an optimal diffusion coefficient proposed by Yamamoto in generalized CMR (GCMR) to improve the spectral radius of CMFD and CMR [14]. This led to the optimal "artificial" diffusion coefficient of odCMFD. This "exact" or "artificial" or "optimally diffusive" diffusion coefficient can be obtained by the addition of a correction term to the actual diffusion coefficient, based on the optical thickness of the mesh and is given as:

$$D_{od} = \frac{1}{3\Sigma_{tr}} + \alpha_{od} h \tag{1}$$

where, Σ_{tr} represents the transport corrected total cross-section, and h is the coarse mesh thickness. The optimally diffusive correction factor, α_{od}, is a function of optical thickness of the coarse mesh ($\Sigma_{tr}h$), as given in Eq. (2).

$$\alpha_{od} = \frac{1}{2} \cdot \frac{\sum_{p=1}^{P} \beta_p \cos\theta_p \, \omega_p}{\sum_{p=1}^{P} \omega_p} \tag{2a}$$

$$\beta_p = \coth\left(\frac{\Sigma_{tr} h}{2\cos\theta_p}\right) - \frac{2\cos\theta_p}{\Sigma_{tr} h} \tag{2b}$$

where, ω_p represents the polar weight, while p and P represent the polar index and number of polar directions, respectively.

The odCMFD scheme uses the formulation of the conventional CMFD, with only the standard coarse mesh diffusion coefficient replaced by the artificial diffusion coefficient given by Eq, (1). Since the CMFD method is well known, its description has not been provided in this paper for brevity. However, interested readers can find a comprehensive review of the CMFD scheme in these references [6][7][8].

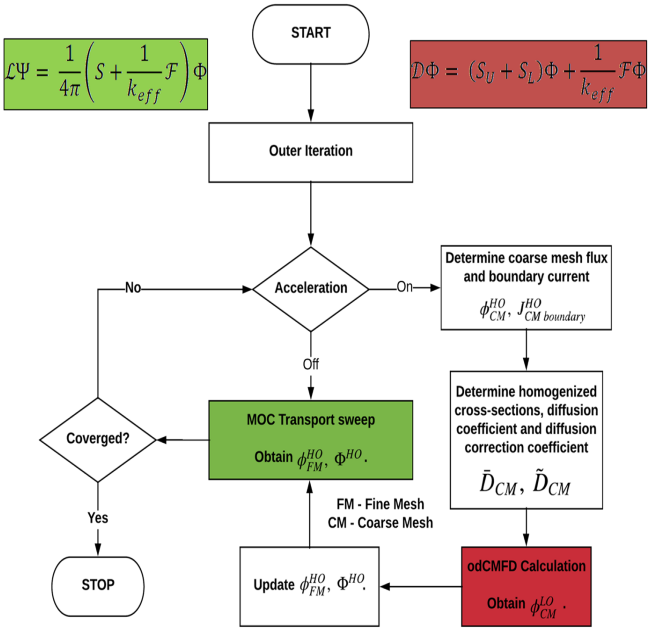

Fig. 1: Flux solver in code DIAMOND

The odCMFD acceleration technique introduced in DIAMOND enables faster convergence in two ways, firstly transferring the computational burden from a high order transport solution to a low order diffusion solver enabling significantly faster and cheaper convergence of the long range scattering effects, and secondly reducing the computational size of the problem by employing a multi-grid fine mesh – coarse mesh solution strategy. A flowchart of implementation of the odCMFD accelerated flux solver in DIAMOND is shown in Figure 1.

NUMERICAL RESULTS

Numerical results from the odCMFD accelerated MOC flux solver used in DIAMOND for the LRA BWR problem [15] have been presented in this section. The 2D Laboratorium für Reaktorregelung (LRA) benchmark is a two energy group, quarter core BWR problem. It is a five material problem consisting of 4 types of homogenized fuel assemblies totalling to 78 cells of size 15 cm x 15 cm surrounded by 43 reflector cells of the same size. The lattice is arranged in an 11 x 11 grid with a total size of 165 cm x 165 cm. The geometry has been illustrated in Figure 2. Reflective boundary condition is applicable on left and bottom boundaries while vacuum boundary condition is applied to the top and right boundaries. This problem was chosen with the aim of showing the convergence stability of odCMFD scheme. This has been done by solving the problem with different sizes of coarse mesh. Since DIAMOND uses the default size of the unique cells as coarse mesh size, varying coarse mesh thickness has been achieved by manually sub-dividing the 15 cm x 15 cm cells into smaller ones. To obtain the reference result, a pure high order transport calculation was also performed by switching off the acceleration. 24 equally spaced angles were used in the azimuthal quadrature along with the 3 angle Tabuchi-Yamamoto angular quadrature

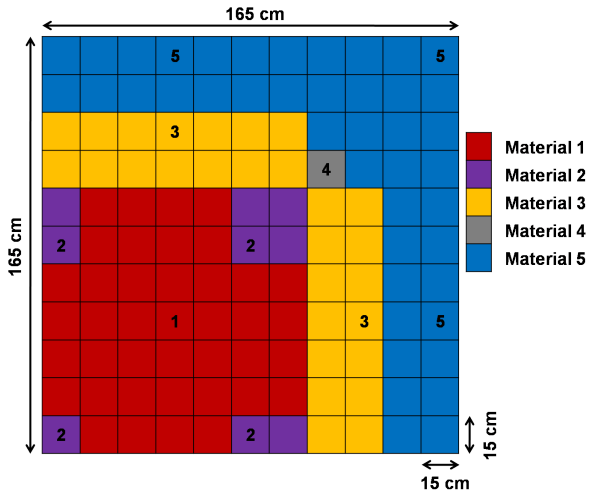

Fig. 2: 2D LRA-BWR benchmark problem description

representing the polar directions for all calculations. The ray density was set to 25 cm^{-1}. The flux and multiplication factor were converged to 10^{-6} and 10^{-7}, respectively. A comparison of the multiplication factor and performance of odCMFD acceleration w.r.t. coventional CMFD and pCMFD techniques, for various cases of this problem has been presented in Table I and Table II.

Table I verifies the unconditional stability of odCMFD acceleration scheme with respect to width of coarse meshes. The high order – low order scheme essentially leads to the same result as obtained from only high order calculations. The variation observed in cases 1, 2 and 5 is due to the different fine mesh structure of these problems with respect to the reference case. Table I also provides the detailed behaviour of odCMFD acceleration for different coarse mesh widths and also shows the execution time for these cases. The actual speed up in terms of time saved, or the effectiveness of the acceleration, initially increases with reducing coarse mesh size but subsequently starts reducing, as shown in Figure 3, due to time consumed for calculation of overheads. Also, the propagation of long range components of the solution is hampered with too small coarse mesh size, which explains the higher number of transport iterations as observed in cases 1, 2 and 3. It is also clear that the odCMFD method can provide speed up of 30-40 times peaking to 65 times when optimized.

Table II confirms that odCMFD performs better than pCMFD without sacrificing its stability w.r.t. optical thickness of the coarse mesh. Although CMFD is the fastest to converge amongst the 3 variants of CMFD, it fails to converge for large coarse meshes, as shown in Figure 4. The number of transport (high order) sweeps reduces 20-40 times for most cases and the computational burden is transferred to the inexpensive diffusion (low order) sweeps. Despite these low order sweeps, numbering to a few tens of thousands, the acceleration achieved is significant.

SUMMARY AND CONCLUSIONS

An optimally diffusive coarse mesh finite difference (odCMFD) method based acceleration technique has been imple-

TABLE I: Results of two group LRA-BWR problem

CASE	COARSE MESH WIDTH (cm)	k_{eff}	DIFF. $(k_{eff}-k_{ref})$ x 10^5 (pcm)	FINE MESHES (#)	COARSE MESHES (#)	TRANSPORT SWEEPS	DIFFUSION SWEEPS	TIME (min)	SPEED UP (x)
Ref. Case	-	1.000592 (k_{ref})	-	123904	-	7217	-	2849	-
Case 1	0.5	1.000723	13.1	217800	108900	1553	28930	1455	1.96
Case 2	1.0	1.000547	-4.5	108900	27225	707	14024	428	6.66
Case 3	1.875	1.000595	0.3	123904	7744	276	6692	140	20.35
Case 4	**3.75**	**1.000596**	**0.4**	**123904**	**1936**	**103**	**3780**	**44**	**64.75**
Case 5	5.0	1.000639	4.7	139392	1089	140	3670	67	42.52
Case 6	7.5	1.000598	0.6	123904	484	218	4596	96	29.68
Case 7	15.0	1.000598	0.6	123904	121	513	7825	228	12.50

TABLE II: CMFD vs pCMFD vs odCMFD performance comparison

CASE	CMFD				pCMFD				odCMFD			
	TS[a]	DS[b]	TIME (min)	SPEED UP (x)	TS	DS	TIME (min)	SPEED UP (x)	TS	DS	TIME (min)	SPEED UP (x)
Case 1	1537	28678	1440	1.98	1809	30928	1695	1.68	1553	28930	1455	1.96
Case 2	672	13371	407	7.00	850	15798	515	5.54	707	14024	428	6.66
Case 3	217	5750	110	25.88	320	7793	162	17.55	276	6692	140	20.35
Case 4	div[c]	div	div	div	107	4271	46	62.33	103	3780	44	64.75
Case 5	div	div	div	div	141	4014	67	42.22	140	3670	67	42.52
Case 6	div	div	div	div	221	4852	97	29.27	218	4596	96	29.68
Case 7	div	div	div	div	513	8038	228	12.50	513	7825	228	12.50

[a] Transport sweeps [b] Diffusion sweeps [c] Diverged

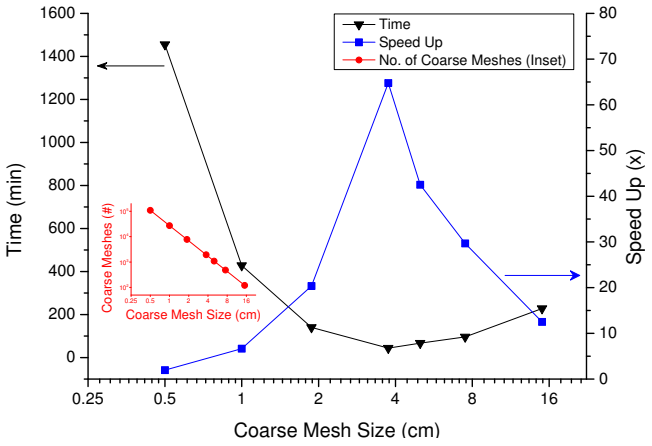

Fig. 3: Performance of odCMFD acceleration scheme for 2D LRA-BWR benchmark

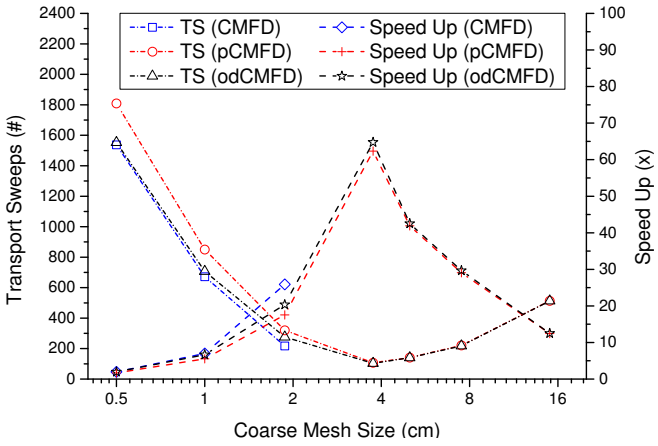

Fig. 4: CMFD vs pCMFD vs odCMFD performance comparison

mented in the code DIAMOND for neutronic analysis of 2D rectangular lattices. This is necessary due to the painfully slow convergence of the MOC flux solvers for realistic problems. The odCMFD accelerator is similar in implementation to the extremely popular CMFD method and requires only a simple modification to the coarse mesh diffusion coefficient based on its optical thickness. Apart from generalizing the pCMFD and CMFD methods, it also combines the speed of CMFD with the unconditional stability of pCMFD.

The odCMFD method accelerates the flux convergence by coupling accurate yet computationally intensive high order transport solutions with fast but approximate low order dif-

fusion solutions. Thus, a significant part of the computation is transferred to the low order approximate problem while the high order problem provides the necessary corrections to the approximate solution. Also, use of a fine mesh – coarse mesh scheme exploits the multi-grid method to reduce the computational size of the problem by spatial homogenization, which speeds the propagation of long range components of the solution. These two properties effectively lead to solving a computationally smaller and simpler problem, and only using the high order solution for finer corrections and accuracy.

Numerical results for the two-group LRA-BWR problem have been provided to show the performance and effectiveness of the acceleration scheme implemented in code DIAMOND. The LRA-BWR problem proves numerically, that the stability of odCMFD scheme is independent of the optical thickness of the coarse mesh, much like the pCMFD scheme, but with higher convergence speeds. It has been observed that with reduction in coarse mesh size, the effective speed gain increases initially but then starts reducing. This is because: 1) the number of coarse meshes increases, leading to higher overhead time for calculation of coarse mesh fluxes, homogenized cross-sections and other coupling terms; and 2) poor propagation of the long range solution components. Thus, maximum acceleration is achieved with a coarse mesh size, which optimizes the two effects. Although the number of high order transport sweeps reduces drastically for all cases, it is important to note that the number of low order iterations is high. The effectiveness of the technique starts reducing since time spent for the significantly high number of low order solutions is no longer insignificant. This is due to the use of traditional power iteration method to solve the low order finite difference equations.

Thus, use of pre-conditioners, Krylov subspace techniques, etc is desirable to obtain faster convergence of the low order problem. The authors plan to take up work in this respect and hope to introduce such advanced schemes in the odCMFD accelerator for further improvement in the convergence speeds. Another facet of the problem that needs attention is the use of multi-grid scheme in energy domain, as has been done in the spatial domain. This will significantly reduce the size of the problem in energy space while dealing with practical problems which involve detailed energy group structures like, XMAS-172, SHEM-281, SHEM-361, etc. Such energy homogenization will also ensure the efficacy of pre-conditioned Krylov subspace techniques by keeping the computational costs minimal.

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REFERENCES

1. J. R. ASKEW, "A Characteristics Formulation of the Neutron Transport Equation in Complicated Geometries," Tech. Rep. AEEW-M 1108, United Kingdom Atomic Energy Establishment, Winfrith (1972).
2. G. S. LEE, N. Z. CHO, and S. G. HONG, "Acceleration and Parallelization of the Method of Characteristics for Lattice and Whole-Core Heterogeneous Calculations," in "Proc. Int. Conf. on Physics of Reactors - Advances in Reactor Physics and Mathematics and Computations into the New Millennium (PHYSOR 2000)," American Nuclear Society, Pittsburgh, USA, May 7–11 (2000).
3. E. E. LEWIS and W. F. MILLER, *Computational Methods of Neutron Transport*, John Wiley and Sons (1984).
4. G. R. CEFUS and E. W. LARSEN, "Stability Analysis of Coarse-Mesh Rebalance," *Nuclear Science and Engineering*, **105**, *1*, 31–39 (1990).
5. K. S. SMITH, "Nodal Method Storage Reduction by Nonlinear Iteration," *Trans. ANS*, **44**, 265–266 (1983).
6. N. Z. CHO and C. J. PARK, "A Comparison of Coarse Mesh Rebalance and Coarse Mesh Finite Difference Accelerations for the Neutron Transport Calculations," in "Proc. Int. Conf. on Nucl. Mathematical and Comp. Sci. - A Century in Review, A Century Anew (M&C 2003)," American Nuclear Society, Gatlinburg, Tennessee, USA, April 6–11 (2003).
7. N. Z. CHO, G. S. LEE, and C. J. PARK, "Partial Current-based CMFD Acceleration of the 2D/1D Fusion Method for 3D Whole-Core Transport Calculations," *Trans. ANS*, **88**, 594 (2003).
8. N. Z. CHO, "Partial Current-based CMFD (p-CMFD) Revisited," in "Trans. KNS," Korean Nuclear Society, Autumn Meeting, Gyeongju, Korea. (2012).
9. L. JAIN, R. KARTHIKEYAN, and U. KANNAN, "Development of Unstructured Meshing Module for Code DIAMOND," in "Trans. ARP," Bhabha Atomic Research Centre, Mumbai, India, December 6–9 (2017).
10. L. JAIN, R. KARTHIKEYAN, and U. KANNAN, "Development of Ray Tracing Module for Code DIAMOND," in "Trans. ARP," Bhabha Atomic Research Centre, Mumbai, India, December 6–9 (2017).
11. A. ZHU, M. JARRETT, Y. XU, B. KOCHUNAS, E. LARSEN, and T. DOWNAR, "An optimally diffusive Coarse Mesh Finite Difference method to accelerate neutron transport calculations," *Annals of Nuclear Energy*, **95**, 116–124 (2016).
12. A. ZHU, B. KOCHUNAS, Y. XU, M. JARRETT, E. LARSEN, and T. DOWNAR, "Theoretical Convergence Rate Lower Bounds for Variants of Coarse Mesh Finite Difference to Accelerate Neutron Transport Calculations," *Nuclear Science and Engineering*, **186**, *3*, 224–238 (2017).
13. E. W. LARSEN, "Infinite-Medium Solutions of the Transport Equation, S_N Discretization Schemes, and the Diffusion Approximation," *Transport Theory and Statistical Physics*, **32**, *5-7*, 623–643 (2003).
14. A. YAMAMOTO, "Generalized Coarse-Mesh Rebalance Method for Acceleration of Neutron Transport Calculations," *Nuclear Science and Engineering*, **151**, *3*, 274–282 (2005).
15. H. PARK, D. A. KNOLL, and C. K. NEWMAN, "Nonlinear Acceleration of Transport Criticality Problems," *Nuclear Science and Engineering*, **172**, *1*, 52–65 (2012).