

Comparative Review of Coarse Mesh Acceleration Methods and the Two-Level p-CMFD Acceleration in the Whole-Core Transport Calculation

Nam Zin Cho

Professor Emeritus

Korea Advanced Institute of Science and Technology (KAIST)

291 Daehak-ro, Yuseong-gu, Daejeon, Korea 34141

nzcho@kaist.ac.kr

March 2022

KEY ACRONYMS

MOC : Method of Characteristics

CMR : Coarse Mesh Rebalance

GCMR : Generalized Coarse Mesh Rebalance

CMFD : Coarse Mesh Finite Difference

p-CMFD : Partial current-based Coarse Mesh Finite Difference

p-IMFD : Partial current-based Intermediate Mesh Finite Difference

PCDF : Partial Current Discontinuity Factor

TL(N)/p-CMFD : Two-Level p-CMFD with N global/local iterations

PI : Power Iteration

G-S : Gauss-Seidel

WS : Wielandt Shift

BiCGSTAB : Bi-Conjugate Gradient Stabilized

JFNK : Jacobian-Free Newton Krylov

INTRODUCTION

Due to the structural design characteristics in the current generation of nuclear reactor cores, the neutron transport theory methods are now called for in the neutronics design and analysis [1]. In typical reactor types such as the thermal and fast reactors, the 2D (method of characteristics)/1D (discrete ordinates method) fusion method [2] is a novel approach and getting increasing attention [3,4]. Still, the 2D method of characteristics calculation takes most of the computing time and thus requires good acceleration schemes [1].

The coarse mesh based acceleration methods [1–11] in neutron transport calculation are widely used, because they are easily applied to the original transport calculation with various geometries. However, they exhibit slow convergence or divergent behavior (in some of the methods) for optically thick coarse mesh cells. This drawback limits the size of coarse mesh cells, incurring significant computational burden per iteration. It is also very important to use converging schemes in the coupling of the neutronics code with the thermal-hydraulics code for feedback [12].

The present article revisits the partial current-based coarse mesh finite difference (p-CMFD) method [7–10] that was developed at KAIST, and that is unconditionally stable and more stable than other coarse mesh based acceleration methods. A recent extension with a two-level (two-grid) convergence speedup scheme [13–16] was made by using the Krylov subspace method. Numerical results of its application to the standard OECD benchmark problem and an enlarged problem show that the two-level scheme wrapped around by the Krylov subspace enhances the convergence rate of p-CMFD significantly, especially for optically thick coarse mesh cells (of assembly size).

COARSE MESH BASED ACCELERATION METHODS AND LIMITATIONS

Coarse mesh based acceleration methods usually consist of two parts: a high-order calculation and a low-order calculation. The high-order calculation employs transport methods (usually based on the discrete ordinates method or the method of characteristics in multigroup transport equations) with fixed fission source. The low-order calculation uses the balance equation, in which the high-order calculation provides parameters over each coarse mesh cell. The low-order calculation gives the multiplication factor (for the whole reactor) and the coarse mesh cell averaged scalar fluxes. The coarse mesh cell averaged scalar fluxes are then “modulated” or prolonged to be used in the fission source of the high-order equation for the next iteration.

To study the efficiency of an acceleration method, Fourier convergence analysis was performed on coarse mesh rebalance (CMR) [5,10], coarse mesh finite difference (CMFD) [10], partial current-based CMFD (p-CMFD) [7–10, 13], and generalized coarse mesh rebalance (GCMR) [11]. The results show that p-CMFD is always stable and more stable than the other methods. CMR shows divergent behavior for optically thin coarse mesh cells. CMFD, GCMR, and p-CMFD are very efficient for optically thin coarse mesh cells but not efficient for optically thick coarse mesh cells; See Fig. 1 (CMFD even diverges for optically thick coarse mesh cells, if \tilde{D} is used from the standard diffusion theory ($\tilde{D} = 1/3 \Sigma_t$)). Note that a recent work on CMFD with linearly interpolating prolongation lp-CMFD [17] stabilizes this divergence).

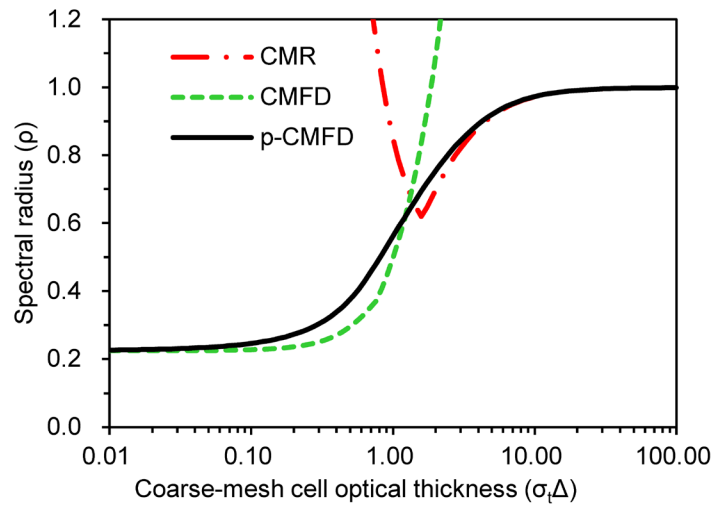


Fig. 1. Results of Fourier stability analysis of CMR, CMFD, and p-CMFD with SC and S16 for the eigenvalue problem (from Ref. 13).

Ref. 18 adjusted (optimized) the diffusion coefficient in CMFD to improve the convergence rate. The diffusion coefficient in p-CMFD can be also adjusted to optimize the spectral radius. Figure 2 shows the results in comparison. Even with the optimized \tilde{D} , CMFD and p-CMFD show slow convergence in optically thick coarse mesh cells. This is a common property for all coarse mesh based acceleration methods; see Ref. 18 for CMFD, Ref. 11 for GCMR, Refs. 10 and 13 for p-CMFD, and Ref. 17 for lp-CMFD. Therefore, the need arises to improve convergence for thick coarse mesh cells.

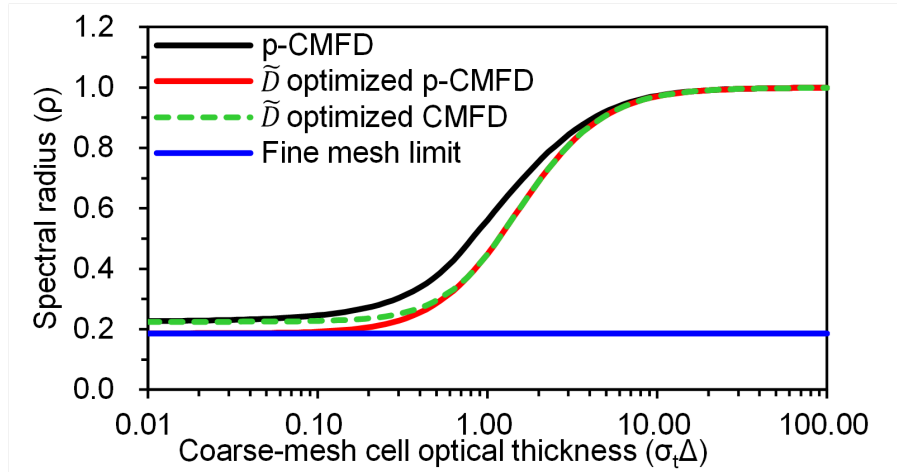


Fig. 2. Spectral radii of the \tilde{D} optimized CMFD and p-CMFD. (See additional results in Ref. 13.)

TWO-LEVEL p-CMFD ACCELERATION

W-Cycle Scheme

The p-CMFD acceleration is a modification of the CMFD acceleration, in that p-CMFD is based on the use of partial currents (instead of net currents used in CMFD), resulting in:

- i) p-CMFD is unconditionally stable,
- ii) p-CMFD provides additional information, that is, transport partial currents on the interface of two coarse mesh cells, and thus,
- iii) the incoming partial current allows a fixed-source problem formulation for a coarse mesh cell, whose solution provides in turn improved flux distribution and outgoing partial current (to the neighboring coarse mesh cell).

Note that CMFD [6] uses one correction coefficient to preserve the surface net current. On the other hand, p-CMFD uses two correction coefficients to preserve the two surface partial currents, respectively (The surface net current is automatically preserved by the two surface partial currents). In p-CMFD, there is little incentive to deal with the optimized \tilde{D} (the improvement is only marginal in thin coarse mesh cells, where it is already very fast), instead we focus on thick coarse mesh cells, utilizing transport partial currents (see Fig. 2). This section describes a two-level spatial coarse grid p-CMFD technique to speedup p-CMFD acceleration, particularly in optically thick coarse mesh cells. To reduce the spectral radius further, we also introduce a global/local iterative

procedure to the low-level calculation in the two-level p-CMFD, as shown in the multi-grid literature notation in Fig. 3 (W-cycle). In Fig. 3, a quarter pin forms an intermediate-mesh cell in p-IMFD and each assembly forms a coarse-mesh cell in p-CMFD. Note that the p-IMFD rebalance calculations are used in restriction and prolongation for the scalar flux and partial currents.

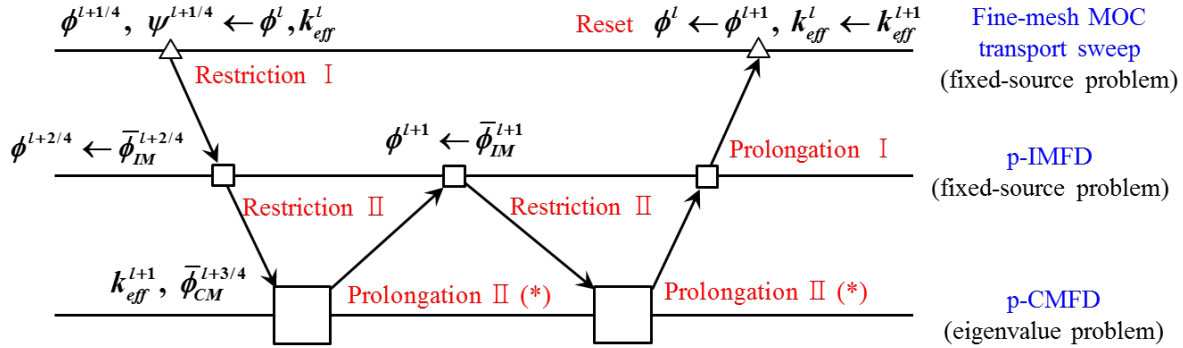


Fig. 3. Two-grid representation of the p-CMFD computational flow for $N = 2$ in W-cycle. (*with updated transport incoming partial currents)

Figure 4 is the convergence result of global/local iterations in the two-level p-CMFD acceleration for a 1D version OECD/NEA benchmark problem. As the number of global/local iterations increases (N goes large), the spectral radius for optically thick coarse mesh cells reduces drastically, approaching that of the fine mesh limit.

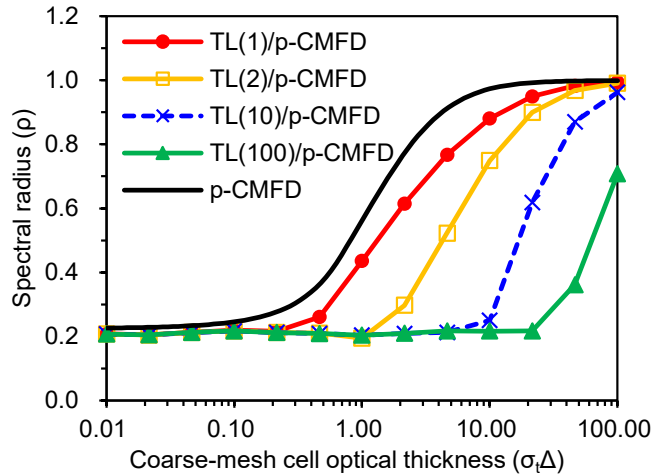


Fig. 4. Spectral radius of global/local iteration in two-level p-CMFD acceleration (TL(N)/p-CMFD: two-level p-CMFD with N global/local iterations).

Krylov Solution Algorithms

In the W-cycle scheme in Fig. 3, Restriction I results in p-IMFD of intermediate-mesh cells and leads to the form,

$$\mathbf{A} \boldsymbol{\phi} = \mathbf{b}, \quad (1)$$

that is a very large problem. It is then followed by the p-CMFD eigenvalue problem in coarse-mesh cells of the form through Restriction II,

$$\mathbf{M} \boldsymbol{\phi} = 1/k_{eff} \mathbf{F} \boldsymbol{\phi}. \quad (2)$$

They are both whole-core problems. Eq. (1) is solved by the BiCGSTAB algorithm [19] and Eq. (2) by the Jacobian-Free Newton-Krylov (JFNK) algorithm [20]. In Eq. (2), $\boldsymbol{\phi}$ and k_{eff} are considered as unknowns simultaneously, rendering them as roots of a nonlinear equation system. They are compared to the traditional methods of Gauss-Seidel (G-S) and power iteration (PI), respectively. The Wielandt shift (WS) acceleration of power iteration (PI) is to be avoided, because it may render the resulting matrix near singular.

NUMERICAL RESULTS

3 x 3 Problem

The two-level p-CMFD is tested on a two-dimensional problem with seven-group cross section data that are specified in the OECD/NEA C5G7 benchmark report [21], and is shown in Figure 5.

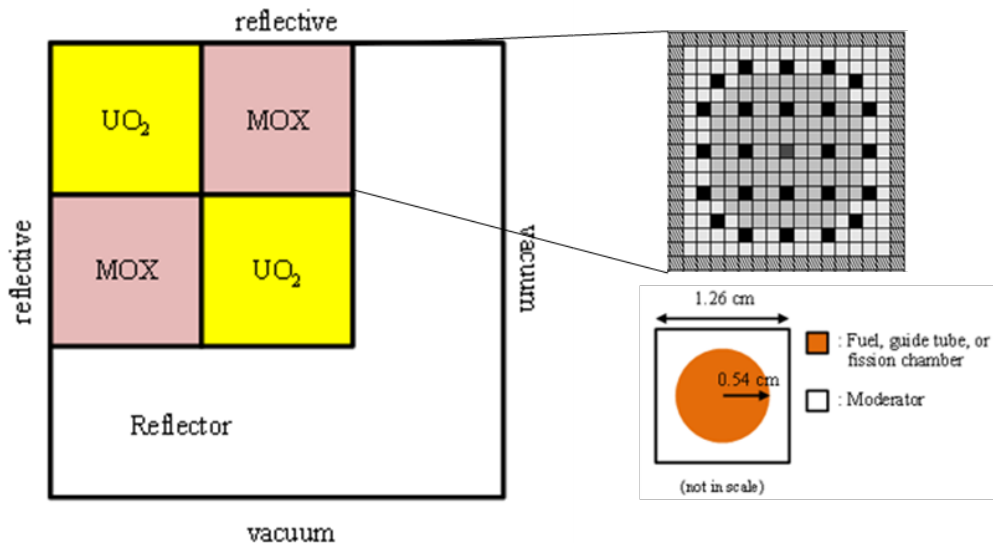


Fig. 5. Geometry of 2D C5G7 benchmark problem.

The computational conditions are as follows: The method of characteristics (MOC) is used, with 40 mesh cells (5 ring divisions and 8 azimuthal sector divisions) per fuel pin cell and 64 mesh cells

(8 by 8 rectangular mesh cells) per reflector (pseudo) pin cell. An intermediate-mesh cell is a quarter of a fuel pin or a reflector pin. Table I shows the various results in comparison. Note that the number of transport sweeps (that is most time-consuming among the various phases of the computation) reduces significantly from No Acceleration to p-CMFD, and more significantly to TL(N)/p-CMFD, as N increases. This effect outweighs well enough the increase in the number of p-CMFD power (or JFNK) iterations.

Table I. Results of 2D C5G7 (3 by 3) Benchmark Problem

Methods	No Acc.	p-CMFD	TL(1)/p-CMFD			TL(4)/p-CMFD		
	a^*	a^*	a^*	b^*	c^*	a^*	b^*	c^*
k_{eff}	1.18658	1.18658	1.18658	1.18658	1.18658	1.18658	1.18658	1.18658
Number of transport sweep iterations	1017	473	28	28	27	18	18	18
Number of p-CMFD Power (or JFNK) Iterations	0	4316	436	436	217	723	723	386
Transport sweep calculation time (sec) †	3148.618	1468.528	87.509	86.188	82.766	55.467	56.747	56.993
Whole-core p-IMFD time (sec)	0	0	5.311	3.034	2.06	2.8	1.859	1.376
Local p-IMFD time (sec)	0	0	4.558	2.834	2.162	8.819	6.602	4.859
Whole-core p-CMFD time (sec)	0	15.802	0.937	0.925	0.944	2.368	2.379	2.581
Total calculation time (sec)	3149.01	1484.67	98.412	93.081	88.017	69.552	67.687	65.9
Speedup	1	2.12	32.00	33.83	35.78	45.28	46.52	47.78
Percentage of transport sweep time in total calculation time	99.99	98.91	88.92	92.59	94.03	79.75	83.84	86.48

a^* : Gauss-Seidel +Power Iteration, b^* : BiCGSTAB +Power Iteration, c^* : BiCGSTAB +JFNK

† : a single thread of a CPU (Intel i7-7700K)

5 x 5 Problem

Additional results on an enlarged OECD/NEA C5G7 benchmark problem [22] are available and included below in Fig. 6 and Table II. As expected, the speedup becomes larger as the problem becomes larger.

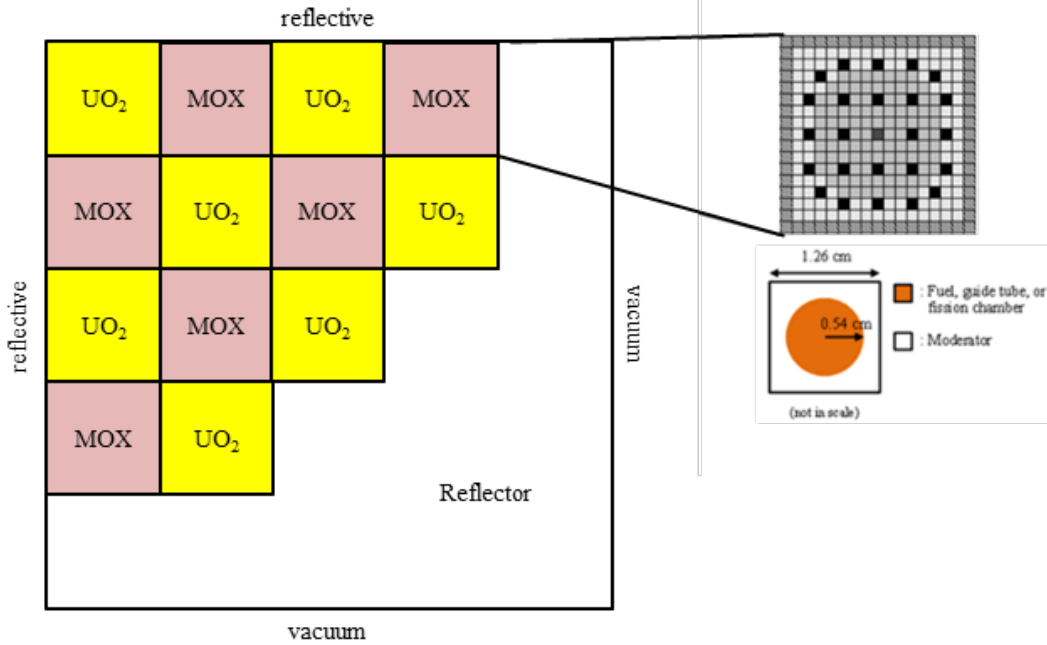


Fig. 6. Geometry of enlarged 2D C5G7 benchmark problem.

Table II. Results of Enlarged 2D C5G7 (5 by 5) Benchmark Problem

Methods	No Acc.	p-CMFD	TL(1)/p-CMFD			TL(4)/p-CMFD		
	a^*	a^*	a^*	b^*	c^*	a^*	b^*	c^*
k_{eff}	1.23141	1.23141	1.23141	1.23141	1.23141	1.23141	1.23141	1.23141
Number of transport sweep iterations	2241	438	48	48	49	18	18	18
Number of p-CMFD Power (or JFNK) Iterations	0	4584	895	893	646	1023	1023	742
Transport sweep calculation time (sec) †	19874.194	3852.734	424.896	433.586	432.902	159.347	159.241	158.804
Whole-core p-IMFD time (sec)	0	0	23.143	13.831	8.467	8.203	5.515	3.536
Local p-IMFD time (sec)	0	0	19.212	12.682	9.307	25.41	18.688	11.893
Whole-core p-CMFD time (sec)	0	38.363	4.177	4.308	4.765	6.353	6.333	6.91
Total calculation time (sec)	19874.33	3891.21	471.662	464.529	455.566	199.425	189.887	181.254
Speedup	1	5.11	42.14	42.78	43.63	99.66	104.66	109.65
Percentage of transport sweep time in total calculation time	100.0	99.01	90.08	93.34	95.03	79.90	83.86	87.61

a^* : Gauss-Seidel +Power Iteration, b^* : BiCGSTAB +Power Iteration, c^* : BiCGSTAB +JFNK

† : a single thread of a CPU (Intel i7-7700K)

CONCLUDING REMARKS

This article presented a further speedup technique for p-CMFD acceleration in the whole-core transport calculation, that is also effective for optically thick coarse mesh cells (of assembly size). It is based on two-level spatial coarse grid p-CMFD with global/local iterations in the low-order calculation. The results show that we obtain fast convergence (even with large coarse-mesh cells), if we use a number of global/local iterations in TL(N)/p-CMFD with Krylov algorithms. This is owing to the availability of transport partial currents on the interface of two coarse mesh cells, allowing rebalance calculation via p-IMFD in each coarse-mesh problem (that can be performed in parallel and thus can reduce the local p-IMFD time further). More importantly, the most time-consuming transport sweep calculation footprint can be reduced further in a major way, if the transport sweep operations are performed characteristics by characteristics in parallel.

As a future work in another direction, the two-level p-CMFD method can be applied to the fast reactor analysis. Since the neutron mean free path is quite long in a fast reactor, the computational cells of super hexagonal- and rhombic-stencils could be considered, following the procedures proposed in Ref. 23, based on the HIRE-theoretic “multigroup” transport equations [24–26] with partial current discontinuity factors (PCDFs).

ACKNOWLEDGMENTS

The author expresses special thanks to Professor T. Kitada of Osaka University, who invited me to write this article for the Reactor Physics Division of the Atomic Energy Society of Japan (AESJ). The author also expresses sincere thanks for special associations and friendships of many years to Professor T. Takeda of Osaka University (now of Fukui University), Professors K. Kobayashi and C. Pyeon of Kyoto University, Professor A. Yamamoto of Nagoya University, Professors H. Sekimoto and T. Obara of Tokyo Institute of Technology, Dr. Y. Tahara of Mitsubishi Heavy Industries, Ltd., and Dr. M. Tatsumi of Nuclear Engineering International.

The author also expresses thanks to Dr. Seungsu Yuk of Korea Atomic Energy Research Institute and Dr. Seongdong Jang of Korea Advanced Institute of Science and Technology, who provided valuable assistance during the preparation of this article.

REFERENCES

1. M. L. ADAMS and E. W. LARSEN, “Fast Iterative Methods for Discrete Ordinates Particle Transport Calculations,” *Prog. Nucl. Energy*, 40, 3 (2002).
2. N. Z. CHO, G. S. LEE, and C. J. PARK, “Fusion of Method of Characteristics and Nodal Method for a 3-D Whole-Core Transport Calculation,” *Trans. Am. Nucl. Soc.*, 86, 322 (2002).
3. B. Collins, et. al., “Stability and Accuracy of 3D Neutron Transport Simulations Using the 2D/1D Method in MvPACT,” *J. of Computational Physics*, 326, 612 (2016).
4. G. Zhang, A. Shieh, W. S. Yang, and Y. S. Jung, “Consistent pCMFD Acceleration Schemes of the Three-Dimensional Transport Code PROTEUS-MOC,” *Nucl.Sci. Eng.*, 193, 828 (2019).

5. G. R. CEFUS and E. W. LARSEN, “Stability Analysis of Coarse-Mesh Rebalance,” Nucl. Sci. Eng., 105, 31 (1990).
6. K. S. SMITH and J. D. RHODES III, “Full-Core, 2-D, LWR Core Calculations with CASMO-4E,” Proc. PHYSOR 2002, Seoul, Korea, October 7–10, 2002, American Nuclear Society (2002) (CD-ROM).
7. N. Z. CHO, G. S. LEE, and C. J. PARK, “On a New Acceleration Method for 3D Whole-Core Transport Calculations,” Annual Meeting, Sasebo, Japan, March 27–29, 2003, Atomic Energy Society of Japan (2003).
8. 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. Am. Nucl. Soc., 88, 594 (2003).
9. N. Z. CHO, “The Partial Current-Based CMFD (p-CMFD) Method Revisited,” Trans. Kor. Nucl. Soc., Gyeongju, Korea, October 25–26, 2012, Korean Nuclear Society (2012).
10. N. Z. CHO and C. J. PARK, “A Comparison of Coarse Mesh Rebalance and Coarse Mesh Finite Difference Accelerations for the Neutron Transport Calculations,” Proc. M&C 2003, Gatlinburg, Tennessee, April 6–11, 2003, American Nuclear Society (2003); see also KAIST internal report NURAPT-2002-02, (with addendum on p-CMFD); https://github.com/nzcho/Nurapt-Archives/blob/master/NurapT2002_2rev2.pdf
11. A. YAMAMOTO, “Generalized Coarse-Mesh Rebalance Method for Acceleration of Neutron Transport Calculations,” Nucl. Sci. Eng., 151, 274 (2005).
12. B. KOCHUNAS, A. FITZGERALD, and E. LARSEN, “Fourier Analysis of Iteration Schemes for k-Eigenvalue Transport Problems with Flux-Dependent Cross Sections,” J. of Comp. Phys., 345, 294 (2017).
13. S. YUK and N. Z. CHO, “Two-Level Convergence Speedup Schemes for p-CMFD Acceleration in Neutron Transport Calculation,” Nucl. Sci. Eng., 188, 1 (2017); and Corrigendum, 188, 303 (2017).
14. N. Z. CHO, “An Overview of p-CMFD Acceleration and Its Applications to Reactor Physics Transport Calculation,” Trans. Am. Nucl. Soc., 117, 1247-1250 (2017).
15. N. Z. CHO, “The Roles of Transport Partial Current Information in Two-Level p-CMFD Acceleration in the Whole-Core Transport Calculation,” Trans. Am. Nucl. Soc., 121, 1323-1326 (2019).
16. N. Z. CHO, “Krylov Subspace Wraps Around the Two-Level p-CMFD Acceleration in the Whole-Core Transport Calculation,” Trans. Am. Nucl. Soc., 123, 1327 (2020).

17. D. WANG and S. XIAO, “A Linear Prolongation Approach to Stabilizing CMFD,” Nucl. Sci. Eng., 190, 45 (2018).
18. A. ZHU, M. JARRETT, Y. XU, B. KOCHUNAS, E. W. LARSEN, and T. DOWNAR, “An Optimally Diffusive Coarse Mesh Finite Difference Method to Accelerate Neutron Transport Calculations,” Ann. Nucl. Energy, 95, 116 (2016).
19. Y. SAAD, “Iterative Methods for Sparse Linear Systems,” SIAM, 2003, pp. 231-234 (BiCGSTAB algorithm for Krylov method).
20. H. PARK, D. A. KNOLL, and C. K. NEWMAN, “Nonlinear Acceleration of Transport Criticality Problems,” Nucl. Sci, Eng., 172, 52 (2012).
21. M. A. SMITH, E. E. LEWIS, and B.-C. NA, “Benchmark on Deterministic Transport Calculations Without Spatial Homogenization: A 2-D/3-D MOX Fuel Assembly 3-D Benchmark,” NEA/NSC/DOC(2003)16, Organisation for Economic Co-operation and Development, Nuclear Energy Agency (2003).
22. N. Z. CHO, “An Enlarged 2-D OECD/NEA Benchmark Problem and Two-Level p-CMFD Solutions,” Korea Advanced Institute of Science and Technology, June 2020; https://github.com/nzcho/Nurapt-Archives/blob/master/NZCho_ANS_W2020_Addendum.4.pdf
23. N. Z. CHO, “A Proposed New Framework for Reactor Physics Analysis with Transport Calculation,” Trans. Kor. Nucl. Soc., Yeosu, Korea, October 24-26, 2018, Korean Nuclear Society (2018); https://www.kns.org/files/pre_paper/40/18A-132_조남진 I.pdf
24. N. Z. CHO, Y. G. JO, and S. YUK, “Multigroup Transport Equations Derived via Homogeneity and Isotropy Restoration Theory,” Trans. Am. Nucl. Soc., 115, 592-595 (2016).
25. N. Z. CHO, Y. G. JO, and S. YUK, “A New Derivation of Multigroup Transport Equations via Homogeneity and Isotropy Restoration Theory,” Ann. Nucl. Energy, 110, 798 (2017).
26. N. Z. CHO, S. Yuk, and Y. G. JO, “Partial Current Discontinuity Factors Determined via JFNK in HIRE-Theoretic Multigroup Transport Equations,” Fall Meeting, Sapporo, Japan, September 13-15, 2017, Atomic Energy Society of Japan (2017).